Journal of the Nigerian Association of Mathematical Physics
Volume 10(November 2006), **583 - 594**

Correlation between perturbation and variation methods in the study of strongly correlated electron systems

Robinson O. Okanigbuan
Department of Physical Sciences
University of Mkar, Mkar, Nigeria.
and
John O.A. Idiodi
Department of Physics,
University of Benin, Benin City, Nigeria.

Abstract

The ground–state wave function and energy are calculated for two electrons subject to a one-band Hubbard Hamiltonian on a one dimensional lattice containing N electronic sites, N = 2,3,4,5,6, and a 3 x 3 cluster of the square lattice, using perturbation and variational methods. The results from these two approximation methods are then compared with the result from exact calculational method.

1.0 Introduction

The study of strongly- correlated electrons has become in the last decade one of the most active fields of condensed matter Physics. The electronic properties of an increasing body of materials cannot be described adequately by Landau's theory of weakly-interacting Oquasiparticles (Fermi liquid theory). The best known cases are the high Tc superconductors and organic conductors. In both cases, a strong anisotropy and a narrow conduction band contribute to make the effects of interactions between electrons (mainly Columbic repulsion) dramatic [ ].

In 1963, Hubbard provided an important physical simplification of the band model of solids [ ] . He pointed out that it is the short-ranged part of the coulomb interaction which is dominant in leading to the instabilities. The long-range part of the coulomb interaction, i.e. the interaction between electrons on different sites, and the interaction between electrons and the ion core of the crystal can be considered to be screened out, and hence, are neglected in the Hubbard model. In a Wannier–state basis, these assumptions lead to a many-body Hamiltonian, of the form

$$H = -t\left\{\sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{+} c_{j\sigma} + h.c\right\} + U\sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (1.1)$$

where $c_{i\sigma,}^{+}, c_{i\sigma}$ are the creation and annihilation operator for an electron of spin σ in the Wannier state. The operators satisfy the fermions anticommutation relations.

$$\left\{c_{i\sigma}^{+}, c_{j\sigma 1}\right\} = \delta_{ij}\delta_{\sigma\sigma'} \qquad (1.2a)$$

$$\left\{c_{i\sigma'}, c_{j\sigma'}\right\} = \left\{c_{i\sigma,}^{+} c_{j\sigma'}^{+}\right\} = 0 \qquad (1.2b)$$

$\langle i, j\rangle$ means summation is only over nearest neighour sites and the spin index $\sigma = \uparrow, \downarrow$ while $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$ is a number operator. t is the electronic hopping parameter between nearest neighour sites i and j, $h.c$ means hermitian

conjugation, while U is the on-site interaction energy. For negative U we have an attractive model, while in the positive case a repulsive one.

In this work we have been able to use perturbation theory [1] to determine the ground state energy and wave function for two electrons interacting in a one-dimensional lattice containing two sites. We then proceed to obtain a general formula for the ground state energy and wavefunction for 2 electrons on N-sites ($N > 2$). The work was then extended to a two-dimensional 3 x 3 square lattice. Comparison was made with the result obtained from the correlated variational approach and exact calculations.

2.0 Perturbation calculation of two interacting electrons in the ground state of the Hubbard Hamiltonian

From equation (1.1)

$$H = -t\left\{\sum_{\langle i,j\rangle\sigma} c^{+}_{i\sigma} c_{j\sigma} + h.c\right\} + U\sum_{i} n_{i\uparrow} n_{i\downarrow}$$

where the unperturbed Hamiltonian H_0 is $$H_o = -t\left\{\sum_{\langle i,j\rangle\sigma} c^{+}_{i\sigma} c_{j\sigma} + h.c\right\} \quad (2.1a)$$

and the perturbation H_1 is $$H_1 = U\sum_{i} n_{i\uparrow} n_{i\downarrow} \quad (2.1b)$$

The perturbation calculation begins by constructing the one-electron Bloch wave functions that diagonalize Ho, and which are

$$\phi_{k\sigma} = \frac{1}{L}\sum_{Rj} e^{i\,k,R_j} c_{j\sigma} \quad (2.2a)$$

$$\phi^{+}_{k\sigma} = \frac{1}{L}\sum_{Rj} e^{-ik,R_j}\, c^{+}_{j,\sigma}|0\rangle \quad (2.2b)$$

where R_j runs over all the cluster sites, and the allowed wave vectors k have the form, $k_{lm} = 2\pi\left[\frac{l}{L}\ \frac{M}{L}\right]$

For two electrons on two sites,

$$\vec{k}_l = \frac{2\pi l}{L}\hat{x},\ L = 1\ ,\ l = 1,2 \quad (2.3)$$

These states satisfy periodic boundary conditions and diagonalize H_o with eigenergies

$$\varepsilon(k_l) = -t\cos\frac{2\pi l}{L} \quad (2.4)$$

In the Hartree-Fock Approximation the wave function for the ground state of the system can be written as

$$\Psi_o = \left[\prod_{E_v \le E_f} A^{+}_{v}\right]\Psi_{vac} \quad (2.5)$$

which contain creation operators referring to all filled levels below the Fermi level E_f. Using (2.5) one can construct many-body wave functions of the Hatree Fock type;

$$\psi_o = \left[\prod_{n=1}^{N} \phi^{+}_{k_n,\sigma_n}\right]|0\rangle \quad (2.6)$$

where N is the total number of electrons in the lattice.

$\psi_{k\sigma} = \left|\phi^{+}_{k_1\sigma_1}\phi^{+}_{k_2\sigma_2}\right|0\rangle$

Choosing $\sigma_1 = \uparrow, \sigma_2 = \downarrow$, we have $$\psi^{1}_{k\sigma} = \frac{1}{2}\left[|1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\rangle + |1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle\right] \quad (2.7)$$

Also choosing $\sigma_1 = \downarrow, \sigma_2 = \uparrow$, $$\psi^{2}_{k\varsigma} = -\frac{1}{2}\left[|1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\rangle + |1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle\right] \quad (2.8)$$

while choosing $\sigma_1 = \uparrow, \sigma_2 = \uparrow$, we get $$\psi^{3}_{k\sigma} = 0 \quad (2.9)$$

and choosing $\sigma_1 = \downarrow, \sigma_2 = \downarrow$, we get $$\psi^{4}_{k\sigma} = 0 \quad (2.10)$$

In this way we classify many-body wave functions according to both wave vector $\vec{k}$ and spin $\vec{\sigma}$. The ground state energy matrix to second order in the perturbation U is given by [1.1]

$$\left\langle \psi_{k\sigma}^{\alpha} \middle| H \middle| \psi_{k\sigma}^{\beta} \right\rangle = T_o + \left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle + \sum_{\delta} \frac{\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\delta} \right\rangle \left\langle \psi_{k\sigma}^{\delta} \middle| H_1 \middle| \psi_{k\sigma}^{f} \right\rangle}{T_o - T_o^{\delta}} \tag{2.11}$$

where T_o is the eigervalue of the uperturbed Hamiltonian H_o.

$T_o = \sum_{n=1}^{N} \varepsilon(k_n)$, N is the number of electrons.

Since $N = 2$,

$T_o = \sum_{n=1}^{2} \varepsilon(k_n)$

$T_o = -2t$

$H_o \psi_{k\sigma}^{1} = -2t \psi_{k\sigma}^{1}$ (2.12a)

Similarly, $H_o \psi_{k\sigma}^{2} = -2t \psi_{k\sigma}^{2}$ (2.12b)

$T_o^1 = -2t, T_o^2 = -2t$

$T_o^1 = T_0^2 = T_0 = -2t$

Thus only two wave functions $\psi_{k\sigma}^{1}$ *and* $\psi_{k\sigma}^{2}$ provides the smallest uperturbed kinetic energy T_0 = - 2t for the two electrons. We now set up the Hamiltonian matrix, using these wave functions, $\left\langle \psi_{k,\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle$.

$$\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle = \begin{pmatrix} \left\langle \Psi_{k\sigma}^{1} \middle| H_1 \middle| \Psi_{k\sigma}^{1} \right\rangle & \left\langle \Psi_{k\sigma}^{1} \middle| H_1 \middle| \Psi_{k\sigma}^{2} \right\rangle \\ \left\langle \Psi_{k\sigma}^{2} \middle| H_1 \middle| \Psi_{k\sigma}^{1} \right\rangle & \left\langle \Psi_{k\sigma}^{2} \middle| H_1 \middle| \Psi_{k\sigma}^{2} \right\rangle \end{pmatrix} \tag{2.13}$$

$$\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle = \begin{pmatrix} \frac{U}{2} & -\frac{U}{2} \\ -\frac{U}{2} & \frac{U}{2} \end{pmatrix} \tag{2.14}$$

Equation (2.14) is the first order matrix energy correction to the ground state energy. The second order matrix energy correction is given by $\sum_{\delta} \frac{\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\delta} \right\rangle \left\langle \psi_{k\sigma}^{\delta} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle}{T_0 - T_0^{\delta}}$

The terms when $\delta = \alpha, \delta = \beta$ are omitted from the summation over δ. Using the wavefunction $\psi_{k\sigma}^{1}$,and $\psi_{k\sigma}^{2}$ we have.

$$\sum_{\delta} \frac{\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{\delta} \right\rangle \left\langle \psi_{k\sigma}^{\delta} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle}{T_0 - T_0^{\delta}} = \frac{\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle \left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k}^{\beta} \right\rangle}{T_0 - T_0^{1}} + \frac{\left\langle \psi_{k\sigma}^{\alpha} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle \left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{\beta} \right\rangle}{T_0 - T_0^{2}} \tag{2.15}$$

$$\left[\begin{array}{c|c} = \dfrac{\left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle}{T_0 - T_0^{2}} & \dfrac{\left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle \left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle}{T_0 - T_0^{2}} \\ \dfrac{\left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle}{T_0 - T_0^{2}} & + \dfrac{\left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle \left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle}{T_0 - T_0^{2}} \\ \hline \dfrac{\left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle}{T_0 - T_0^{1}} & \dfrac{\left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle \left\langle \psi_{k\sigma}^{1} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle}{T_0 - T_0^{1}} \\ + \dfrac{\left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{1} \right\rangle}{T_0 - T_0^{2}} & + \dfrac{\left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle \left\langle \psi_{k\sigma}^{2} \middle| H_1 \middle| \psi_{k\sigma}^{2} \right\rangle}{T_0 - T_0^{2}} \end{array}\right]$$

$\alpha, \beta = 1,2.$

Since $T_0 = T_0^1 = T_0^2 = -2t$, the second order matrix energy correction to the ground state energy vanishes. This also follows from the fact that all the terms in the summation over δ contain the terms $\alpha = \delta, \beta = \delta$.

$$\left\langle \psi_{k\sigma}^{\alpha} \middle| H \middle| \psi_{k\sigma}^{\beta} \right\rangle = \begin{pmatrix} -2t & 0 \\ 0 & -2t \end{pmatrix} + \begin{pmatrix} \frac{U}{2} & \frac{-U}{2} \\ \frac{-U}{2} & \frac{U}{2} \end{pmatrix} = \begin{pmatrix} -2t+u/2 & -u/2 \\ -u/2 & -2t+U/2 \end{pmatrix} \tag{2.16}$$

Let $A = \begin{pmatrix} -2t+u/2 & -U/2 \\ -U/2 & -2t+U/2 \end{pmatrix}$. Solving the non-trivial solution of the equation $(A - I\lambda_j)\vec{x} = 0$, gives

$$\lambda = -2t + U, \ \lambda_2 = -2t$$

The ground state energy is given by $E_g = -2t + U$ (2.17)

The ground state wavefunction is given by $\psi_{g.s} = \sum_{\alpha} C\alpha \psi_{k\sigma}^{\alpha} + \sum_{\delta} D_{\delta} \psi_{k\sigma}^{\delta}$ (2.18)

where zero-order coefficient C_{α} are obtained from the diagonalization of the second-order Hamiltonian matrix (Equation 2.18)] whereas first-order coefficients D_{δ} are given by

$$D_{\delta} = \sum_{\alpha} \frac{\left\langle \psi_{k\sigma}^{\delta} \middle| H_1 \middle| \psi_{k\sigma}^{\alpha} \right\rangle}{T_0 - T_o^{\delta}} c_{\alpha} \tag{2.19}$$

from equation (2.18), $\psi_{gs} = c_1 \psi_{k\sigma}^1 + c_2 \psi_{k\sigma}^2 + D_1 \psi_{k\sigma}^1 + D_2 \psi_{k\sigma}^2$ (2.20)

and from equation (2.19) $D_1 = \frac{\left\langle \psi_{k\varsigma}^1 \middle| H_1 \middle| \psi_{k\sigma}^1 \right\rangle}{T_o - T_o^1} C_1 + \frac{\left\langle \psi_{k\varsigma}^2 \middle| H_1 \middle| \psi_{k\sigma}^2 \right\rangle}{T_o - T_o^1} C_2$ (2.21)

$$D_2 = \frac{\left\langle \psi_{k\varsigma}^2 \middle| H_1 \middle| \psi_{k\sigma}^1 \right\rangle}{T_o - T_o^2} C_1 + \frac{\left\langle \psi_{k\varsigma}^2 \middle| H_1 \middle| \psi_{k\sigma}^2 \right\rangle}{T_o - T_o^2} C_2 \tag{2.23}$$

since $T_o^1 = T_o^2 = T_o = -2t$, the first order coefficient D_1 and D_2 vanishes. Zero-order coefficient obtained from the diagonalization of equation (2.16) are;

$C_1 = \frac{1}{\sqrt{2}}, C_2 = -\frac{1}{\sqrt{2}}$ from equation (2.20), $\Psi_{g.s} = \frac{1}{\sqrt{2}} \psi_{k\sigma}^1 - \frac{1}{\sqrt{2}} \psi_{k\sigma}^2$

$$\Psi_{g.s} = \frac{1}{2}\left[\left| 1\uparrow 1\downarrow \right\rangle + \left| 2\uparrow 2\downarrow \right\rangle + \left| 1\uparrow 2\downarrow \right\rangle - \left| 1\downarrow 2\uparrow \right\rangle \right] \tag{2.24}$$

where $\Psi_{g.s}$ is normalized.

2.0 Variational calculation of two-interacting electrons in the ground state of the Hubbard Hamiltonian.

We write the correlated ground-state wave function in the form.

$$\left| \Psi \right\rangle = \sum_{i=j} x(i,j) \left\{ \left| i\uparrow i\downarrow \right\rangle - \left| i\downarrow, j\uparrow \right\rangle \right\}^2 \tag{3.1}$$

Here, $\left| i\uparrow, j\downarrow \right\rangle$ means that one electron is on lattice site i with spin up and the other electron on lattice site j with spin down. The $X(i,j)$ are variational parameters. Let us consider the case of two electrons on two sites. Equation (3.1) can be written as

$\left| \Psi \right\rangle = \sum_{l=0}^{k} x_l \left| \Psi_l \right\rangle$, $k = N/2$ *for even N*

$\left| \Psi \right\rangle = x_o \left| \Psi_o \right\rangle + x_1 \left| \Psi_1 \right\rangle$

$\left| \Psi_o \right\rangle = \sum_{i=1}^{2} \left| i\uparrow, j\downarrow \right\rangle$

$\left| \Psi_l \right\rangle = \sum_{|i-j|=l} \left\{ \left| i\uparrow, j\downarrow \right\rangle - \left| i\downarrow, j\uparrow \right\rangle \right\}$

$$\therefore |\Psi_1\rangle = |1\uparrow, 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle$$

$$\therefore |\Psi\rangle = x_o\left[|1\uparrow,1\downarrow\rangle + |2\uparrow,2\downarrow\rangle\right] + x_1\left[|1\uparrow,2\downarrow\rangle - |1\downarrow,2\uparrow\rangle\right]$$

$$\langle\Psi|\Psi\rangle = 2\left(x_0^2 + x_1^2\right) \tag{3.2}$$

$$\langle\Psi|H|\Psi\rangle = 2t\left[4\left(\frac{U}{4t}\right)x_0^2 - 4x_0x_1\right] \tag{3.3}$$

Variational ground state energy is of the form

$$Eg = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{3.4}$$

Therefore,
$$Eg = \frac{2t\left[4\left(\frac{U}{4t}\right)x_o^2 - 4x_0x_1\right]}{2\left(x_0^2 + x_1^2\right)}$$

$$E = \frac{Eg}{t} = \frac{4\left(\frac{U}{4t}\right)x_o^2 - 4x_0x_1}{\left(x_0^2 + x_1^2\right)} \tag{3.5}$$

Minimization of the expression (3.5) with respect to all the variational parameters, leads immediately to the variational ground state energy

$$E_g == -2t\left[\sqrt{\left(\frac{U}{4t}\right)^2 + 1} \quad - \frac{U}{4t}\right] \tag{3.6}$$

The corresponding ground state wavefunction is given by

$$|\Psi\rangle = \frac{1}{2^{1/2}}\left[\frac{\left[\sqrt{U^2+16}+2\right]-U}{\sqrt{U^2+16t^2}}\right]^{1/2}\left[|1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\rangle\right]$$

$$+\frac{1}{2^{1/2}}\left[\frac{\sqrt{U^2+16}+2+U}{\sqrt{U^2+16t^2}}\right]^{1/2}\left[|1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle\right] \tag{3.7}$$

3.0 Two electrons in a one dimensional lattice containing N sites (N > 2)

4.1 Perturbation calculation.

Using the perturbation procedure of section 2.0, we obtain the following energies and wavefunction for N = 3, 4, 5.

For N = 3,

$$E_g = -4t + \frac{2U}{3} \tag{4.1}$$

and
$$\Psi_g = -\frac{1}{3}\begin{bmatrix}|1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\rangle + |3\uparrow 3\downarrow\rangle + |1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle + |1\uparrow 3\downarrow\rangle \\ -|1\downarrow 3\uparrow\rangle + |2\uparrow 3\downarrow\rangle - |2\downarrow 3\uparrow\rangle\end{bmatrix} \tag{4.2}$$

If N = 4,

$$E_g = -4t + \frac{U}{2} \tag{4.3}$$

and
$$\Psi_g = -\frac{1}{4}\begin{bmatrix}|1\uparrow 1\uparrow\rangle + |2\uparrow 2\downarrow\rangle + |3\uparrow 3\downarrow\rangle + |4\uparrow 4\downarrow\rangle + |1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle \\ +|1\uparrow 4\downarrow\rangle - |1\downarrow 4\uparrow\rangle + |2\uparrow 3\downarrow\rangle - |2\downarrow 3\uparrow\rangle + |3\uparrow 4\downarrow\rangle - |3\downarrow 4\uparrow\rangle \\ +|1\uparrow 3\downarrow\rangle - |1\downarrow 3\uparrow\rangle + |2\uparrow 4\downarrow\rangle - |2\downarrow 4\uparrow\rangle\end{bmatrix} \tag{4.4}$$

If N = 5,

$$E_g = -4t + \frac{u}{2} \tag{4.5}$$

and $$\Psi_g = -\frac{1}{5}\begin{bmatrix} |1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\rangle + |3\uparrow 3\downarrow\rangle + |4\uparrow 4\downarrow\rangle + |5\uparrow 5\downarrow\rangle + |1\uparrow 2\downarrow\rangle \\ + |1\uparrow 4\downarrow\rangle - |1\downarrow 2\uparrow\rangle + |2\uparrow 3\downarrow\rangle - |2\downarrow 3\uparrow\rangle + |3\uparrow 4\downarrow\rangle - |3\downarrow 4\uparrow\rangle \\ + |4\uparrow 5\downarrow\rangle - |4\downarrow 5\uparrow\rangle + |1\uparrow 5\downarrow\rangle - |1\downarrow 5\uparrow\rangle + |1\uparrow 3\downarrow\rangle - |1\downarrow 3\uparrow\rangle \\ + |3\uparrow 5\downarrow\rangle - |3\downarrow 5\uparrow\rangle + |1\uparrow 4\downarrow\rangle - |1\downarrow 4\uparrow\rangle + |2\uparrow 5\downarrow\rangle - |2\downarrow 5\uparrow\rangle \\ + |2\uparrow 4\downarrow\rangle - |2\downarrow 4\uparrow\rangle \end{bmatrix}. \tag{4.6}$$

In general, for 2 electrons on N sites (N > 2 where N is an integer).

$$E_g = -4t + \frac{2U}{N} \tag{4.7}$$

In general, the ground state wave function is given by

$$\Psi_g = \pm\frac{1}{N}\left\{\sum_{i=l}^{N}|i\uparrow, i\downarrow\rangle + \sum_{\substack{i,j=1 \\ i=j}}^{N}\left[|i\uparrow\ j\downarrow\rangle - |i\downarrow\ j\uparrow\rangle\right]\right\} \tag{4.8}$$

5.0 Two electrons in a one dimensional lattice containing N sites (N > 2)

5.1 Variational calculation

Using the variation method as demonstrated in section 3.0 we obtain the following energies and wavefuction for N = 3,5 (odd lattice sites) and N =4 ,6 (even lattice sites).

If N = 3,

$$E_g = -t + 2t(U/4t) - \frac{t}{2}\sqrt{16(U/4t)\left(1+\frac{U}{4t}\right)+36} \tag{5.1}$$

and $$\Psi_g = -\frac{1}{\sqrt{2}}\left[\frac{\sqrt{u^2+4ut+36+^2}-(u+2t)}{\sqrt{2u^2+4ut+28t^2-(u+2t)\sqrt{u^2+4ut+36t^2}}}\right]$$

$$\times\left\{|1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\rangle + |3\uparrow 3\downarrow\rangle\right\} - \frac{1}{\sqrt{2}}\left[\frac{4t}{\sqrt{2U^2+4Ut+28t^2-(U+2t)\sqrt{U^2+4Ut+36t^2}}}\right] \tag{5.2}$$

$$\times\left\{|1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle + |1\uparrow 3\downarrow\rangle - |1\downarrow 3\uparrow\rangle + |2\uparrow 3\downarrow\rangle - 2\downarrow 3\uparrow\right\}$$

If N = 5, the ground state energy in matrix form is

$$A = \begin{bmatrix} 4(U/4t) & -4 & 0 \\ -2 & -2 & 0 \\ 0 & -2 & -2 \end{bmatrix} \tag{5.3a}$$

If N = 4, the ground state energy matrix take the form

$$B = \begin{bmatrix} 4(U/4t) & -4 & 0 \\ -2 & 0 & -2 \\ 0 & -4 & 0 \end{bmatrix} \tag{5.3b}$$

If N = 6, the ground state energy matrix is given by

$$C = \begin{bmatrix} 4(U/4t) & -4 & 0 & 0 \\ -2 & 0 & -2 & 0 \\ 0 & -2 & 0 & -2 \\ 0 & 0 & -4 & 0 \end{bmatrix} \tag{5.3c}$$

6.0 Two Electrons in a (3 x 3) cluster of the square lattice perturbation calculation.

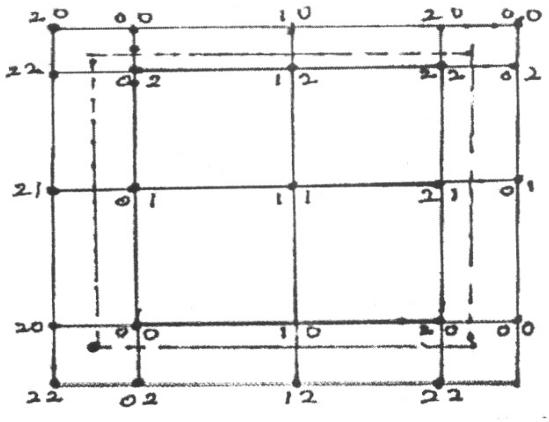

Figure 2D 3 x 3 square lattice with periodic boundary conditions.

Using the perturbation procedure of section 2.0, we construct the one-electron Bloch wave functions that diagonalize H_o, that is,

$$\phi^{+}_{k\sigma} = \frac{1}{L}\sum_{Rj} e^{-ik.R_j}\ C^{+}_{j\sigma}\,|\,0\rangle$$

$$H_o\,\phi^{+}_{k\uparrow} = -2t\left[\cos 2\pi l/L + \cos 2\pi m/L\right]\phi^{+}_{k\uparrow} \qquad (6.1a)$$

$$\varepsilon(k_{lm}) = -2t\left[\cos 2\pi l/L + \cos 2\pi m/L\right] \qquad (6.1b)$$

and $k_{lm} = \frac{2\Pi l}{L}\hat{x} + \frac{2\Pi m\,\hat{y}}{L}$, $\hat{x}, \hat{y}$ are unit vectors along the axes.

$l, m = 0,1,2,3;\ \ L = 3.$

where H_o is the unperturbed Hamiltonian (2.1a) of the Hubbard Hamiltonian equation (1.1)
The allowed wave vectors K_{lm} are, K_{00}, k_{01}, $k_{02,}$ k_{10}, k_{11}, k_{12}, k_{20},k_{21}, and k_{22}.

We classify many-body wavefunctions according to these wave vector $\overrightarrow{k_{lm}}$ and spin σ. The ground state is given by k_{oo}, wavevector subspace.

There are a total of 90 wavefunctions for $(\sigma_1 = \uparrow, \sigma_2 = \downarrow)$, $(\sigma_1 = \downarrow, \sigma_2 = \uparrow)$ *and wavevector* $\overrightarrow{k_{lm}}$
The ground state energy matrix is given by equation (2.11)

$$\left\langle \psi^{\alpha}_{k\sigma}\middle|H\middle|\psi^{\beta}_{k\sigma}\right\rangle = T_0 + \left\langle \psi^{\alpha}_{k\sigma}\middle|H_1\middle|\psi^{\beta}_{k\sigma}\right\rangle + \sum_{\delta}\frac{\left\langle \psi^{\alpha}_{k\sigma}\middle|H_1\middle|\psi^{\delta}_{k\sigma}\right\rangle\left\langle \psi^{\delta}_{k\sigma}\middle|H_1\middle|\psi^{\beta}_{k\sigma}\right\rangle}{T_o - T^{\delta}_o}$$

where
$$T_o = \sum_{n=1}^{2}\varepsilon(k_n) = -8t \qquad (6.2)$$

Out of the 90 many body wavefunctions constructed, only two, defined by the k_{oo} vector provide the smallest kinetic energy T_o=-8t for two electrons. We label them as, $\psi^{1}_{k\sigma}$ *and* $\psi^{46}_{k\sigma}$

$$\psi^{1}_{k\sigma} = \frac{1}{9}\left\{\begin{array}{l}\left|00\uparrow 00\downarrow\right\rangle + \cdots + \left|01\uparrow 01\downarrow\right\rangle + \cdots + \left|02\uparrow 02\downarrow\right\rangle + \cdots + \left|10\uparrow 10\downarrow\right\rangle + \cdots \\ + \left|11\uparrow 11\downarrow\right\rangle + \cdots + \left|12\uparrow 12\downarrow\right\rangle + \cdots + \left|20\uparrow 20\downarrow\right\rangle + \cdots + \left|21\uparrow 21\downarrow\right\rangle \\ + \left|22\uparrow 22\downarrow\right\rangle\end{array}\right\} \qquad (6.3a)$$

$$\psi^{46}_{k\sigma} = \frac{1}{9}\left\{\begin{array}{l}\left|00\uparrow 00\downarrow\right\rangle + \cdots + \left|01\uparrow 01\downarrow\right\rangle + \cdots + \left|02\uparrow 02\downarrow\right\rangle + \cdots + \left|10\uparrow 10\downarrow\right\rangle + \cdots \\ + \left|11\uparrow 11\downarrow\right\rangle + \cdots + \left|12\uparrow 12\downarrow\right\rangle + \cdots \left|20\uparrow 20\downarrow\right\rangle + \cdots + \left|21\uparrow 21\downarrow\right\rangle + \cdots \\ + \left|22\uparrow 22\downarrow\right\rangle\end{array}\right\} \qquad (6.3b)$$

and

$$H_o \psi^1_{k\sigma} = -8t\psi^1_{k\sigma} \tag{6.4a}$$

$$H_o \psi^{46}_{k\sigma} = -8t\psi^{46}_{k\sigma} \tag{6.4b}$$

$$\left\langle \psi^{\alpha}_{k\sigma} | H_1 | \psi^{\beta}_{k\sigma} \right\rangle = \begin{pmatrix} \left\langle \psi^1_{k\sigma} | H_1 | \psi^1_{k\sigma} \right\rangle & \left\langle \psi^1_{k\sigma} | H_1 | \psi^{46}_{k\sigma} \right\rangle \\ \left\langle \psi^{46}_{k\sigma} | H_1 | \psi^1_{k\sigma} \right\rangle & \left\langle \psi^{46}_{k\sigma} | H_1 | \psi^{46}_{k\sigma} \right\rangle \end{pmatrix} = \begin{pmatrix} \frac{U}{9} & \frac{-U}{9} \\ \frac{-U}{9} & \frac{U}{9} \end{pmatrix} \tag{6.5}$$

$$\sum_{\delta} \frac{\left\langle \psi^{\alpha}_{k\sigma} | H_1 | \Psi^{\delta}_{k\sigma} \right\rangle \left\langle \psi^{\delta}_{k\sigma} | H_1 | \psi^{\beta}_{k\sigma} \right\rangle}{T_o - T^{\delta}_o}$$

$$= \left(\begin{array}{c|c} \sum_{\delta=1}^{90} \left\langle \psi^1_{k\sigma} | H_1 | \psi^{\delta}_{k\sigma} \right\rangle \left\langle \psi^{\delta}_{k\sigma} | H_1 | \psi^1_{k\sigma} \right\rangle & \sum_{\delta=1}^{90} \left\langle \psi^{46}_{k\sigma} | H_1 | \psi^{\delta}_{k\sigma} \right\rangle \left\langle \psi^{\delta}_{k\sigma} | H_1 | \psi^1_{k\sigma} \right\rangle \\ \hline \sum_{\delta=1}^{90} \left\langle \psi^1_{k\sigma} | H_1 | \psi^{\delta}_{k\sigma} \right\rangle \left\langle \psi^{\delta}_{k\sigma} | H_1 | \psi^{46}_{k\sigma} \right\rangle & \sum_{\delta=1}^{90} \left\langle \psi^{46}_{k\sigma} | H_1 | \psi^{\delta}_{k\sigma} \right\rangle \left\langle \psi^{\delta}_{k\sigma} | H_1 | \psi^{46}_{k\sigma} \right\rangle \end{array} \right) = \begin{pmatrix} \frac{-U^2}{81t} & \frac{U^2}{81t} \\ \frac{U^2}{81t} & \frac{-U^2}{81t} \end{pmatrix} \tag{6.6}$$

$$\left\langle \psi^{\alpha}_{k\sigma} | H_1 | \psi^{\beta}_{k\sigma} \right\rangle = \begin{pmatrix} -8t & 0 \\ 0 & -8t \end{pmatrix} + \begin{pmatrix} U/9 & -U/9 \\ -U/9 & U/9 \end{pmatrix} + \begin{pmatrix} -U^2/81t & U^2/81t \\ U^2/81t & -U^2/81t \end{pmatrix}$$

$$\begin{pmatrix} -8t + \frac{U}{9} - \frac{U^2}{81t} & \frac{-U}{9} + \frac{U^2}{81t} \\ \frac{-U}{9} + \frac{U^2}{81t} & -8t + \frac{U}{9} - \frac{U^2}{81t} \end{pmatrix} \tag{6.7}$$

$$Let\ A = \begin{pmatrix} -8t + \frac{u}{9} - \frac{u^2}{81t} & \frac{-u}{9} + \frac{u^2}{81t} \\ \frac{-u}{9} + \frac{u^2}{81t} & -8t + \frac{u}{9} - \frac{u^2}{81t} \end{pmatrix}$$

Solving the non trivial solution of the equation.

$(A - I\lambda j)\vec{x} = 0, gives$

$$\lambda_1 = -8t + \frac{2u}{9} - \frac{2u^2}{81t}, \lambda_2 = -8$$

$$\lambda_1 = E_g = -8t + \frac{2U}{9} - \frac{2U^2}{81t} \tag{6.8}$$

The ground state wavefuncfion is given by equation (2.19) of section 2.0

$$\Psi_{g.s} = \sum_{\alpha=1}^{2} C_{\alpha} \psi^{\alpha}_{k\sigma} + \sum_{\delta=1}^{90} D_{\delta} \psi^{\delta}_{k\delta}$$

where $C_1 = \frac{1}{\sqrt{2}}, C_2 = C_{46} = -\frac{1}{\sqrt{2}}$ are the zero order coefficients obtained from the diagonalization of matrix A. First order coefficients D_{δ} is obtained from equation (2.19) of section (2.0).

$$D_{18} = -\frac{-U}{27\sqrt{2t}}, D_{33} = \frac{-U}{27\sqrt{2t}}, D_{39} = \frac{-U}{54\sqrt{2t}}$$

$$D_{41} = -\frac{-U}{54\sqrt{2t}}, D_{63} = \frac{U}{27\sqrt{2t}}, D_{78} = \frac{U}{27\sqrt{2t}}$$

$$D_{84} = \frac{U}{54\sqrt{2t}}, D_{86} = \frac{U}{54\sqrt{2t}}$$

$$\Psi_{k\sigma} = \frac{2}{\sqrt{2}}\psi^1_{k\sigma} + \psi^{18}_{k\sigma}(D_{18} - D_{63}) + \psi^{33}_{k\sigma}(D_{33} - D_{78}) + \psi^{39}_{k\sigma}(D_{39} - D_{84}) + \psi^{41}_{k\sigma}(D_{41} - D_{86})$$

where $\psi^{18}_{k\sigma}$ is given by [k_{01},k_{02}] wavevector subspace is given by the

$\psi_{k\sigma}^{33}$ is given by the wavevector space [k_{10},k_{20}]

$\psi_{k\sigma}^{39}$ is given by [k_{11},k_{22}], $\psi_{k\sigma}^{41}$ is given by [k_{12},k_{21}]

$$\psi_{k\sigma}=\frac{1}{\sqrt{2}}\psi_{k\sigma}^{1}-\frac{U}{27\sqrt{2t}}\left(\psi_{k\sigma}^{18}+\psi_{k\sigma}^{33}+\psi_{k\sigma}^{39}+\psi_{k\sigma}^{41}\right)$$

7.0 Two electrons in a (3 x 3) clusters of the square lattice

7.1 Variational calculation.

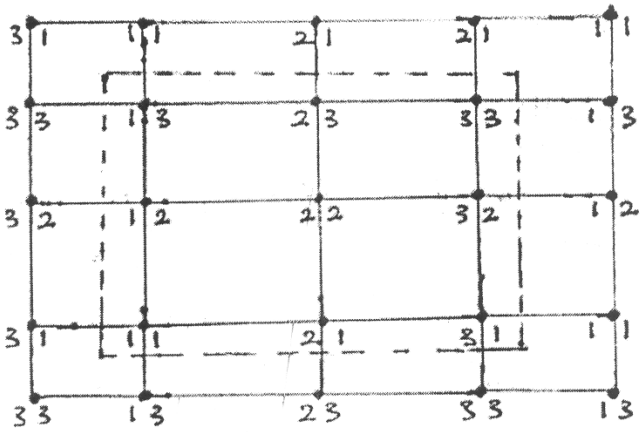

Figure 2D 3 x 3 Square lattice with periodic boundary conditions.

We make use of the correlated ground state wavefunction given by eqn. (3.1) to obtain.

$$\begin{aligned}|\Psi\rangle &= x_0\{|11\uparrow 11\downarrow\rangle+|12\uparrow 12\downarrow\rangle+|13\uparrow 13\downarrow\rangle+\cdots+|33\uparrow 33\downarrow\rangle\}+\times_1\{|11\uparrow 12\downarrow\rangle-|11\downarrow 12\uparrow\rangle\\ &+|11\uparrow 21\downarrow\rangle-|11\downarrow 21\downarrow\rangle+\cdots\}+|32\uparrow,33\downarrow\rangle-|32\downarrow,33\uparrow\rangle\\ &+\times_2\{|11\uparrow,22\downarrow\rangle-|11\downarrow 22\uparrow\rangle+|11\uparrow 23\downarrow\rangle-|11\downarrow 23\uparrow\rangle+\cdots+|23\uparrow 31\downarrow\rangle-|23\downarrow,31\uparrow\rangle\}\end{aligned} \tag{7.1}$$

Variational ground state energy is of the form (3.4) in section 3.0.

$$\langle\Psi|\Psi\rangle = 9x_0^2+36x_1^2+36x_2^2 \tag{7.2a}$$

and

$$\langle\psi|H|\psi\rangle = 9t\left\{4\left(\frac{U}{4t}\right)x_0^2-16x_0x_1-32x_1x_2-8x_1^2-16x_2^2\right\} \tag{7.2b}$$

$$E_g(x_0,x_1,x_2)=9t\frac{\left\{4\left(\frac{u}{4t}\right)x_0^2-16x_0x_1-32x_1x_2-8x_1^2-16x_2^2\right\}}{9x_0^2+36x_1^2 36x_2^2} \tag{7.3}$$

Minimization of the expression (7.3) with respect to all the variational parameters, lead immediately to the variational ground state energy matrix.

$$A=\begin{bmatrix}4(u/4t) & -8 & 0\\ -2 & -2 & -4\\ 0 & -4 & -4\end{bmatrix} \tag{7.4}$$

8.0 Numerical results and discussion

We have obtained total energies and wave functions, using Poturbation method and correlated variational approach for 2 electrons on N sites, N = 2,3,4,5,6 and the (3 x 3) cluster of the square lattice. The results obtained are shown in the tables below.

Table 1: Ground State Energy E_g/t as a Function of U/4t for 2 Electrons on 2 Sites.

U/4t	Perturbation	Variational	Exact
-50	-202.00	-200.02	-200.02
-30	-122.00	-120.03	-20.03
-20	-82.00	-80.05	-80.05
-3.0	-14.00	-12.32	-12.32
-2.0	-10.00	-8.47	-8.47
-1.0	-6.00	-4.83	-4.83
-0.05	-2.20	-2.10	-2.10
-0.02	-2.08	-2.04	-2.04
-0.01	-2.04	-2.02	-2.02
0	-2.00	-2.00	-2.00
0.02	-1.96	-1.96	-1.96
0.01	-1.60	-1.81	-1.81
0.50	0.00	-1.23	-1.23
1.00	2.00	-0.83	-0.83
1.50	4.00	-0.61	-0.61
2.0	6.00	-0.47	-0.47

Table 2: Ground State Energy E_g/t as a Function of (U/4t) for 2 Electrons on 3 Sites.

U/4t	Perturbation	Variation	Exact
-50	-137.333	-200.0404	-200.0404
-30	-84.000	-120.0678	-120.0678
-20	-57.333	-80.1024	-80.1024
-3.0	-12.000	-12.7446	-12.7446
-2.0	-9.333	-9.1231	-9.1231
-1.0	-6.6667	-6.0000	-6.0000
-0.05	4.1333	-4.0682	-4.0682
-0.02	-4.0530	-4.0269	-4.0269
-0.01	-4.0267	-4.0134	-4.0134
0	-4.0000	-4.0000	-4.0000
0.02	-3.9467	-39736	-3.9736
0.1	-3.7333	-3.8725	-3.8725
0.5	-2.6667	-3.4641	-3.4641
1.0	-1.3333	-3.1231	-3.1231
1.5	0.0000	-2.8990	-2.8990
2.0	1.3333	-2.7446	-2.7446

Table 3: Ground State Energy E_g/t as a Function of (U/4t) for 2 Electrons on 4 Sites.

U/4t	Perturbation	Variational	Exact
-50	-104.0000	-200.0400	-200.0400
-30	-64.0000	-120.0667	-120.0667
-20	-44.0000	-80.1000	-80.1000
-3.0	-10.0000	-12.6648	-12.6648
-1.0	-6.0000	-5.8064	-5.8064
-0.05	-4.1000	-4.0516	-4.0516
-0.02	-4.0100	-4.0203	-4.0203
-0.01	-4.0200	-4.0101	-4.0101
0	-4.0000	-4.0000	-4.0000
0.02	-3.9600	-3.9802	-3.9802
0.1	-3.8000	-3.9060	-3.9060
0.5	-3.0000	-3.6272	-3.6272
1.0	-2.0000	-3.4186	-3.4186
1.5	-1.0000	-3.2915	-3.2915
2.0	0.0000	-3.2078	-3.2078

Table 4: Ground State Energy E_g/t as a Function of U/4t for 2 Electrons on 5 Sites.

U/4t	Perturbation	Variational	Exact
-50	-84.0000	-200.0404	-200.0404
-30	-52.0000	-120.0678	-120.0678
-20	-36.0000	-80.1024	-80.1024

U/4t	Perturbation	Variational	Exact
-3.0	-8.80000	-12.7446	-12.7446
-2.0	7.2000	-9.1231	-9.1231
-1.0	-5.6000	-6.0000	-6.0000
-0.05	-4.0800	-4.0682	-4.0682
-0.02	-4.0320	-4.0269	-4.0269
-0.01	-4.0160	-4.0134	-4.0134
0	-4.0000	-4.0000	-4.0000
0.02	-3.968	-3.9736	-3.9736
0.1	-3.8400	-3.8725	-3.8725
0.5	-3.2000	-3.4641	-3.64641
1.0	-2.4000	-3.7016	-3.7016
1.5	-1.6000	-2.8990	-2.8990
2.0	-0.8000	-2.7446	-2.7446

Table 5: Ground State Energy E_g/t as a Function of U/4t for 2 Electrons on 6 Sites.

U/4t	Perturbation	Variational	Exact
-50	-70.6650	-200.040	-200.040
-30	43.9990	-120.0666	-120.0666
-20	30.6660	-80.0999	-80.09999
-3.0	-7.9999	-12.6495	-12.6495
-2.0	6.6666	-8.9467	-8.9467
-1.0	-5.3333	-5.6845	-5.6845
-0.05	-4.0667	-4.0350	-4.0350
-0.02	-4.0267	-4.0136	-4.0136
-0.01	-4.0133	-4.0067	-4.0067
0	-4.0000	-4.0000	-4.0000
0.02	-3.9733	-3.9869	-3.9868
0.1	-3.8667	-3.9394	-3.9394
0.5	-3.3333	-3.7824	-3.7824
1.0	-2.6667	-3.6845	-3.6845
1.5	-2.0000	-3.6313	-3.6313
2.0	-1.3333	-3.5984	-3.5984

Table 6: Ground State Energy E_g/t as a Function of U/4t for 2 Electrons on a (3x3) cluster of the Square Lattice.

U/4t	Perturbation	Variational	Exact
-50	-1040.195	-1200.0808	-200.0808
-30	390.257	-120.1356	-120.1356
-20	-183.818	-80.2051	-80.2051
-3.0	-14.2226	-13.6090	-13.6090
-2.0	-11.3582	-10.5941	-10.5941
-1.0	-9.284	-8.7446	-8.7446
-0.05	-8.0454	-8.0227	-8.0227
-0.02	-8.01793	-8.0090	-8.0090

U/4t	Perturbation	Variational	Exact
-0.01	-8.0089	-8.0045	-8.0045
0	-8.0000	-8.0000	-8.0000
0.02	-7.9822	-7.9912	-7.9912
0.1	-7.9121	-7.9579	-7.9579
0.5	-7.5802	-7.8190	-7.8190
1.5	-6.8889	-7.6090	-7.6090
2.0	-6.6173	-7.5440	-7.5440

From the results show in the tables, perturbation method gives correct results of the ground state energies E_g/t for negative values of u/4t in the range $-1 \leq \frac{u}{4t} \leq 0$.

For large values of U/4t, say -50, perturbation methods breaks down. In general, the result obtained using the variational method is closer to that obtained from the method of exact diagonalization than perturbation calculation.

Second order perturbation calculation, leads to diagonalization of a second order Hamiltonian matrix for any number of lattice sites, one and two dimensions. For variational calculation, dimension of Hamiltonian matrix increase as lattice sites increases. As U/4t increases to zero, ground state energy (E_g/t) tend to a common value of -2.0000 for 2 electrons on 2 sites, -4.0000 for 2 electrons on N sites N=3, 4, 5, 6 and -8.0000 for 2 electrons on a 3 x 3 cluster. These results reflect the usual trend.

9.0 Conclusion

We have studied in this paper the use of two approximate methods to calculate the energies and wavefunctions of systems described by the single-band Hubbard Hamiltonian. In the infinite U/4t limit, the results obtained from the perturbation calculation seems not to be appealing. This is not surprising, since as U becomes large, perturbation theory is expected to break down.

The variational method is therefore a better approximation for all values of U.

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