

Ground State Energy of the Two Electrons on 2 Site of Aid Lattice Using the Lanczos Technique

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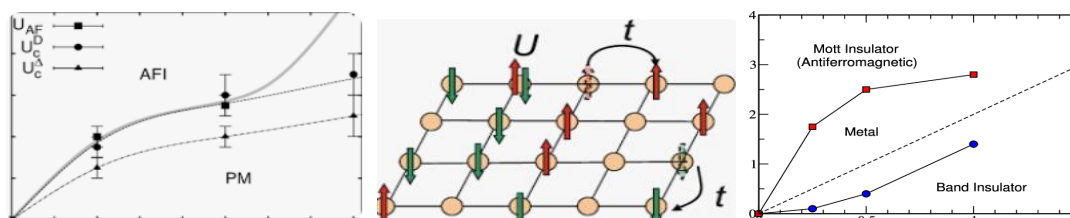
Abstract

Standard approaches to evaluate the ground-state properties of the Hubbard model via the Lanczos method have convergence problems upon the growing difference between hopping and Coulomb interaction strength. This issue is quite relevant since energy convergence does not necessarily translate into convergence of the ground-state itself. The ground state energy and wave function of the single band Hubbard model on the one dimensional lattice is computed using the Lanczos methods. Ground state energy for two electron system on two sites was analytically solved using 4x4 matrixes. It is shown that the ground state energies obtained for different values of the interaction strength, compare nicely with that obtained using the method exact calculation.

Keywords: Ground-State, Hubbard Model, Lanczos Method, Electron System.

Introduction

The Hubbard model is the simplest model that is capable of describing the essential physics of strongly correlated electron systems. It is believed that the competition between electronic mobility and on-site Coulomb repulsion described by the Hubbard model, which favors the localization of electrons, (Macedo, 2013). The Hubbard model is an approximate model used, especially in solid state physics, to describe the transition between conducting and insulating systems. It is widely believed to be a good model for correlated electron systems including high temperature superconductors. The Hubbard model is solvable for a few electrons and a few sites but is extremely difficult to solve for many electrons on many sites.



Figures: The phase diagram of the ionic Hubbard model (Souza et al., 2016a)

Ground state phase diagram of the Hubbard model on the anisotropic triangular lattice in t' - U plane. AFI and PM denote an antiferromagnetic insulating phase and a paramagnetic metallic phase. The dash-dotted curve represents the metal insulator transition determined by the opening of the charge gap. The broken curve denotes a possible phase boundary between different insulating states. The curves are the guides for eyes. See the text for details.

The Hubbard model, named after John Hubbard 1963 is the simplest model of interacting particles in lattices, with the only two terms in the Hamiltonian; a kinetic term allowing for hopping of particles between holes of the lattice and a potential term consisting of an on sites interaction. The particles can either be fermions or bosons (Schrieffer, 2018). Standard approaches to evaluate the ground-state properties of the Hubbard model via the Lanczos method have convergence problems upon the growing difference between hopping and Coulomb interaction strength. This issue is quite relevant since energy convergence does not necessarily translate into convergence of the ground-state itself. (Souza et al., 2016b). In particular, the Hubbard model is applied to study the behavior of strongly correlated electron systems. It describes a lattice of fixed sites where electrons can tunnel among next-neighbor sites at the same time it can locally interact with another electron via Coulomb repulsion or attraction. The Hamiltonian of the Hubbard model read (Souza & Macedo, 2016)

The Hubbard model is a good approximation for particles in a periodic potential, at sufficiently low temperature that all the particles are in the lowest Bloch band, as long as any long-range interactions between the particles can be ignored. If interactions between particles on different sites of the lattice are included, the model is often referred to as the extended Hubbard model. (Charles K 2004).

The model was originally proposed to describe electrons in solids and has since been the focus of particular interest as a model for high temperature super conductivity. For electron in a solid, the Hubbard model can be considered as an improvement on the tight-binding model, which includes only the hopping term for strong interaction, it can give qualitatively different behavior from the tight. (Macedo, 2013). Binding model, and correctly predicts the existence of so called mott insulators, which are prevented from becoming conducting by the strong repulsion between the particles. (Schrieffer, 2018, Souza et al., 2016).

The Hubbard model is based on the tight –binding approximation. In the tight-binding approximation, electrons are viewed as occupying the standard orbital of their hopping between atoms, and then hopping between atoms, and then hopping between atoms during conduction. Mathematically, this is represented as hopping integral or transfer integral between neighboring atoms, which can be viewed as the physical principle that creates electrons bonds in crystalline

Materials (Chen, 1989; Dagotto, 1994). The Hubbard Hamiltonian takes the form:

$$H = -t \sum_{(i,j)\sigma} C_{i\sigma}^{\dagger} C_{j\sigma} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} \quad 1.1.0$$

Where $C_{i\sigma}^+ C_{j\sigma}$ and $n_i \uparrow n_j \downarrow$ are the creation, annihilation and number operations, respectively for an electron of spin in the wannier state on the i^{th} the j^{th} lattice $F_{i,j}$ means that only interest neighbor site hopping are allowed (Dagotto, 1994).

The Hubbard model has been extensively studied the single band Hubbard model in both one dimensional ring and dimensional torus. By the exact calculation of the pair correlation function $F_{i,j}$ defined as the possibility of finding an electron at site j when there has been an electron of opposite at site i , it is shown that for two electrons, the interaction is always repulsive in the ground state for any positive value of the on-site coulomb interaction U Okanigbuan OR, (2015) studied the single –band tight-binding model with on-site repulsion U and nearest neighbor-exchange interaction j (the so called Hubbard Hirsch Hamiltonian) with the help of a correlated variation approach.

Theoretical Background, The Lanczos Technique

In order to deal with the Hubbard model in finite lattice sizes, a diagonalization of its Hamiltonian, Eq. (1) is required. In grand-canonical systems, however, the size of the array grows exponentially with the number of sites, (Musco et al., 2018)

The general formulae for the lanczos technique is

$$|\phi_{n+1}\rangle = H|\phi_n\rangle - \frac{\langle\phi_n|H|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle}|\phi_n\rangle - \frac{\langle\phi_n|\phi_n\rangle}{\langle\phi_{n-1}|\phi_{n-1}\rangle}|\phi_{n-1}\rangle \quad 1.1.1$$

In the lanczos technique, a special basis is constructed so that the Hamiltonian has a tri-diagonal representation], firstly we select an arbitrary vector $|\phi_0\rangle$ in the Hilbert space of the model being studied for a two site system containing 2 electrons we have the following many body state Standard diagonal techniques aim for computing the whole Eigen state spectrum. However, our aim is to efficiently compute the ground state of the Hubbard model. Then, the Lanczos method arises as a great tool for this task, allocating as less memory as possible.(Macedo, 2013)

Ground state energy of the two electrons on 2 sites of aid lattice using the lanczos method In the Lanczos method, a special basis is constructed such that the Hamiltonian has a tridigonal representation Firstly, we select an arbitrary vector ϕ_0 in the Hilbert space of the model being studied for a two site system containing 2 electrons, we have the following many body states. (Okanigbuan OR, 2015, Aaron et al; 2017)

$$|1\rangle = |1 \uparrow 1 \downarrow\rangle$$

$$|2\rangle = |2 \uparrow 2 \downarrow\rangle$$

$$|3\rangle = |1 \uparrow 2 \downarrow\rangle$$

$$|4\rangle = |1 \downarrow 2 \uparrow\rangle$$

$$\text{Let } |\phi_0\rangle = |1 \uparrow 2 \downarrow\rangle$$

Recall equation 1.1

$$H = -t \sum_{(i,j)\sigma} C_{i\sigma}^+ C_{j\sigma} + U \sum_{i=1}^N n_i \uparrow n_j \downarrow \quad 1.1.2$$

The expanded Hubbard model is given by;

$$H = -t[C_{1\uparrow}^+C_{2\uparrow} + C_{2\uparrow}^+C_{1\uparrow} + C_{1\downarrow}^+C_{2\downarrow} + C_{2\downarrow}^+C_{1\downarrow}] + U[C_{1\uparrow}^+C_{1\uparrow}C_{1\downarrow}^+C_{1\downarrow} + C_{2\uparrow}^+C_{2\uparrow}C_{2\downarrow}^+C_{2\downarrow}] \quad 1.1.3$$

$$H|\phi_0\rangle = -t[|0\rangle + |2\uparrow 2\downarrow\rangle + |1\uparrow 1\downarrow\rangle + 0 + U|0\rangle] = -t|2\rangle - t|1\rangle \quad 1.1.4$$

$$\langle\phi_0|\phi_0\rangle = \langle 3| - t|2\rangle + \langle 3| - t|1\rangle = 0 \quad 1.1.5$$

$$\langle\phi_0|\phi_0\rangle = 1 \quad 1.1.6$$

$$|\phi_1\rangle = -t|2\rangle - t|1\rangle - 0 \quad 1.1.7$$

$$\phi_1\rangle = -t|2\rangle\uparrow 2\downarrow\rangle - t|1\uparrow 1\downarrow\rangle \quad 1.1.8$$

$$H|\phi_1\rangle = t^2|1\uparrow 2\downarrow\rangle + t^2|2\uparrow 1\downarrow\rangle - tu|2\uparrow 2\downarrow\rangle + t^2|2\uparrow 1\downarrow\rangle + t^2|1\uparrow 2\downarrow\rangle - tu|1\uparrow 1\downarrow\rangle \quad 1.1.9$$

$$H|\phi_1\rangle = t^2|1\uparrow 2\downarrow\rangle - t^2|1\downarrow 2\uparrow\rangle - tu|2\uparrow 2\downarrow\rangle - t^2|1\downarrow 2\uparrow\rangle + t^2|1\uparrow 2\downarrow\rangle - tu|1\uparrow 1\downarrow\rangle \quad 1.2.0$$

$$H|\phi_1\rangle = 2t^2|1\uparrow 2\downarrow\rangle - 2t^2|1\downarrow 2\uparrow\rangle - tu|1\uparrow 1\downarrow\rangle - tu|2\uparrow 2\downarrow\rangle \quad 1.2.1$$

$$|\phi_1\rangle = 2t^2|3\rangle - 2t^2|4\rangle - tu|1\rangle - tu|2\rangle \quad 1.2.2$$

$$\langle\phi_1|H|\phi_1\rangle = -2t^3\langle 1|3\rangle + 2t^3\langle 1|4\rangle + t^2u\langle 1|1\rangle + t^2u\langle 1|2\rangle - 2t^3\langle 2|3\rangle + 2t^3\langle 2|4\rangle + t^2u\langle 2|1\rangle + t^2u\langle 2|2\rangle \quad 1.2.3$$

$$\langle\phi_1|H|\phi_1\rangle = t^2u + t^2u = 2t^2u \quad 1.2.4$$

$$\langle\phi_1|\phi_1\rangle = (t^2(1|1) + t^2(1|2) + t^2(2|1) + t^2(2|2)) = 2t^2 \quad 1.2.5$$

Now,

$$|\phi_2\rangle = H|\phi_1\rangle - \frac{\langle\phi_1|H|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle}|\phi_1\rangle - \frac{\langle\phi_1|\phi_1\rangle}{\langle\phi_0|\phi_0\rangle}|\phi_0\rangle \quad 1.2.6$$

$$= 2t^2|3\rangle - 2t^2|4\rangle - tu|1\rangle - tu|2\rangle - \frac{2t^2u(-t|2\rangle - t|1\rangle)}{2t^2} - \frac{2t^2}{1}/3 \quad 1.2.7$$

$$= 2t^2|3\rangle - 2t^2|4\rangle - tu|1\rangle - tu|2\rangle + tu|2\rangle + tu|1\rangle - 2t^2|3\rangle \quad 1.2.8$$

$$|\phi_2\rangle = 2t^2|4\rangle = -2t^2|1\downarrow 2\uparrow\rangle \quad 1.2.9$$

$$\langle\phi_2|\phi_2\rangle = 4t^4 \quad 1.3.0$$

$$H|\phi_2\rangle = 2t^3|2\downarrow 2\uparrow\rangle + 2t^3|1\downarrow 1\uparrow\rangle = -2t^3|2\uparrow 2\downarrow\rangle - 2t^3|1\uparrow 1\downarrow\rangle \quad 1.3.1$$

$$H|\phi_2\rangle = -2t^3|2\rangle - 2t^3|1\rangle \quad 1.3.2$$

$$\langle\phi_2|H|\phi_2\rangle = 0 \quad 1.3.3$$

$$|\phi_3\rangle = H|\phi_2\rangle - \frac{\langle\phi_2|H|\phi_2\rangle}{\langle\phi_2|\phi_2\rangle}|\phi_2\rangle - \frac{\langle\phi_2|\phi_2\rangle}{\langle\phi_1|\phi_1\rangle}|\phi_1\rangle \quad 1.3.4$$

$$|\phi_3\rangle = -2t^3|2\rangle - 2t^3|1\rangle - 0 - \frac{4t^4}{2t^2}(-t|2\rangle - t|1\rangle) \quad 1.3.5$$

$$|\phi_3\rangle = -2t^3|2\rangle - 2t^3|1\rangle + 2t^3|2\rangle + 2t^3|1\rangle \quad 1.3.6$$

$$|\phi_3\rangle = 0 \quad 1.3.7$$

Now,

$$H = \begin{bmatrix} a_n & b_{\frac{1}{2}n+1} & 0 & 0 \\ b_{\frac{1}{2}n+1} & a_{n+1} & b_{\frac{1}{2}n+2} & 0 \\ 0 & b_{\frac{1}{2}n+2} & a_{n+2} & b_{\frac{1}{2}n+3} \\ 0 & 0 & b_{\frac{1}{2}n+3} & a_{n+3} \end{bmatrix}$$

$$a_n = \frac{\langle \phi_n | H | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle} \quad 1.3.8$$

$$b^{\frac{1}{2}}_n = \left(\frac{\langle \phi_n | \phi_n \rangle}{\langle \phi_{n-1} | \phi_{n-1} \rangle} \right)^{\frac{1}{2}} \quad 1.3.9$$

$$H = \begin{bmatrix} a_0 & b^{\frac{1}{2}}_1 & 0 & 0 \\ b_1 & a_1 & b^{\frac{1}{2}}_2 & 0 \\ 0 & b^{\frac{1}{2}}_2 & a_2 & b^{\frac{1}{2}}_3 \\ 0 & 0 & b^{\frac{1}{2}}_3 & a_3 \end{bmatrix}$$

$$a_0 = \frac{\langle \phi_0 | H | \phi_0 \rangle}{\langle \phi_0 | \phi_0 \rangle} = 0 \quad 1.4.0$$

$$a_1 = \frac{\langle \phi_1 | H | \phi_1 \rangle}{\langle \phi_1 | \phi_1 \rangle} = \frac{2t^2 u}{2t^2} = u \quad 1.4.1$$

$$b_1 = \left(\frac{\langle \phi_1 | \phi_1 \rangle}{\langle \phi_0 | \phi_0 \rangle} \right)^{\frac{1}{2}} = \left(\frac{2t^2}{1} \right)^{\frac{1}{2}} = \sqrt{2} t \quad 1.4.2$$

$$a_2 = \frac{\langle \phi_2 | H | \phi_2 \rangle}{\langle \phi_2 | \phi_2 \rangle} = 0 \quad 1.4.3$$

$$b_2 = \left(\frac{\langle \phi_2 | \phi_2 \rangle}{\langle \phi_1 | \phi_1 \rangle} \right)^{\frac{1}{2}} = \left(\frac{4t^4}{2t^2} \right)^{\frac{1}{2}} = \sqrt{2} t \quad 1.4.4$$

Therefore,

$$H = \begin{bmatrix} 0 & \sqrt{2}t & 0 \\ \sqrt{2}t & u & \sqrt{2}t \\ 0 & \sqrt{2}t & 0 \end{bmatrix}$$

To find the eigenvalues of the Hamiltonian;

$$\text{Det}(H - \lambda I) = 0$$

$$\text{Det} \begin{bmatrix} 0 - \lambda & \sqrt{2}t & 0 \\ \sqrt{2}t & u - \lambda & \sqrt{2}t \\ 0 & \sqrt{2}t & 0 - \lambda \end{bmatrix} = 0$$

$$\text{Det} \begin{bmatrix} -\lambda & \sqrt{2}t & 0 \\ \sqrt{2}t & u - \lambda & \sqrt{2}t \\ 0 & \sqrt{2}t & -\lambda \end{bmatrix} = 0$$

$$-\lambda[(u - \lambda)(-\lambda) - 2t^2] - \sqrt{2}t[-\lambda(\sqrt{2}t) - 0] = 0 \quad 1.4.5$$

$$-\lambda[\lambda^2 - u\lambda - 2t^2] + 2\lambda t^2 = 0 \quad 1.4.6$$

$$-\lambda^3 + u\lambda^2 + 2\lambda t^2 + 2\lambda t^2 = 0 \quad 1.4.7$$

$$-\lambda^3 + u\lambda^2 + 4\lambda t^2 = 0 \quad 1.4.8$$

$$\lambda^3 - u\lambda^2 - 4\lambda t^2 = 0 \quad 1.4.9$$

$$\lambda(\lambda^2 - u\lambda - 4t) = 0 \quad 1.5.0$$

This implies that;

$$\lambda_1 = 0 \quad \text{or} \quad \lambda_{2,3} = \frac{u \pm \sqrt{u^2 - 4x^4xt^2}}{2}$$

$$\lambda_2 = \frac{u}{2} - \frac{1}{2}\sqrt{u^2 + 16t^2} \quad 1.5.1$$

$$\lambda_3 = \frac{u}{2} + \frac{1}{2}\sqrt{u^2 + 16t^2} \quad 1.5.2$$

Result and Discussion

Ground state energy for two electron system on two sites were analytically solved using 4×4 matrix and the result is the lowest energy eigenvalues given by as compared with the exact;

$E_g = \frac{u}{2} - \frac{1}{2}\sqrt{u^2 + 16t^2}$ Compare to the exact result given by

$$E_G = -\frac{1}{2}(\sqrt{U^2 + 16t^2} - U)$$

Result and Discussion Ground state energy for two electron system on two sites were analytically solved using 4×4 matrix and the results obtained (Okanigbuan OR, 2015) are presented in the figures and table below. Figure 1 shows ground state energy as a function of positive U energy for 2 electrons on 2 sites for Lanczos method while Figure 2 shows ground state energy as a function of positive U for 2 electrons on 2 sites for exact method. Thus, the correlation between the two graphs are in perfect agreement. Table 1 below shows the numerical results of Lanczos method and exact method which is in a good agreement with experimental values.

Conclusion

In this study, we have successfully calculated the Ground state energy of the two electrons on 2 site of aid lattice using the Lanczos technique and this revealed Lanczos technique is a reliable numerical method in determining the ground state energy of a system described by the Hubbard Hamiltonian. Ground state energies obtained using the Lanczos method compare nicely with that obtained using exact method. The size of the Hamiltonian matrix to diagonalized is 4×4 matrix when Lanczos technique is applied. (Okanigbuan OR, 2015).

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