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Superconductivity in Correlated Fermions System

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Abstract

We have studied the Hubbard model which is a model that is used to describe the physics of strongly correlated Fermions systems. Using the Hubbard model, we worked on some systems in one dimension (1-D) at half fillings. We employed the numerical exact diagonalization technique and found out that there was a transition from metallic state to a superconducting state as we move from the positive value of the On-site interaction strength to the negative value of the On-site interaction strength U.

Keywords: Hubbard model, exact diagonalization, superconducting state and interaction strength.

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1.0 Introduction

Electron correlation in narrow-band systems has been studied extensively using the Hubbard model [1], in which the magnitude of the on-site interaction strength U and the one-electron band width W control the properties of the system [2]. Despite intensive theoretical work, the physics of strongly correlated fermions still contains numerous unsolved problems, even in its simplest formulation such as the single band Hubbard model [3]. It is also believed that the Hubbard model can describe some of the properties of the transition-metal oxides, and possibly high-temperature superconductors. Some researchers have worked on the Hubbard model in infinite dimension [3,4,5], and results on the thermodynamic quantities, resistivity, and optical conductivity were presented in their work[6].

Following the discovery of high-T_c superconductivity [7], the two-dimensional (2D) Hubbard model with a repulsive Coulomb interaction has been suggested as one of the simplest models that may contain the basic interactions to explain superconductivity in the cuprates [8]. However, evidence for a super-conducting ground state has not been found in numerical calculation [9]. In one dimension the U<0 ground state wave function can be obtained exactly [10], but it is too complicated to decide whether it could lead to the superconductivity.

In this paper, we will study the behaviour of the lowest energy levels of the Hubbard model at half fillings on finite one-dimensional systems as a function of U/t. We will consider the value of U/t ranging from the positive value of U to the negative value of U. It has been observed that the negative-U Hubbard model is a superconductor not only at half filling but for all fillings [9,11]. There are several mechanisms which can induce an effective attraction among the electrons which overcomes the repulsive electromagnetic interaction (coupling of the electrons with the lattice and with quasi-bosonic excitations, chemical mechanisms, e.t.c.), so that the Hubbard model with negative U is also of considerable interest [12]. We also look at the phase transition from metallic to superconducting state for the various systems by plotting the ground state energy (energy band gap) of the system with the on-site Coulomb interaction. A reduction in the energy gap is analogous to the overlapping of the Hubbard sub-band which describes a metallic state.

The Hubbard model in one-dimension for systems at half fillings is given by Eqs. (1) [13]

$$H = -t\sum_{\langle ij\rangle\sigma}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + h.c\right) + U\sum_i n_{i\uparrow}n_{i\downarrow} \qquad (1)$$

Where t is the hopping integral, $c_{i\sigma}^{\dagger}$and $c_{j\sigma}$ are the creation and annihilation operators of electron in lattice site *i* and spin σ(↑↓) respectively. U is the on-site interaction strength. $n_{i\uparrow}$ is the particle number which is given as $n_{i\uparrow} = c_{i\uparrow}^{\dagger}c_{j\uparrow}$.

2.0 Methodology

The exact diagonalization technique is employed in this work [14]. The Hubbard model for 2 electrons on 2 sites is given as

$$H = -t\left\{c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\uparrow}^{\dagger}c_{1\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow}\right\} + U\{n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\}$$

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$$H = -t\{c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\uparrow}^{\dagger}c_{1\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow}\} + U\{c_{1\uparrow}^{\dagger}c_{1\uparrow}c_{1\downarrow}^{\dagger}c_{1\downarrow} + c_{2\uparrow}^{\dagger}c_{2\uparrow}c_{2\downarrow}^{\dagger}c_{2\downarrow}\}$$

where $n_{1\uparrow} = c_{1\uparrow}^{\dagger}c_{1\uparrow}$ (2)

There are six possible states which the electrons can have:

$$\left.\begin{aligned} |1\rangle &= |1\uparrow 1\downarrow\rangle \\ |2\rangle &= |2\uparrow 2\downarrow\rangle \\ |3\rangle &= |1\uparrow 2\downarrow\rangle \\ |4\rangle &= |1\downarrow 2\uparrow\rangle \\ |5\rangle &= |1\uparrow 2\uparrow\rangle \\ |6\rangle &= |1\downarrow 2\downarrow\rangle \end{aligned}\right\} \quad (3)$$

If we act Eqs. (2) on Eqs. (3) a matrix will be formed which is given below

$$H = \begin{bmatrix} u & 0 & -t & t & 0 & 0 \\ 0 & u & -t & t & 0 & 0 \\ -t & -t & 0 & 0 & 0 & 0 \\ t & t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4)$$

The ground state energy of the system is given by (5):

$$\mathrm{E} = \frac{\mathrm{E_g}}{\mathrm{t}} = -2\left[\sqrt{\left(\frac{\mathrm{U}}{4\mathrm{t}}\right)^2 + 1} - \left(\frac{\mathrm{U}}{4\mathrm{t}}\right)\right] \quad (5)$$

The Hubbard model for 3 electrons on 3 sites is given as

$$H = -t\{c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\uparrow}^{\dagger}c_{1\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow} + c_{2\uparrow}^{\dagger}c_{3\uparrow} + c_{2\downarrow}^{\dagger}c_{3\downarrow} + c_{3\uparrow}^{\dagger}c_{2\uparrow} + c_{3\downarrow}^{\dagger}c_{2\downarrow} + c_{1\uparrow}^{\dagger}c_{3\uparrow} + c_{1\downarrow}^{\dagger}c_{3\downarrow} + c_{3\uparrow}^{\dagger}c_{1\uparrow} + c_{3\downarrow}^{\dagger}c_{1\downarrow}\} + U\{c_{1\uparrow}^{\dagger}c_{1\uparrow}c_{1\downarrow}^{\dagger}c_{1\downarrow} + c_{2\uparrow}^{\dagger}c_{2\uparrow}c_{2\downarrow}^{\dagger}c_{2\downarrow} + c_{3\uparrow}^{\dagger}c_{3\uparrow}c_{3\downarrow}^{\dagger}c_{3\downarrow}\} \quad (6)$$

There are twenty possible states which the electrons can have. If Eqs. (6) acts on the twenty possible states, a matrix will be generated and the ground state energy of the system is given as:

$$\mathrm{E} = \frac{1}{2}(-3t + u - \sqrt{9t^2 + 2tu + u^2}) \quad (7)$$

The Hubbard model for 4 electrons on 4 sites is given as

$$H = -t\{c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\uparrow}^{\dagger}c_{1\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow} + c_{2\uparrow}^{\dagger}c_{3\uparrow} + c_{2\downarrow}^{\dagger}c_{3\downarrow} + c_{3\uparrow}^{\dagger}c_{2\uparrow} + c_{3\downarrow}^{\dagger}c_{2\downarrow} + c_{1\uparrow}^{\dagger}c_{3\uparrow} + c_{1\downarrow}^{\dagger}c_{3\downarrow} + c_{3\uparrow}^{\dagger}c_{1\uparrow} + c_{3\downarrow}^{\dagger}c_{1\downarrow} + c_{1\uparrow}^{\dagger}c_{4\uparrow} + c_{1\downarrow}^{\dagger}c_{4\downarrow} + c_{4\uparrow}^{\dagger}c_{1\uparrow} + c_{4\downarrow}^{\dagger}c_{1\downarrow} + c_{4\uparrow}^{\dagger}c_{3\uparrow} + c_{4\downarrow}^{\dagger}c_{3\downarrow} + c_{3\uparrow}^{\dagger}c_{4\uparrow} + c_{3\downarrow}^{\dagger}c_{4\downarrow} + c_{2\uparrow}^{\dagger}c_{4\uparrow} + c_{2\downarrow}^{\dagger}c_{4\downarrow} + c_{4\uparrow}^{\dagger}c_{2\uparrow} + c_{4\downarrow}^{\dagger}c_{2\downarrow}\} + U\{c_{1\uparrow}^{\dagger}c_{1\uparrow}c_{1\downarrow}^{\dagger}c_{1\downarrow} + c_{2\uparrow}^{\dagger}c_{2\uparrow}c_{2\downarrow}^{\dagger}c_{2\downarrow} + c_{3\uparrow}^{\dagger}c_{3\uparrow}c_{3\downarrow}^{\dagger}c_{3\downarrow} + c_{4\uparrow}^{\dagger}c_{4\uparrow}c_{4\downarrow}^{\dagger}c_{4\downarrow}\}$$

(8)

There are seventy possible states which the electrons can have. If we act Eqs. (8) on the seventy possible states, a matrix will be generated and the ground state energy of the system for a particular case when t=1 and U=5 is given as -2.38. We have decided to solve for a particular case because the matrix formed is so large and a generalized ground state cannot be found easily using the software we employed.

Discussion of Results

From computation, Fig. 3.1 of the Hubbard model for a system of 2 electrons on 2sites in one-dimension is divided into three parts: the part on the right hand side of the vertical axis is the metallic part while, above it is the insulating part (i.e $Eg \geq 0$ is the insulating part and $Eg < 0$ is the metallic part) [15]. As the on-site interaction strength, U is increased; the energy band width also increased and got to a point where it remained constant within the metallic regime. As long as the value of U kept on increasing the energy band width became stable very close to the zero energy gap and there was no transition from the metallic region to the insulating region. But as the value of U becomes more negative, there was a sudden transition from the metallic state to the superconducting state. The value of

E_g=-2.00 where U=0 is the point at which the system becomes superconductor [9] and [10].

From computation, Fig. 3.2 of the Hubbard model for a system of 3 electrons on 3 sites in one-dimension shows that, as the on-site interaction strength, U is increased; the energy band width also increased and got to a point where it remained constant within the metallic regime. As long as the value of U kept on increasing the energy band width became metallic in the sense that the overlapping of the Mott-Hubbard sub-bands increased and there was no transition from the metallic region to the insulating region. There was transition from the metallic state to the superconducting state. The value of E_g where U=0 is the point at which the system becomes superconductor [9] and [10], and at that point the corresponding value of E_g= -3.00

From the computation of Table 3.3, Fig. 3.3 of the Hubbard model for a system of 4 electrons on 4 sites in one-dimension shows that, as the on-site interaction strength, U is increased; the energy band width also increased and got to a point where it remained constant within the metallic regime. As long as the value of U kept on increasing the energy band width became metallic which is analogous to the overlapping of the Mott-Hubbard sub-bands being increased and there was no transition from the metallic region to the insulating region. Transition from the metallic state to the superconducting state takes place at the point E_g= -4.00. This work is just the preliminary stage, a detailed work will be published in the next volume.

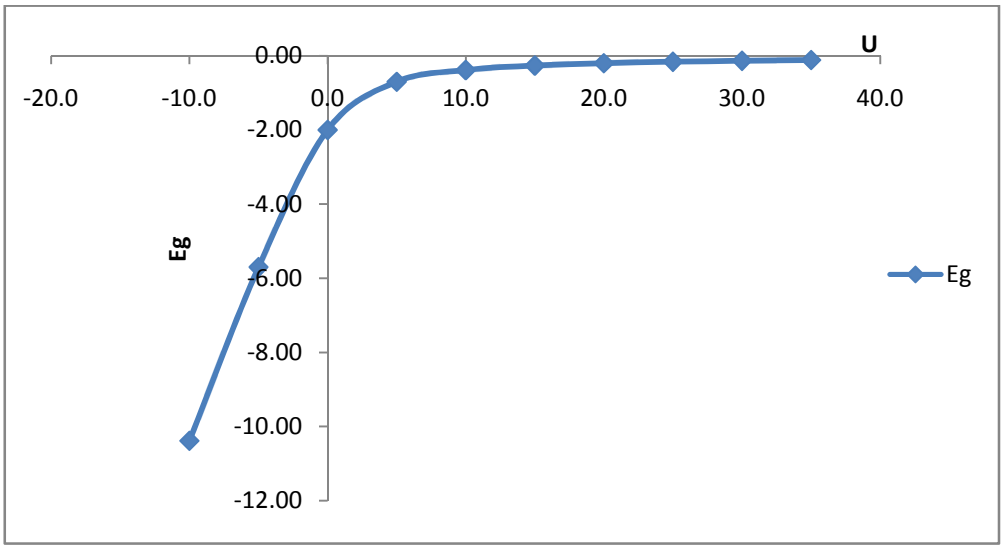

Fig 3.1: Graph of the ground state energy (Eg) plotted against U, for a system of 2 electrons on 2-sites.

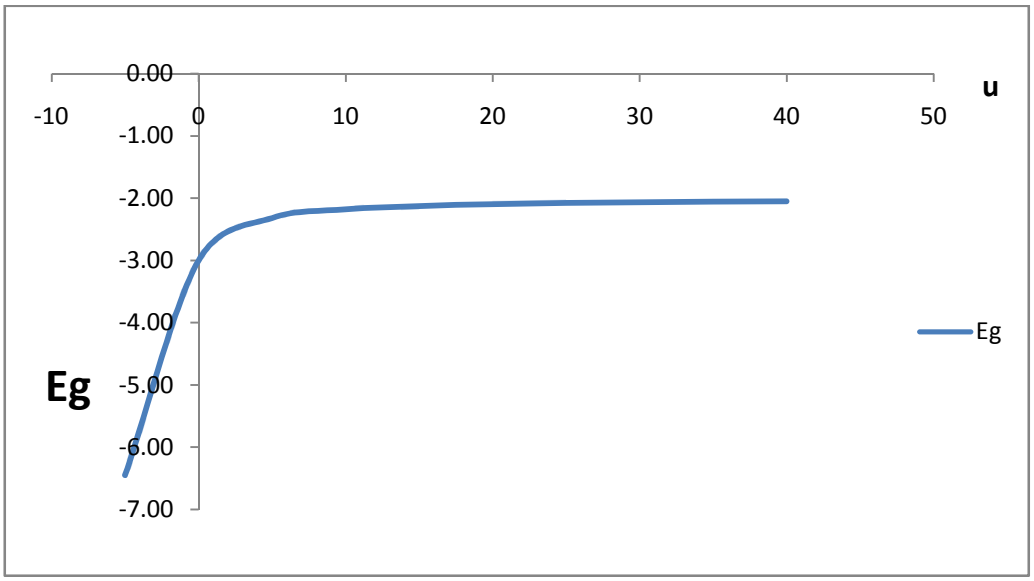

Fig 3.2: Graph of the ground state energy (Eg) plotted against U, for a system of 3 electrons on 3-sites.

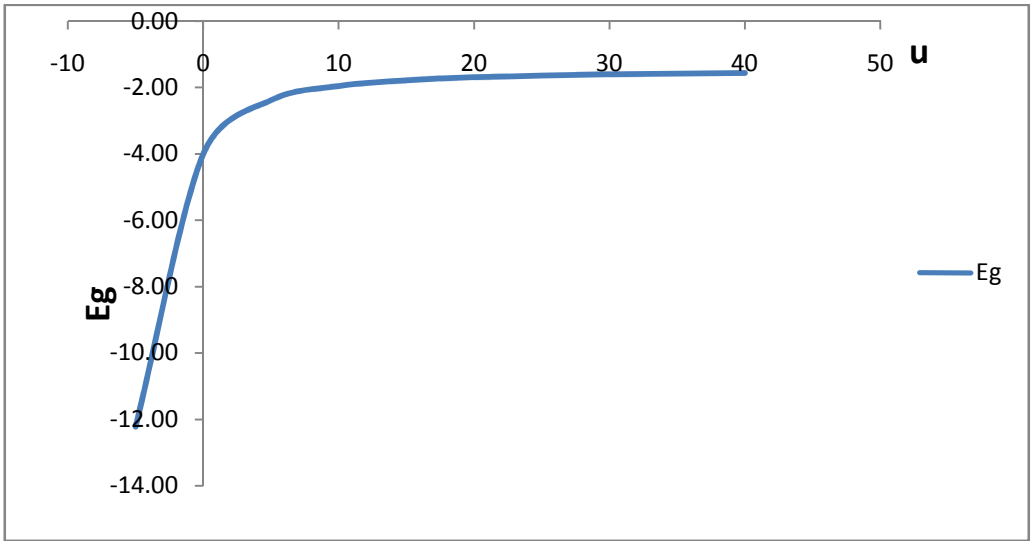

Fig 3.3: Graph of the ground state energy (Eg) plotted against U, for a system of 2 electrons on 2-sites.

Conclusion

In this work, we have shown that superconductivity exist in the one-dimensional finite Hubbard model at half fillings using the exact diagonalization technique. As the number of sites increases, the value of E_g at which the transition from metallic state to superconducting state also increases. It is interesting to know that no matter the value of U for a finite one-dimension Hubbard model, transition from metallic state to insulating state was difficult to achieve. The positive-U Hubbard model is known as the repulsive Hubbard model while the negative-U Hubbard model is called the attractive Hubbard model, under certain conditions the presence of an attractive short range interaction may lead to the formation of electron pairs in the real space and many physical systems exhibit properties related to the existence of local electrons (superconductors, transition metal oxides, alternating-valence compounds, etc. [12].

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