Ground State Energy of the Two-dimensional Hubbard Model at Low Filling

Okanigbuan O.R., Idiodi J.O.A. Okanigbuan P.N.

1Department of Physics, Ambrose Alli University, Ekpoma, Nigeria. 2Department of Physics, University of Benin, Benin-City, Nigeria. 3Department of Basic Sciences, Benson Idahosa University, Benin-City, Nigeria.

Abstract: The ground state of the Hubbard model for $L \times L$ Square Lattices ($L=2,3,4,5$) at low fillings (2 electrons) is studied using perturbation theory. It is shown that for the ratio $\frac{U}{N}$ of the positive on-site coulomb interaction $U$ and the number of sites $N$, result obtained from perturbation theory is in agreement with that obtained using correlated variational approach for small values of the ratio $\frac{U}{N}$.

Key words: On-site coulomb interaction, ground state energy, perturbation theory.

INTRODUCTION

The renewed interest in simple models of interacting electrons stimulated by the discovery of high temperature superconductivity, has shown the weakness of the usual theoretical treatments of these systems and the lack of general consensus on their physical properties\(^{[1]}\).

In spite of considerable effort devoted to the analysis of these systems, it is clear that the necessary theoretical skills and tools to deal with strongly correlated fermion systems are lacking\(^{[2]}\). Many analytical and numerical techniques have been developed to accommodate a good theoretical framework.

The two commonly used approximate analytical calculations, applied to many-body systems, are perturbation method and variational method. Perturbation method, relies on us being able to write down convergent or asymptotic series expansion of the observables we are interested in, and therefore works only in restricted ranges of parameter values in the many-body Hamiltonian. On the other hand, variational calculations requires us to make a biased first guess as to what form the many-body wave function may take, thus closing the door to discovering unusual and unexpected, behaviours in the many-body ground state\(^{[3]}\). The two numerical techniques by far most intensively used are Lanczos\(^{[4,5]}\) and Monte-Carlo (M.C.) methods, but regretfully these methods have also limitations. The MC approach allows to handle sufficiently large systems so that the results are physically of great interest in trying to predict the behaviour of the system in the thermodynamic limit. However, because of the so-called sign problem, which enormously enhances the statistical uncertainties of simulations, the maximum size of the lattice to be described is confined to a few tens of sites.

The minus sign problems do not arise in the diagonalization procedures, based on the Lanczos method\(^{[6]}\) and its modifications\(^{[7]}\), where all quantities (static and dynamical) can be computed from the ground state.

In spite of these advantages, memory limitations impose severe restrictions on the size of clusters that can be studied within this method. Usually the basis set of vectors employed in the diagonalization procedure grows exponentially with the system size.

Accordingly, the Hubbard Hamiltonian\(^{[8]}\)

\[ H = -\sum_{\langle i,j \rangle} [C_{i \sigma}^+ C_{j \sigma} + H.c.] + U \sum_{i} n_{i \uparrow} n_{i \downarrow} \quad [1.1] \]

proposed by J. Hubbard\(^{[9]}\), has spurred renewed interest, since it is widely considered that it is a good description of the low energy physics of high-Tc superconductors.

Corresponding Author: Okanigbuan O.R., Department of Physics, Ambrose Alli University, Ekpoma, Nigeria.
The terms in $H$ are:
1. a band “hopping” interaction between states on adjacent sites, with transfer integral $t$;
2. the creation (destruction) operator written as $C_{i\sigma}^+ (C_{i\sigma})$
3. an on-site (intra-atomic) interaction $U$ which can be either repulsive or attractive. The model, once the lattice is defined is determined by:
   a. defining the cluster with $N$ sites,
   b. defining the dimensionless parameter $(U/t)$
   c. defining the sign of $U$ and
   d. determining the number of particles $n$ in the cluster, where $0 \leq n \leq 2N$, and the number of particles per site may vary between 0 and 2. The total number of available many-body states for each $N$-cluster is $2^{2N}$, regardless of particle occupation. The number of many-body states for given $N$ and $n$ is $\frac{2N!}{n!(2N-1)!}$.

The aim of the present work is to evaluate the ground state energy of the Hubbard Hamiltonian on $LxL$ square lattice using standard perturbation theory.

The validity and convenience of stationary perturbation theory in the context of the Hubbard model has been proved for intermediate $U$ values as large as $U=4$ (in units where the hopping $t=1$)\([10]\). It is shown in reference\([11]\), that for a one-dimensional lattice the accuracy of perturbation calculation is enhanced when the ratio $\left(\frac{U}{N}\right)$, is small. That is, the crucial parameter in the perturbation expansion, is not just the interaction strength $U$, but the ratio $\left(\frac{U}{N}\right)$. The aim of this work is to investigate this behaviour by considering a more realistic system, the 2 dimensional square lattice. One important aspect of our study will be to compare our results with those obtained from the correlated variational approach\([12]\). The remaining sections of the paper are organized as follows:

In section II, we give a short description of the perturbation method. In section III, we calculate the ground state energy of two interacting electrons as a function of the $\left(\frac{U}{N}\right)$. Results obtained are discussed in section IV, while in section V we draw up conclusions.

II Method: The Hubbard Hamiltonian, equation (1 .1) is divided into 2 part, i.e.

$$H = H_0 + H_1$$\([10]\)

$$H_0 = -t \sum_{<i,j>,\sigma} C_{i\sigma}^+ C_{j\sigma} + H.C$$\([1.2]\)

$$H_1 = U \sum n_i \overrightarrow{n_j}$$\([1.3]\)

$H_0$ is the non-interacting part of the Hamiltonian, while $H_1$ is the interacting part of the Hamiltonian or the perturbed part.

The perturbation calculation proceed by constructing the one-electron Bloch wave function that diagonalise $H_0$, that is,

$$\phi_{k,\sigma}^+ = \frac{1}{L} \sum_{R_j} e^{-ik \cdot R_j} C_{j\sigma}^+ |0\rangle$$\([1.4]\)

where $R_j$ runs over all the sites, $L$ is the lattice size, and $k$ are the allowed wave vectors for the given lattice and take the form

$$K_{l,m} = -2\pi L \frac{x}{x} + \frac{2\pi m}{y}$$\([1.5]\)

The single-electron Bloch state (1.4) diagonalise $H_0$ with eigenenergies,

$$\varepsilon_k (K_{lm}) = -\left[\cos \textfrac{2\pi l}{L} + \cos \textfrac{2\pi m}{L}\right]$$\([1.6]\) for the 2x2 cluster

and

$$\varepsilon_k (K_{lm}) = -2\left[\cos \textfrac{2\pi l}{L} + \cos \textfrac{2\pi m}{L}\right]$$\([1.7]\) for the LxL cluster $L>2$

Many-body wavefunctions which are eigenstate of...
Ho are classified according to wavevector $\vec{k}$ and spin $\vec{\sigma}$. The ground state energy matrix, constructed with in every $k$ subspaces is given by

$$
\langle \psi_{k\sigma}^\alpha | H | \psi_{k\sigma}^\beta \rangle = T_o + \langle \psi_{k\sigma}^\alpha | H_1 | \psi_{k\sigma}^\beta \rangle + \sum_\delta \frac{\langle \psi_{k\sigma}^\alpha | H_1 \psi_{k\sigma}^\delta \rangle \langle \psi_{k\sigma}^\delta | H_1 | \psi_{k\sigma}^\beta \rangle}{T_o - T_o^\delta} \tag{1.8}
$$

The ground state wave function is

$$
\psi_{gs} = \sum_\alpha C_\alpha \psi_{k\sigma}^\alpha + \sum_\delta D_\delta \psi_{k\sigma}^\delta \tag{1.9}
$$

where zero-order coefficient $C_\alpha$ are obtained from diagonalization of the second order Hamiltonian matrix eqn (1.8), whereas first order $D_\alpha$ are given by

$$
D_\delta = \sum_\alpha \frac{\langle \psi_{k\sigma}^\delta | H | \psi_{k\sigma}^\alpha \rangle}{T_o - T_o^\delta} C_\alpha \tag{1.10}
$$

**RESULTS AND DISCUSSION**

From the application of the perturbation method in section II, the following ground state energies are obtained for 2 electrons on (LxL) cluster of the square lattice. For the (2x2) cluster, that is $L = 2$,

$$
E_g = -4t + \frac{2U}{4} - 2.5 \left( \frac{U^2}{t} \right) \tag{1.11}
$$

And for $L > 2$,

$$
E_g = -8t + 2 \left( \frac{U}{N} \right) - \alpha \left( \frac{U}{t} \right)^2 \tag{1.12}
$$

$\alpha$ in eqn (1.12) is dependent on $N$, the number of sites. $\alpha = 8$ for 3x3 cluster, $\alpha = 19.667$ for the 4x4 cluster, $\alpha = 30.3996$ for the 5x5 cluster and $\alpha = 348.75$ for a 30x30 cluster.

**Table 1:** Comparison between the ground state energy of 2 interacting electrons obtained from perturbation calculation $\left( \frac{E_p}{t} \right)$ and variational calculation $\left( \frac{E_v}{t} \right)$ of a 2D Hubbard model for various values of the interaction strength $\left( \frac{U}{t} \right)$.

<table>
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<th>$N$</th>
<th>$U$</th>
<th>$E_v$</th>
<th>$\frac{E_v}{t}$</th>
<th>$\frac{E_p}{t}$</th>
<th>$E_v$</th>
<th>$\frac{E_v}{t}$</th>
<th>$\frac{E_p}{t}$</th>
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<td>-4.000</td>
<td>0</td>
<td>-8.000</td>
<td>-8.000</td>
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<td>-8.000</td>
<td>-8.000</td>
<td>0</td>
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</tr>
</tbody>
</table>

Number of sites $N = L^2$. 

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911
We have computed ground state energies using equations (1.11) and (1.12) for (LxL) cluster of the 2 dimensional square lattices. Results obtained are shown in Table1. Given $\frac{U}{t} = 10$, $N = 4$ which implies $L = 2$ and $\frac{U}{N} = 2.5$ in units hopping intergral $t=1$, $E_v = -3.1489$ and $E_p = -14.6250$ with error $|E_p - E_v| = 11.4761$. On the other hand when $N = 25$ and $\frac{U}{N} = 0.4$, $E_v = -7.8446$ and $E_p = -12.0689$ with error $|E_p - E_v| = 4.2243$. The error indicates that the ground state energies obtained from perturbation methods gets better when $\frac{U}{N} \to 0$ that is $N \to \infty$. For a 30x30 cluster when $\frac{U}{t} = 16$, $E_p = -8.0746$, while the result shown in reference (12) is - 7.9970. The total energy given by Gutzwiller ansatz $^{[13]}$ in the 2D case is

$$-8t \left(1 - \frac{1}{N^2}\right)$$

and that given by correlated ground state (variational approach) is $-8t \left(1 - \frac{\beta}{N^2}\right)$. These two results agree with eqn (1.12) in the limit of $N \to \infty$.

5. Conclusion: It is generally believed that, in the large $U$ limit the Hubbard Hamiltonian cannot be treated with perturbative methods$^{[10,13,14,15]}$. In this work it is shown that for a two dimensional square lattice, perturbation theory is valid for any value of the interaction $U$, provided one increases the number of sites $N$ sufficiently, such that ratio $\frac{U}{N}$ is small that is $N \to \infty$. Thus, the crucial parameter is not just $U$ but $\frac{U}{N}$.

REFERENCES