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On strongly correlated N-electron systems

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Abstract

An attempt is made in this work to extend the correlated variational approach of Chen and Mei [1], which was developed for two-electron systems, to N-electron systems (N>2). Preliminary results are reported here for four electrons interacting under a Hubbard-type potential in a one-dimensional lattice with only four sites.

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1.0 Introduction

Electronic correlation is largely responsible for the various interesting properties (magnetic, electrical, optical, etc) of solid materials. Owing to the recognition that the band structure of a metal has important influence on the stability of its electron gas, it is then obvious that to develop a theory of electronic correlations, one must take into account the atomic structure of the solid. In 1963, Hubbard [2] proposed a Hamiltonian model, the so-called t-U model, that describes a single band and which contains only two terms. While the *t*-part of the Hamiltonian model describes electrons hopping from site to site controlled by the Pauli exclusion principle, the U-part of the model describes the Coulomb interaction of two electrons of opposite spins occupying the same ionic site. The Hubbard Model, as it is known today, is widely believed to be the simplest model that describes the behaviour of correlated electrons in a solid [3-5].

Several mathematical methods (Exact Diagonalization Approach, Quantum Monte Carlo Method, etc) have been developed to study the physics of strongly correlated electron systems. For an excellent review of the methods, [see Reference 6].

In this work, we shall utilize the variational method. Though any variational approach is an approximation to an exact treatment, an important advantage of the variational method is that the explicit form of the variational trial wavefunction allows us to keep track of the physics. One can identify clearly which part of the wavefunction is relevant to any given physical situation. In spite of this obvious advantage, our literature search appears to reveal that the variational method has not enjoyed as much patronage as, for instance, Quantum Monte Carlo (QMC) calculational approach.

In 1989, Chen and Mei [1] developed a correlated variational approach (CVA) to study a quantum system of two electrons interacting in the ground state of the Hubbard Hamiltonian in a finite-sized lattice containing M lattice sites. Only one dimensional (ID) and two dimensional (2D) lattices were considered in their work. The extension of the work of Chen and Mei to 3D lattices has been carried out by one of us [7].

The variational wavefunction employed in the work of Chen and Mei [1] is suitable for studying the Hubbard Hamiltonian and the antiferromagnetic or singlet states that arise from it. The wavefunction is therefore highly inadequate for the study of quantum systems that admit triplet states, as in ferromagnetic materials. The construction of an appropriate variational wavefunction for studying quantum systems that admit both singlet and triplet states has been carried out by Enaibe and Idiodi [8]. In addition, simplified formulations of the work of Chen and Mei have been provided by Akpojotor and Idiodi [5,9]. These simplifications lead to a general expression for the variational ground state energy applicable to ID, 2D and 3D lattices.

So far we have considered a system consisting of only two electrons. Clearly, the variational wavefunction for a system of more than two electrons will be different from that for two electrons. It is desirable to have such a general variational wavefunction for a system of *N* electrons (N > 2). In this preliminary report, an attempt is made to extend the correlated variational approach of Chen and Mei [1] to a quantum system consisting of 4 electrons interacting in the ground state of the Hubbard model in a 1D lattice containing only 4 lattice sites. Periodic boundary conditions have been adopted in order to ensure that all lattice sites are equivalent.

The plan of this paper is as follows:
A brief review of the relevant features of the CVA are discussed in sections II and III for the Hubbard Hamiltonian and the Hubbard-Hirsch Hamiltonian, respectively. Section IV discusses the application of the CVA to a system of 4 electrons on 4 sites, and concluding remarks are given in section V.

2.0 Variational wavefunction for two-interacting electrons in the ground state of the Hubbard Hamiltonian

The single-band Hubbard Hamiltonian may be written as [1, 5-7].

$$H = -t\left\{\sum_{\langle ij\rangle\sigma} C_{i\sigma}^{+}\, C_{j\sigma} + H.c.\right\} + U\sum_{i} n_{i\uparrow}\, n_{i\downarrow} \qquad (2.1)$$

where $C_{i\sigma}^{+}, C_{j\sigma}$ and $n_{i\sigma}$ are the creation, annihilation, and number operators, respectively, for an electron of spin σ (= $\uparrow$ or $\downarrow$) in the Wannier state on the i^{th} lattice site. The notation $\langle ij\rangle$ means nearest neighbours, while t is the electronic hopping parameter between nearest neighbour sites i and j. H.c. denotes Hermitian conjugation and its inclusion in the Hamiltonian guarantees that the expectation values of all dynamical quantities will be real.

The motion of the two electrons interacting in the ground state of the Hubbard Hamiltonian is modeled by Chen and Mei [1], by a correlated variational trial wavefunction, suitable for studying singlet states, of the form

$$|\psi\rangle = \sum_{i} X_0\left\{|i\uparrow, i\rangle\right\} + \sum_{i\neq j} X_{|i-j|}\left\{|i\uparrow, j\downarrow\rangle - |i\downarrow, j\uparrow\rangle\right\} \qquad (2.2)$$

where X_0, X_1, …, and so on are variational parameters.

The wavefunction (2.2) was successfully applied to solve the problem of the dynamics of two electrons interacting under the Hubbard potential on various finite sized lattices with periodic boundary conditions. Detailed results emerging from these studies can be found in references 1, 5, and 7.

3.0 Variational wavefunction for two-interacting electrons in the ground state of the Hubbard-Hirsch Hamiltonian

The single-band Hubbard-Hirsch Hamiltonian may be written as [10]

$$H = -t\left\{\sum_{\langle ij\rangle\sigma} C_{i\sigma}^{+}\, C_{j\sigma} + H.c.\right\} + U\sum_{i} n_{i\uparrow}\, n_{i\downarrow} + J\sum_{\langle ij\rangle\sigma\sigma'} C_{i\sigma}^{+}\, C_{j\sigma'}^{+}\, C_{i\sigma'} C_{j\sigma} \qquad (3.1)$$

where the various operators in (3.1) are as defined in Section 2. The Hamiltonian consists of three parts: the t-term which describes the hopping of electrons from site to site, the on-site Coulomb interaction U and the nearest neighbour exchange interaction J. Clearly, if J is set equal to zero in equation (2.1), we recover the t-U model which is precisely the Hubbard Hamiltonian.

Enaibe and Idiodi [8], studied the motion of two electrons interacting in the ground state of the Hubbard-Hirsch Hamiltonian by a correlated variational trial wavefunction of the form

$$|\Psi\rangle = \sum_{i} X_o\left\{|i\uparrow, i\downarrow\rangle\right\} + \sum_{i\neq j} -X_{|i-j|}\left\{|i\uparrow, j\downarrow\rangle - |i\downarrow, j\uparrow\rangle\right\} + \sum_{i\neq j} Y_{|i-j|}\left\{|i\uparrow, j\uparrow\rangle\right\} \qquad (3.2)$$

where the $X_{|i-j|}$ and the $Y_{|i-j|}$ are variational parameters for the antiferromagnetic phase and ferromagnetic phase of the trial wavefunction, respectively.

The wavefunction given by equation (3.2) can be seen as an extension of that of Chen and Mei given by equation (2.2).

This approach was successfully applied to solve the problem of the dynamics of two electrons interacting in the ground state of the Hamiltonian (3.1) in various finite sized lattices with periodic boundary conditions. Detailed results emerging from theses studies can be found in references 8 and 11.

4.0 Variational wavefunction for four-interacting electrons in the ground state of the Hubbard Hamiltonian

When we have four electrons in a ID lattice that has only four lattice sites (half-filling), there are a total of 70 possible electronic states. Out of these, 36 are singlet states (unit of spin is zero) and 34 are triplet states (unit of spin is $\pm S$, where $S = 1$ or 2).

Since we are interested only in the singlet states for the ground state of the Hubbard Hamiltonian, an exact calculation to determine the ground state energy and wavefunction will definitely yield a 36 x 36 matrix. The exact diagonalization of this matrix produced the ground state energies and eigen vectors as a function of

the interaction strength U/4t. It is from these eigen vectors that the correlated variational trial wavefunction, utilized in this section, was constructed. This trial wavefunction may be written in the form

$$
\begin{aligned}
|\Psi\rangle = {} & X_1 \{|1\uparrow,1\downarrow,2\uparrow,2\downarrow\rangle + |3\uparrow,3\downarrow,4\uparrow,4\downarrow\rangle\} + X_2 \{|2\uparrow,2\downarrow,3\uparrow,3\downarrow\rangle + |4\uparrow,4\downarrow,1\uparrow,1\downarrow\rangle\} \\
& X_3 \{|1\uparrow,1\downarrow,3\uparrow,3\downarrow\rangle + |2\uparrow,2\downarrow,4\uparrow,4\downarrow\rangle\} + X_4 \{|1\uparrow,1\downarrow,2\uparrow,4\downarrow\rangle - |1\uparrow,1\downarrow,2\downarrow,4\uparrow\rangle| \\
& + |2\uparrow,2\downarrow,3\uparrow,1\downarrow\rangle - |2\uparrow,2\downarrow,3\downarrow,1\uparrow\rangle| + |3\uparrow,3\downarrow,4\uparrow,2\downarrow\rangle - |3\uparrow,3\downarrow,4\downarrow,2\uparrow\rangle| \\
& + \{|4\uparrow,4\downarrow,1\uparrow,3\downarrow\rangle - |4\uparrow,4\downarrow,1\downarrow,3\uparrow\rangle\} + X_5 \{|1\uparrow,1\downarrow,2\uparrow,3\downarrow\rangle - |1\uparrow,1\downarrow,2\downarrow,3\downarrow\rangle| \\
& + |2\uparrow,2\downarrow,4\uparrow,1\downarrow\rangle - |2\uparrow,2\downarrow,4\downarrow,1\uparrow\rangle| + |3\uparrow,3\downarrow,4\uparrow,1\downarrow\rangle - |3\uparrow,3\downarrow,4\downarrow,1\uparrow\rangle| \qquad (4.2) \\
& + |4\uparrow,4\downarrow,2\uparrow,3\downarrow\rangle - |4\uparrow,4\downarrow,2\downarrow,3\uparrow\rangle|\} + X_6 \{|1\uparrow,1\downarrow,3\downarrow,4\uparrow\rangle - |1\uparrow,1\downarrow,3\uparrow 4\downarrow\rangle| \\
& + |2\uparrow,2\downarrow,3\downarrow,4\uparrow\rangle - |2\uparrow,2\downarrow,3\uparrow,4\downarrow\rangle| + |3\uparrow,3\downarrow,1\downarrow,2\uparrow\rangle - |3\uparrow,3\downarrow,1\uparrow,2\downarrow\rangle| \\
& + |4\uparrow,4\downarrow,1\downarrow,2\uparrow\rangle - |4\uparrow,4\downarrow,1\uparrow,2\downarrow\rangle|\} + X_7 \{|1\uparrow,2\uparrow,3\downarrow,4\downarrow\rangle + |1\downarrow,2\downarrow,3\uparrow,4\uparrow\rangle\} \\
& X_8 \{|1\uparrow,2\downarrow,3\downarrow,4\uparrow\rangle + |1\downarrow,2\uparrow,3\uparrow,4\downarrow\rangle\} + X_9 \{|1\uparrow,2\downarrow,3\uparrow,4\downarrow\rangle + |1\downarrow,2\uparrow,3\downarrow,4\uparrow\rangle\}
\end{aligned}
$$

which is clearly patterned after the singlet state obtained when the 36 x 36 matrix for the electronic states is diagonalized exactly. The variational ground state energy E_g is given by

$$E_g = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \qquad (4.2)$$

where H is the Hubbard Hamiltonian given by equation (2.1) and $|\psi\rangle$ is the trial wavefunction given by equation (4.1).

It can easily be shown that

$$\langle\psi|\psi\rangle = 2X_1^2 + 2X_2^2 + 2X_3^2 + 8X_4^2 + 8X_5^2 + 8X_6^2 + 2X_7^2 + 2X_8^2 + 2X_9^2 \qquad (4.3)$$

and

$$
\begin{aligned}
\langle\psi|H|\psi\rangle = t \Big\{ & 16\left(\frac{U}{4t}\right) X_1^2 + 16\left(\frac{U}{4t}\right) X_2^2 + 16\left(\frac{U}{4t}\right) X_3^2 + 32\left(\frac{U}{4t}\right) X_4^2 + 32\left(\frac{U}{4t}\right) X_5^2 + 32\left(\frac{U}{4t}\right) X_6^2 \\
& - 16X_1 X_5 + 16X_2 X_6 - 16X_3 X_5 + 16X_3 X_6 - 16X_5 X_7 + 16X_5 X_9 \\
& - 16X_6 X_8 + 16X_6 X_9 \Big\} \qquad (4.4)
\end{aligned}
$$

where $U/4t$ is the on-site pair-interaction strength. Taking into account (4.2) and (4.3), Equation. (4.1) can be minimized with respect to the variational parameters to yield a 9 x 9 matrix of the form

$$
\begin{pmatrix}
E-8p & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\
0 & E-8p & 0 & 0 & 0 & -4 & 0 & 0 & 0 \\
0 & 0 & E-8p & 0 & 4 & -4 & 0 & 0 & 0 \\
0 & 0 & 0 & E-4p & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & E-4p & 0 & 1 & 0 & -1 \\
0 & -1 & -1 & 0 & 0 & E-4p & 0 & 1 & -1 \\
0 & 0 & 0 & 0 & 4 & 0 & E & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 4 & 0 & E & 0 \\
0 & 0 & 0 & 0 & -4 & -4 & 0 & 0 & E
\end{pmatrix}
\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ X_9 \end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad (4.5)
$$

where $E = E_g/t$ is the total energy of the four electrons and $p = U/4t$ The minimization was done subject to the normalization constraint

$$\sum_{i=1}^{9} X_i^2 = 1 \qquad (4.6)$$

The total energies for various values of $U/4t$ and the corresponding variational parameters can be determined. Clearly, the lowest energy for any given $U/4t$ is the variational ground state energy.

The results obtained are presented in Table 1.

Table 1: Variational Total Energies and the Corresponding Variational Parameters as a Function of the Interaction Strength $U/4t$

Interaction Strength $U/4t$	Total Energy E	Variational parameters								
		X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9
50.000	-0.0600	-0.0001	0.0001	0	0	-0.0061	-0.0061	-0.4082	-0.4082	0.8165
20.00	-0.1498	-0.0004	0.0004	0	0	-0.0153	-0.0153	-0.4082	-0.4082	0.8163
10.00	-0.2981	-0.0015	0.0015	0	0	-0.0304	-0.0304	-0.4079	-0.4079	0.8157
1.00	-2.1027	0.0808	-0.0808	0	0	0.2040	0.2040	0.3881	0.3881	-0.7762
0.25	-3.3408	0.2187	-0.2187	0	0	0.2921	0.2921	0.3497	0.3497	-0.6994
0.00	-4.0000	-0.4472	0	-0.4472	0	-0.4472	0	-0.4472	0	0.4472
-0.01	-4.0502	-0.3179	-0.3179	-0.6359	0	-0.3156	0.3156	-0.3117	0.3177	0
-1.00	-10.1027	0.3881	0.3881	0.7762	0.2040	0.2040	-0.2040	0.0808	-0.0808	0
-1.50	-13.6346	0.3964	0.3964	0.7929	0	0.1620	-0.1620	0.0475	-0.0475	0
-2.00	-17.3202	0.4007	0.4007	0.8013	0	0.1322	-0.1322	0.0305	-0.0305	0

Table 2 Comparison of the Variational Total Energy for 2 Electrons and 4 Electrons on a 4-site lattice. A case of quarter and half-filling, respectively.

Interaction Strength U/4t	Variational Total Energy for 2 electrons on 4 Sites [7]	Variational Total Energy for 4 electrons on 4 Sites
50.00	-2.8480	-0.0600
20.00	-2.8771	-0.1498
10.00	-2.9230	-0.2981
1.00	-3.4183	-2.1027
0.25	-3.7853	-3.3408
0.0	-4.0000	-4.0000
-0.01	-4.0100	-4.0502

4.1 Numerical results and discussion

It is evident from Table 1 that as the interaction strength U/4t is made positively large; the four electrons prefer to stay at different adjacent sites thereby forming an antiferromagnetic state. This is monitored by the variational parameter X_9 in the trial wavefunction. Double occupancy of a site, on the other hand, is less favoured in this parameter regime. But as the parameter U/4t decreases, the tendency to double occupancy of nearest neighbour sites, which is monitored by the variational parameters X_1 and X_2, increases. In this parameter regime the antiferromagnetic phase of the wavefunction, monitored by X_9, is permanently vacant.

From Table 1, the total energy of the four interacting electrons decreases as the on-site interaction strength decreases. As is evident in Table 2, when the pair-interaction strength is large, the total energies of the four interacting electrons in a one dimensional lattice system is greater at half-filling than at quarter filling. But as U decreases to zero, both energies tend to the common value of –4. These results reflect the usual trend.

5.0 Conclusion

We have in this study constructed a variational wavefunction for four electrons interacting under the Hubbard type potential in a ID lattice with four lattice sites. The trial wavefunction was patterned after an exact calculation. It is therefore not surprising that the variational calculation reproduced the energies obtained from an exact calculation. The matrix size encountered in the variational calculation was much smaller than the 36 x 36 matrix encountered in the exact calculation. This is another advantage of the variational method. It is desirable, however, to have a method of obtaining the trial wavefunction without first doing an exact calculation. This will allow one to apply the correlated variational approach to a general quantum system consisting of N-electrons on M-sites. This interesting problem is currently being studied with the help of group theory.

References

[1] Chen, L. and Mei, C. (1989). Phys. Rev. B39, 9006.
[2] Hubbard, J. (1963). Proc. Roy. Soc. London A276, 238.
[3] Ten Haaf, D.F.B. and Leeuwen, J.M.J. (1992). Phys. Rev. B46, 6313.
[4] Vollhardt, D., Blumer, N., Held, K., Koller, M., Schlipf, J. and Ulmke, M. (1997) Z. Phys. Bl03, 238.
[5] Akpojotor, G.E. and Idiodi, J.O.A. (2004). Zuma J. Pure and Applied Sciences 6(1), 124.
[6] Dagotto, E. (1994) Rev. Mod. Phys. 66, 772.
[7] Enaibe, A.E. (2003). A variational approach to the study of highly correlated electron systems. Ph.D thesis, University of Benin, Benin City, Nigeria.

[8] Enaibe, A.E. and Idiodi, J.O.A (2003). J. Nig. Assoc. Math. Phys. 7, 275.
[9] Akpojotor, G.E. and Idiodi, J.O.A. (2004). Nig. J. Phys. 16(2), 125.
[10] Amadon, J.C. and Hirsh, J.E. (1996). Phys. Rev. B54, 6364.
[11] Enaibe, A.E. and Idiodi, J.O.A. (2003). Benin Sci. Dig. Vol. 1, 96.