

Full Length Research Paper

# Properties of the $U \gg t$ 2-electrons in two dimensions using the Hubbard model

E.O. Aiyohuyin\* and Amen Oni-Ojo

Department of Physics University of Benin, Benin City, Nigeria.

Accepted 17 June, 2009

We examine the behaviour of 2 electrons on a  $2 \times 2$  square lattice sites. The Hubbard model was used to model the system and was diagonalized using the configuration interaction method which is a variational method. The variations of the ground state energy  $E/t$  ground state double occupied sites  $D$ , and the ground state kinetic energy  $E_{kin}/t$  with the interaction strength  $u/t$  ( $u < 0$  and  $u > 0$ ) were examined. The functions  $E/t$  and  $E_{kin}/t$  were found to be parabolic functions of  $u/t$ . This suggests that superconductivity is driven by both electron and hole doping.

**Key words:** Hubbard model, superconductivity, configuration interaction and electron correlation.

## INTRODUCTION

The parent materials for cuprate high- $T_c$  superconductors like  $\text{La}_2\text{Cu}_2\text{O}_4$  and  $\text{YBa}_2\text{Cu}_3\text{O}_6$  are antiferromagnetic insulators before doping. With doping the compounds become spin liquids and then transform into metals (Akira, 1993). Doping creates holes which can move. In the insulating phase, the electrons are tightly bound to their atoms. Their energy bands are narrow and kinetic energy is too small to allow hopping. This much is known about these fascinating materials.

On the other hand the Hubbard model has a stable antiferromagnetic phase at exactly half-filling (Schrieffer et al., 1989; Anderson, 1952) for all values of the interaction strength  $u/t$ . The attractive Hubbard model shows the sim-

plest Hamiltonian that incorporates the basic physics of electron pairing correlations in lattice. It is frequently applied to explain the appearance of super conductivity (Kocharian et al., 1999; Allen, 1990).

The purpose of this paper is to investigate the whole electron  $u > 0$  and electron-electron  $u < 0$  couplings [6] and their relationships to some ground state properties. The character of the pairing can be tuned by varying the in-

teraction strength  $u/t$  and the sign of the parameter  $u$ . Solution of the Hubbard model for the infinite number of electrons in a solid-state lattice requires an approximation scheme. Using the dynamical cluster approximation, for cluster of four sites, Maier et al's., results (Maier et al., 2005) showed that the properties of high-temperature superconductors were reproduced. This is one motivation for this work.

The paper is organized as follows. After the introduction, we review the Hubbard model and the basic formalism for the configuration interactions method, in section 2. Section 3 presents the calculations of the ground state properties. Section 4 is the summary of the results.

## Hubbard model and configuration interactions

In second quantization the Hubbard Hamiltonian is

$$-t \sum_{\langle ij \rangle} c_{ia}^+ c_{j\sigma} + u \sum_i n_i n_i \quad 2.1$$

Where;  $c_{i\sigma}^+$  ( $c_{i\sigma}$ ) creates (annihilates) an electron with spin  $\sigma$  in the Wannier state localized at site  $i$  and  $n_i \sigma$  is the number operator,  $t$  is the energy associated with an elec-

\*Corresponding author. E-mail: aiyohuyin@yahoo.com.

tron hopping between adjacent sites,  $u$  is the on-site Coulomb repulsion energy, and  $\langle ij \rangle$  restricts the sum to over nearest neighbours.

The Hubbard model is used effectively for narrow bands. If  $\frac{u}{t} \gg 1$  the Coulomb interaction is very strong and hopping is negligible. In the limit  $\frac{u}{t} \rightarrow \infty$  (Akira, 1993), no two electrons can occupy the same site unless their spins are antiparallel. In this limit, each electron occupies its own site and the system is similar to the case of non-interacting electrons. The electrons are localized. For finite but large  $\frac{u}{t}$ , electrons with antiparallel spins on adjacent site hop back and forth and can lower the energy of the system. The system is effectively in antiferromagnetic interaction between the spins. If  $\frac{u}{t} \rightarrow 0$ , the model becomes the nearest neighbour tight binding model.

The configuration interactions technique is a variational method (Post Hartree-Fock Techniques, 2009). We begin with the expansion of the ground-state wave function.

$$|\psi_o\rangle = \left( 1 + \sum_{i\mu} \alpha_{\mu}^i c_i^+ c_{\mu} + \sum_{\substack{i<j \\ \mu<\nu}} \alpha_{\mu\nu}^{ij} c_i^+ c_j^+ c_{\nu} c_{\mu} + \dots \right) |\phi_{SCF}\rangle$$

$c^+$  ( $c$ ) creates (annihilates) an electron. The subscripts on the operators refer to electronic orbitals. The Greek indices  $\mu, \nu$  etc are used for occupied orbitals and latin indices  $i, j$  etc for unoccupied orbitals.

The self-consistent field (SCF) occupied ground state is

$$D \quad V_S \quad \frac{u}{t}$$

defined as:

$$|\phi_{SCF}\rangle = \prod_{\mu=1}^N c_{\mu}^+ |0\rangle$$

$|0\rangle$  is the vacuum state. The electrons are in delocalized molecular orbitals.

The values of  $\alpha_{\mu}^i, \alpha_{\mu\nu}^{ij}$ , etc are obtained by diagonalizing (Peter Fulde, 1995) the Hamiltonian  $H$  within a Hilbert space of a given dimension. The coefficients may be seen also as variational parameters fixed by minimizing the energy.

The dimension of the Hilbert space is of the order  $\binom{2L}{N}$

and equals the number of different  $N$ -electron configurations.

Where  $L$  is the number of basis functions and  $N$  is the number of electrons. For a  $2 \times 2$  square lattice sites, there are four basis functions. Here the Hilbert space has dimension  $\binom{8}{2} = 28$  configurations. The configuration interactions technique enables a drastic reduction of the Hilbert space to only two from 28 namely;

$$|\phi_{SCF}\rangle \text{ and } c_1^+ c_2^+ c_2 c_1 |\phi_{SCF}\rangle.$$

The system of equations of the configuration interactions takes the form

$$\sum_J H_{IJ} \alpha_J = E \alpha_I \tag{2.1}$$

Here  $H_{IJ} = \langle \phi_I | H | \phi_J \rangle$ , Provided the  $|\phi_I\rangle$  are orthogonal otherwise, the right hand side of equation 2.1 has to be multiplied by the overlap matrix. The  $\alpha_I$  can be found by iteration; if approximate starting values are chosen. From  $\sum_J \alpha_J^{(0)} \langle \phi_I | H | \phi_J \rangle$  the  $\alpha_I^{(1)}$  are determine requiring  $\sum_I |\alpha_I^{(1)}|^2 = 1$ . The iteration is continued until the results converge.

### Calculations of the ground state properties

the number of particles. Thus the number of configurations is 28. The ground-state wave function is expanded in terms of only two configurations namely:

$$|\phi_{SCF}\rangle \text{ and } c_1^+ c_2^+ c_2 c_1 |\phi_{SCF}\rangle$$

The system of configuration interactions

The ground-state energy is

$$[20u^2 - 45.8u + 360.9t^2]^{1/2}$$

equations are:

$$\alpha_1^{(0)} \langle \phi_1 | H | \phi_1 \rangle + \alpha_2^{(0)} \langle \phi_1 | H | \phi_2 \rangle = E \alpha_1^{(1)} \tag{1}$$

$$\alpha_1^{(0)} \langle \phi_2 | H | \phi_1 \rangle + \alpha_2^{(0)} \langle \phi_2 | H | \phi_2 \rangle = E \alpha_2^{(1)} \tag{2}$$

$$|\alpha_1^{(1)}|^2 + |\alpha_2^{(1)}|^2 = 1 \tag{3}$$

The Hubbard Hamiltonian is expanded thus:

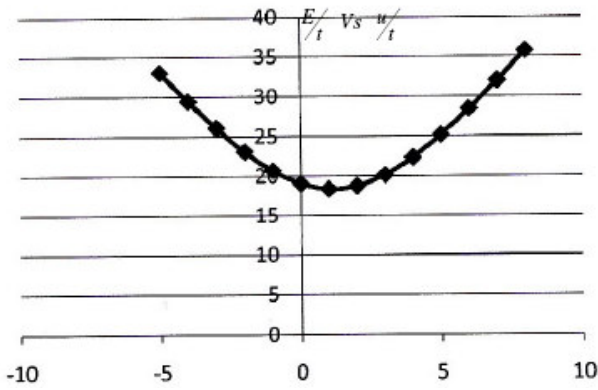


Figure 1. The ground-state energy vs.  $u/t$ .

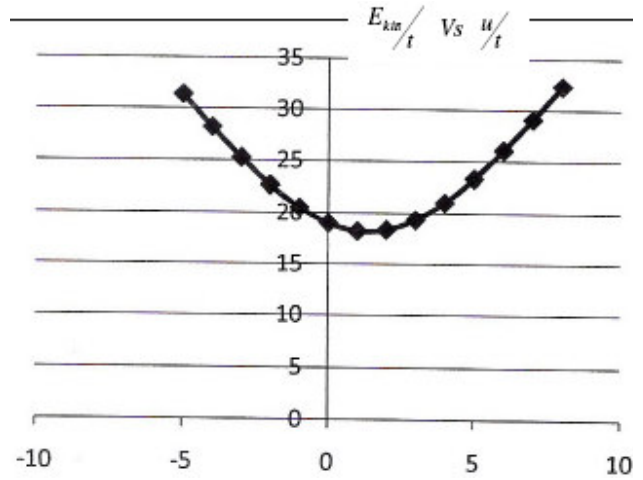


Figure 3. The ground-state kinetic energy vs.  $u/t$ .

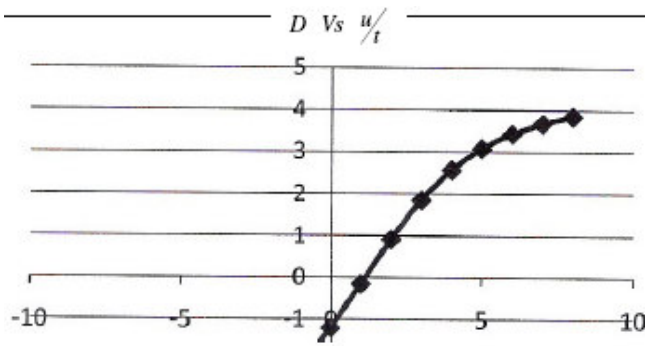


Figure 2. The ground-state doubly occupied sites vs.  $u/t$ .

$$H = -2 \left[ c_1^\dagger c_2 + c_1^\dagger c_3 + c_1^\dagger c_4 + c_2^\dagger c_1 + c_2^\dagger c_3 + c_2^\dagger c_4 + c_3^\dagger c_1 + c_3^\dagger c_2 + c_3^\dagger c_4 + c_4^\dagger c_1 + c_4^\dagger c_2 + c_4^\dagger c_3 \right] + 4u$$

The ground-state doubly occupied sites are:

$$D = \left( 20u^2/t^2 - 28/t^2 \right) \left( \frac{20u^2}{t^2} - 46u/t^2 + 361 \right)^{1/2}$$

and the ground-state kinetic energy is:

$$\frac{E_{kin}}{t} = \left( 20u^2/t^2 - u/t^2 \cdot 46 + 361 \right)^{1/2} + \frac{1}{2t} \left( \frac{2u}{t} - 4 \left( \frac{u}{t} \right)^2 \right) \left( 20 \left( \frac{u}{t} \right)^2 + 46 u/t^2 + 361 \right)^{-1/2}$$

### Summary

The ground-state properties of energy, kinetic energy are parabolic functions of the interaction strength  $\left( \frac{u}{t} < 0 \text{ and } \frac{u}{t} > 0 \right)$ . This is indicated by Figure 1. This suggests that electron-electron interaction is as important

as hole-electron interaction in the ground state. At large  $u/t$  the free-single particle motion of electrons or holes inside the band is strongly suppressed by increasing  $\left| \frac{u}{t} \right|$  due to the large occupation of doubly occupied sites in the bound state.

The local attraction of electrons or holes favours the formation of the local pairs with opposite spins while the local repulsion of electrons or holes suppresses the pair formation from Figure 2.  $D$  increases monotonically with  $\left| \frac{u}{t} \right|$  for  $u > 0$  and  $u < 0$ .

However, from Figure 3 the kinetic energy increases with increasing  $u/t$  for  $u > 0$  and  $u < 0$ .

### REFERENCE

Akira Ishihara (1993). Electron Liquids (Springer-Verlag Berlin).  
 Allen PB (1990). Electronic pairing: How and why? Edited by Lynn JW (1952). High temperature superconductivity (Springer-Verlag Berlin 303).  
 Anderson PW (1952). New approach to the theory of superexchange interactions Phys. Rev. 86: 694.  
 Hubbard J (1963). Electron correlations in narrow energy bands. Proc. Roy. Soc. London Ser. A276. 238.  
 Kocharian AN, Yang Chiang YL (1999). Phase Transitions and exact ground-state properties of the one dimensional Hubbard model in a magnetic field Phys. Rev. B59: 7458.  
 Maier TA, White JB, Jarrel M, Kent P, Schulthess TC (2005). New insights into high temperature superconductivity from a computational solution of the two-dimensional Hubbard model J. Phys. Conference Series 16: 257.  
 Peter Fulde (1995). Electron Correlations in molecules and solids (Third Enlarged Edition Springer-Verlog Heidelberg).  
 Post Hartree-Fock Techniques Address: www.physics.uc.edu/~plcent/the\_sis/plcthnnode14.html (Assessed on June 15, 2009).  
 Schrieffer JR, Wen XG, Zhang SC (1989). Dynamic flutuations and the

bag mechanism of the high- $T_c$  superconductivity Phys. Rev. B39: 11663.

Yang C, Kocharian AN, Chiang YL (2000). New insights into high temperature superconductivity from a computational solution of the two-dimensional Hubbard model J. Phys. Condens. Matter 12: 7433.