Properties of the $U >> t$ 2-Electrons in Two Dimensions Using the Hubbard Model

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We examine the behaviour of 2 electrons on a 2 x 2 square lattice sites. The Hubbard model was used to model the system and was diagonalized using the configuration interaction method, which is essentially a variational method. Variations of the ground state energy $\left(E/t\right)$, the 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, D and $\frac{E_{kin}}{t}$ were found to be symmetric functions of u/t. This suggests that superconductivity is driven by both electron and hole doping.

1. Introduction

The parent materials for cuprate high-T_c superconductors like La_2 Cu_2O_4 and YBa_2 Cu_3 O_6 are antiferromagnetic insulators before doping. With doping, these compounds become spin liquids and then transform into metals [1]. 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 [2] has a stable antiferromagnetic phase at exactly half-filling [3,4] for all values of the interaction strength u/t. The attractive Hubbard model shows the simplest Hamiltonian that incorporates the basic physics of electron pairing correlations in lattice. It is frequently applied to explain the appearance of super conductivity [5,6].

The purpose of this paper is to investigate the hole –electron $(u<0)$ and electron-electron $(u>0)$ couplings [7] and their relationships to some ground state properties. The character of the pairing can be tuned by varying the interaction strength u/t and the sign of the parameter u.

The solution of Hubbard model for an infinite number of electrons in a solid-state lattice requires an approximation scheme. Using the dynamical cluster approximation, for cluster of four sites, Mark Jarrell's results [8] showed that the properties of high-temperature superconductors can be 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 Sec. 2. Sec. 3 presents the calculations of the ground state properties and Sec. 4 gives a summary of the results.

2. Hubbard model and configuration interactions

In second quantization, the Hubbard Hamiltonian is

$$-t\sum_{\langle ij\rangle\sigma}c_{i\sigma}^{+}c_{j\sigma}+u\sum_{i}n_{i\uparrow}n_{i\downarrow} \qquad (2.1)$$

where $c_{i\sigma}^{+}\left(c_{i\sigma}\right)$ creates (annihilates) an electron with spin σ in the Wannier state localized at site i, $n_{i\sigma}$ is the number operator, t is the energy associated with an electron hopping between adjacent sites, and u is the on-site Coulomb repulsion energy, whereas $\langle ij\rangle$ restricts the sum over to nearest neighbours.

The Hubbard model is used effectively only for the narrow bands. For u/t >>1, the coulomb interaction is very strong and the hopping is negligible. In the limit $u\to\infty$ [1], 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. For finite but large u, 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. For $t\to 0$, the electrons are localized. The electrons are uniformly spaced and behave

classically. This is the atomic limit. For $u \to 0$, the model becomes the nearest neigbour tight binding model.

The configuration interactions technique is a variational method. We begin with the expansion of the ground-state wavefunction

$$|\psi_0\rangle = \left(1 + \sum_{i\mu} \alpha_\mu^i c_i^+ c_\mu + \sum_{\substack{i<j \\ \mu<\nu}} \alpha_{\mu\nu}^{ij} c_i^+ c_j^+ c_\nu c_\mu + ... \right) |\phi_{SCF}\rangle$$

Here, $c_i^+ c_\mu$, $c_i^+ c_j^+ c_\nu c_\mu$, and so on are creation and annililation operators respectively. They do so in delocalized canonical molecular orbitals.

The values of α_μ^i, $\alpha_{\mu\nu}^{ij}$, etc. are obtained by diagonalizing [9] H within a Hilbert space of given dimension. The coefficients may also be seen as variational parameters fixed by minimizing the energy.

The system of equations of the configuration interactions takes the form

$$\sum_J H_{IJ}\, \alpha_J = E\alpha_I \qquad (2.2)$$

Here, $H_{IJ} = \langle \phi_I | H | \phi_J \rangle$.

Provided $|\phi_I\rangle$ are orthogonal otherwise, the right-hand side of equation (2.2) has to be multiplied by the overlap matrix.

The α_I can be found by iteration if the approximate starting values are chosen. From $\sum_J \alpha_J^{(0)} \langle \phi_I | H | \phi_J \rangle = E\alpha_I^{(1)}$, $\alpha_I^{(1)}$ are determined by requiring that $\sum_I \left| \alpha_I^{(1)} \right|^2 = 1$.

The iteration is continued until the results converge.

3. Calculations of the ground state properties

In this system, the number of actual configurations is: $\binom{2L}{N}$ Here L is the number of sites or basis functions and N is 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:

$|\phi_{SCF}\rangle$ and $|\phi_2\rangle = c_1^+ c_2^+ c_2 c_1 |\phi_{SCF}\rangle$. The system of configuration interactions equations are:

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

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

$$\left|\alpha_1^{(1)}\right|^2 + \left|\alpha_2^{(1)}\right|^2 = 1 \quad 3$$

The Hubbard Hamiltonian is expanded thus:

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

The ground-state energy is

$$E = \left[20u^2 - 45.8u + 360.9t^2 \right]^{1/2}$$

The ground-state double occupied sites are

$$D = \left[20 u^2/t^2 - 27.9/t^2 \right] \left[20\left(\frac{u}{t}\right)^2 - \frac{45.8u}{t^2} + 360.9 \right]^{-1/2}$$

And, the ground-state kinetic energy is

$$\frac{E_{kin}}{t} = \left[20\left(\frac{u}{t}\right)^2 - \frac{u}{t^2}\, 45.8 + 360.9 \right]^{1/2} + \frac{1}{2t} \left[\frac{2u}{t} - 4\left(\frac{u}{t}\right)^2 \right] \left[20\left(\frac{u}{t}\right)^2 + 45.8\, u/t^2 + 360.9 \right]^{-1/2}$$

4. Summary

The ground-state properties of energy and the kinetic energy are symmetric functions of the interaction strength (u < 0 and u > 0). This suggests that electron-electron interaction is as important as hole-electron interaction in the ground state. At large u/t $(u>0),(u<0)$ the free-single particle motion of electrons or holes inside the band is strongly suppressed by increasing $|u|$ due to the large occupation of doubly occupied sites in the bound state.

The local attraction of electrons or holes favours the formation of local pairs with opposite spins, while the local repulsion of electrons or holes suppresses the pair formation D that increases with u/t for $(u>0),(u<0)$.

However, the kinetic energy increases with increasing value of $u(u<0,\ u>0)$. This, taken with the similar behaviour of D, shows that the system moving from an insulator of a spin liquid, a metal, to a super conductor thereafter [1].

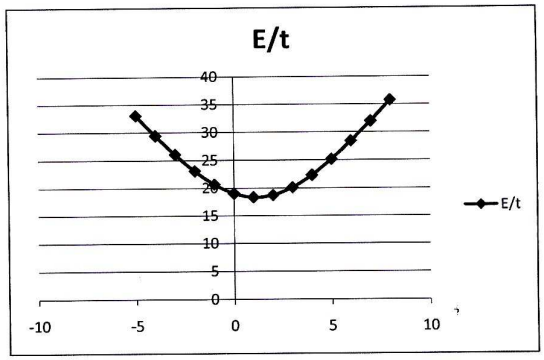

Fig. 1: The ground-state energy vs u/t.

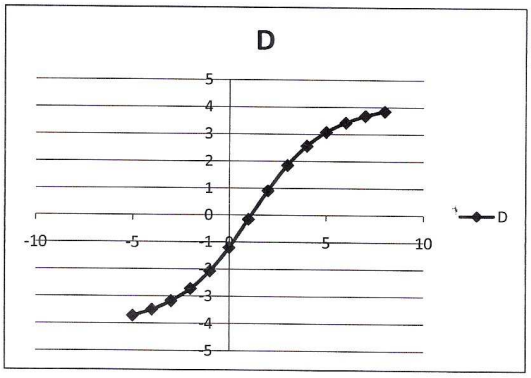

Fig. 2: The ground-state double occupied sites vs u/t.

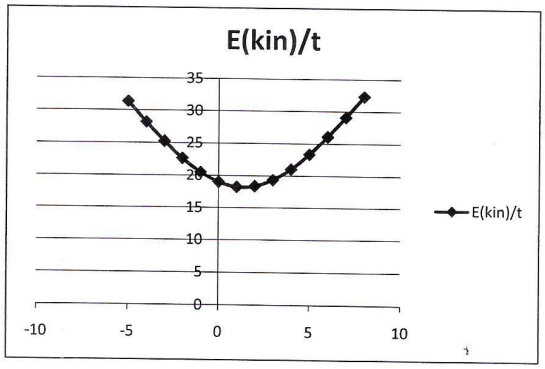

Fig. 3: The ground-state kinetic energy vs u/t.

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