

THE EXACT DIAGONALIZATION TECHNIQUE FOR THE ATTRACTIVE HUBBARD MODEL

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The one-dimensional attractive Hubbard model ($U \ll 0$) is discussed assuming periodic boundary conditions and the half-filling case. The considered chains have N nodes, the same number of electrons, where $N - 1$ of them have the same spin projection. The discussed translational and unitary symmetries provide the exact diagonalization of the Hamiltonian for even $N < 7$ via various applications of the unitary group.

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1. Introduction

The Hubbard model derived in [1], and independently by Gutzwiller in [2, 3] and Kanamori in [4], is based on the tight-binding approximation. The model is one of the simplest with main aspects of the physical image of interacting electrons in the crystal. The electrons occupying the atoms can move between them by the so-called *hopping* during conduction and provide electron bands in a crystal. In spite of a substantial simplification of the model compared to the real physical situation of interacting electrons in a crystal, obtained results may explain the insulating, magnetic, and even superconducting effects in a solid. The Hubbard model has been important for understanding of many sophisticated, physical problems like ferromagnetism, antiferromagnetism, the Mott transition, high-temperature superconductivity, the Bose–Einstein condensate in cold optical lattice [5–7], *etc.* Despite its apparently simple structure, the exact solution exists only for one spatial dimension, given in year 1968 by Lieb and Wu [8], by using the method of Yang [9], and [10] from the year after, and is not

easy to analyse. In general, there are several approximation techniques, among the others mean field-theory, various Green's function decoupling schemes and functional methods. We continue the work with one spatial dimension, which is of much importance for its possible generalizations to higher dimensions, and as the exactly solvable model [11, 12]. In addition, the one-dimensional case may become more important due to its possible applications in intensively studied carbon nanotubes [13], one-dimensional organic superconductors [14], or one-dimensional organic ferromagnet [15]. There is also possibility of modelling the one-dimensional Hubbard model of fermionic quantum gas loaded into an optical lattice [16], which is a promising candidate for quantum information processing.

2. The Hamiltonian and its symmetries

The dynamics of the finite set of interacting electrons, occupying the one-dimensional chain, consisting of N atoms, can be described by the Hubbard Hamiltonian in the following form

$$\hat{H} = t \sum_{i \in \tilde{2}} \sum_{j \in \tilde{N}} \left(\hat{a}_{ji}^\dagger \hat{a}_{j+1i} + \hat{a}_{j+1i}^\dagger \hat{a}_{ji} \right) + U \sum_{j \in \tilde{N}} \hat{n}_{j+} \hat{n}_{j-}, \quad (1)$$

where $\tilde{N} = \{j = 1, 2, \dots, N\}$ denotes the set of atoms of the chain, $\tilde{2} = \{i = +, -\}$, $\hat{n}_{ji} = \hat{a}_{ji}^\dagger \hat{a}_{ji}$, and finally $\hat{a}_{ji}^\dagger$, $\hat{a}_{ji}$ are the canonical Fermi operators, that is creation and annihilation operators of electron of spin i , on the site j . One can observe that electrons behave as *waves* in the first component of the Hamiltonian (1), while they behave as *particles* in the second one, with the assumption of the occurrence of electron–electron interaction with the characteristic constant interaction denoted by U [17]. In general, U can be of any value, with $U < 0$ ($U \ll 0$ — the case presented in this article) and $U > 0$ ($U \gg 0$ [18, 19]) being responsible for attraction and repulsion, respectively, and $U = 0$ standing for no effect or plain gas of fermions.

The *single-node* space h_j has the basis consisting of n vectors denoting all possible occupations of one node, since we are dealing with fermions

$$\dim h_j = n = 4, \quad h_j = lc_{\mathbb{C}}\{\pm, \emptyset, +, -\}, \quad (2)$$

where $\emptyset$ denotes the empty node, $+$ and $-$ stand for one-node spin projection equal to $\frac{1}{2}$ and $-\frac{1}{2}$, respectively, $\pm$ denotes the double occupation of the one node by two electrons with different spin projections, and $lc_{\mathbb{C}}A$ stands for the linear closure of a set A over the complex field $\mathbb{C}$. One can obtain the final Hilbert space $\mathcal{H}$ of all quantum states of the system in the following

way

$$\mathcal{H} = \prod_{j=1}^N \otimes h_j, \quad \mathcal{H} = \sum_{N_e=0}^{2N} \oplus \mathcal{H}^{N_e}, \quad (3)$$

where $\mathcal{H}^{N_e}$ denotes the space with fixed number of electrons N_e . The set of all linearly independent vectors called *electron configurations* [20] provides the initial, orthonormal basis of the Hilbert space $\mathcal{H}$. These configurations are defined by the following mapping

$$f : \tilde{N} \longrightarrow \tilde{4}, \quad \tilde{4} = \{\pm, \emptyset, +, -\}, \quad (4)$$

and constitute the N -sequences of the elements from the set $\tilde{4}$

$$|f\rangle = |f(1)f(2)\dots f(N)\rangle = |i_1 i_2 \dots i_N\rangle, \quad i_j \in \tilde{4}, \quad j \in \tilde{N}, \quad (5)$$

with

$$\tilde{4}^{\tilde{N}} = \left\{ f : \tilde{N} \longrightarrow \tilde{4} \right\}, \quad (6)$$

$$\mathcal{H} = lc_{\mathbb{C}} \tilde{4}^{\tilde{N}}. \quad (7)$$

The one-dimensional Hubbard model has many symmetries, systematically studied by many researchers, starting from Lieb and Wu [8], Yang [9] and continued in, *inter alia*, Refs. [17, 21, 22], with the book of Essler *et al.* being the eminent summary and supplement of their work [23]. Since the periodic boundary condition are assumed, the Hamiltonian (1) has the obvious translational symmetry ($\hat{a}_{N+1i} = \hat{a}_{1i}$), this means that one-particle Hamiltonian of the form (1) is completely diagonalized by a Fourier transformation. Apart from the cyclic symmetry, system reveals, among others, two independent SU(2) symmetries [23, 24], that is SU(2) $\times$ SU(2), in spin and pseudospin space [25]. This symmetry involves spin and charge degrees of freedom, thus, one has two sets of generators, $\{\hat{S}_z, \hat{S}^+, \hat{S}^-\}$ and $\{\hat{J}_z, \hat{J}^+, \hat{J}^-\}$, for spin and charge, respectively. These generators can be written in the following forms

$$\hat{S}_z = \frac{1}{2} \sum_{j \in \tilde{N}} \left(\hat{a}_{j+}^\dagger \hat{a}_{j+} - \hat{a}_{j-}^\dagger \hat{a}_{j-} \right), \quad \hat{S}_+ = \hat{S}_-^\dagger = \sum_{j \in \tilde{N}} \hat{a}_{j+}^\dagger \hat{a}_{j-}, \quad (8)$$

$$\begin{aligned} \hat{J}_z &= \frac{1}{2} \sum_{j \in \tilde{N}} \left(\hat{a}_{j+}^\dagger \hat{a}_{j+} + \hat{a}_{j-}^\dagger \hat{a}_{j-} - 1 \right), \quad \hat{J}_+ = \sum_{j \in \tilde{N}} (-1)^j \hat{a}_{j+}^\dagger \hat{a}_{j-}^\dagger, \\ \hat{J}_- &= \sum_{j \in \tilde{N}} (-1)^j \hat{a}_{j+} \hat{a}_{j-} \end{aligned} \quad (9)$$

and the transfer between these two sets is known as the Shiba transformation [8, 23].

3. Exact diagonalization

The action $A : \Sigma_N \times \tilde{4}^{\tilde{N}} \longrightarrow \tilde{4}^{\tilde{N}}$ of the symmetric group Σ_N on the set $\tilde{4}^{\tilde{N}}$ provides orbits $\mathcal{O}_\mu$ of the group Σ_N labelled by the *weight* μ , which is a sequence of non-negative integers $\mu = (\mu_1, \mu_2, \mu_3, \mu_4)$, with relation $\sum_{i \in \tilde{4}} \mu_i = N$, defined by the following equation

$$\mu_i = \left| \left\{ i_j = i \mid j \in \tilde{N} \right\} \right|, \quad i \in \tilde{4}. \quad (10)$$

From now on, we confine our considerations only to the case of $U \ll 0$, and to the half-filling magnetic rings, that is with N nodes occupied by $N_e = N$ electrons, including $N - 1$ electrons with the same spin projection. Since we are dealing with $U \ll 0$, the set of electron configurations no longer contains the elements with two atoms singly occupied by opposite spin projection (unpaired spins). Thus, the weights belong to the set

$$\{(1, 1, N - 2, 0), (1, 1, 0, N - 2)\}. \quad (11)$$

Since the numbers of up- and down-spin electrons are separately conserved, the matrix representation of the Hamiltonian (1), within the postulated set (11), gets reduced to the sectors characterized by elements of the subset

$$\{(N - 1, 1), (1, N - 1)\} \quad (12)$$

of the Cartesian product $N_+ \times N_-$, where N_+ and N_- denote the number of electrons with the spin projection equal to $\frac{1}{2}$ and $-\frac{1}{2}$, respectively. We proceed with the total magnetization $M = \frac{N}{2} - 1$, and with the initial basis given by Table I, where f^i denotes the *initial* electron configuration of the orbit $\mathcal{O}_{f^i}$ of the translational symmetry group C_N , and F is the set of f^i differing from each other by transposition of the elements $\pm$ and $\emptyset$. As we consider the case of $U \ll 0$ — the nodes with the $-$ alone will never appear.

The first step in the process of diagonalization of the system Hamiltonian is application of the so-called *basis of wavelets* [26] *i.e.* Fourier transform on the orbits $\mathcal{O}_{f^i}$ of the group C_N , as the aftermath of the translational symmetry of the magnetic ring. The appropriate amplitude takes the form

$$|k, f^i\rangle = \frac{1}{\sqrt{N}} \sum_{j \in \tilde{N}} e^{i2\pi k j / N} |f_j, f^i\rangle, \quad (13)$$

where $|f_j, f^i\rangle$ denotes the j th electron configuration of the orbit $\mathcal{O}_{f^i}$, and the quasi-momentum $k \in B$, with

$$B = \{k = 0, \pm 1, \pm 2, \dots, \left\{ \begin{array}{ll} \pm(N/2 - 1), N/2 & \text{for } N \text{ even} \\ \pm(N - 1)/2, & \text{for } N \text{ odd} \end{array} \right\}\}. \quad (14)$$

TABLE I

The decomposition of the set of electron configurations, for the case of $\mu = (1, 1, 4, 0)$, and $U \ll 0$ into orbits $\mathcal{O}_{f^i}$ of the translational symmetry group C_6 .

i	M	μ	f^i	$\mathcal{O}_{f^i}$
1	2	$(1, 1, 4, 0)$	$ \pm \emptyset + + + +\rangle$	$ \pm \emptyset + + + +\rangle$ $ + \pm \emptyset + + +\rangle$ $ + + \pm \emptyset + +\rangle$ $ + + + \pm \emptyset +\rangle$ $ + + + + \pm \emptyset\rangle$ $ \emptyset + + + + \pm\rangle$
2			$ \emptyset \pm + + + +\rangle$	$ \emptyset \pm + + + +\rangle$ $ + \emptyset \pm + + +\rangle$ $ + + \emptyset \pm + +\rangle$ $ + + + \emptyset \pm +\rangle$ $ + + + + \emptyset \pm\rangle$ $ \pm + + + + \emptyset\rangle$
3			$ \pm + \emptyset + + +\rangle$	$ \pm + \emptyset + + +\rangle$ $ + \pm + \emptyset + +\rangle$ $ + + \pm + \emptyset +\rangle$ $ + + + \pm + \emptyset\rangle$ $ \emptyset + + + \pm +\rangle$ $ + \emptyset + + + \pm\rangle$
4			$ \emptyset + \pm + + +\rangle$	$ \emptyset + \pm + + +\rangle$ $ + \emptyset + \pm + +\rangle$ $ + + \emptyset + \pm +\rangle$ $ + + + \emptyset + \pm\rangle$ $ \pm + + + \emptyset +\rangle$ $ + \pm + + + \emptyset\rangle$
5			$ \pm + + \emptyset + +\rangle$	$ \pm + + \emptyset + +\rangle$ $ + \pm + + \emptyset +\rangle$ $ + + \pm + + \emptyset\rangle$ $ \emptyset + + \pm + +\rangle$ $ + \emptyset + + \pm +\rangle$ $ + + \emptyset + + \pm\rangle$

The representation of the Hamiltonian in the basis of wavelets includes the complex elements. To get rid of them, one can use the gauge transformation, as the second step of the procedure of the exact diagonalization, by adding to the amplitude (13) the additional phase as follows

$$|k, f^i, F\rangle = \frac{1}{\sqrt{N}} e^{i\pi k t_{\pm\emptyset}/N} \sum_{j \in \tilde{N}} e^{i2\pi k j/N} |f_j, f^i\rangle, \quad (15)$$

where $t_{\pm\emptyset}$ denotes the distance between the elements $\pm$ and $\emptyset$ in the initial electron configuration f^i , equal to the number of singly occupied nodes between them plus 1. The transformation (15) constitutes the local gauge field dependent on the quasi-momentum k and the parameter $t_{\pm\emptyset}$ characterizing the set F . The example of the representation of the Hamiltonian for the case $N = 6$, $N_e = 6$, $N_+ = 5$, $k = 1$ in the *gauged basis of wavelets* takes the form

$$\check{H} = \begin{bmatrix} U & 0 & -\sqrt{3}t & 0 & 0 \\ 0 & U & 0 & -\sqrt{3}t & 0 \\ -\sqrt{3}t & 0 & U & 0 & -\sqrt{3}t \\ 0 & -\sqrt{3}t & 0 & U & \sqrt{3}t \\ 0 & 0 & -\sqrt{3}t & \sqrt{3}t & U \end{bmatrix}. \quad (16)$$

The third step in the diagonalization procedure of the Hamiltonian is taking into account the $SU(2) \times I$ symmetry in the pseudo-spin space, where I denotes the identity element of the group $SU(2)$, since the singly occupied atoms have the same spin projection. The appropriate amplitude constructed on the gauged basis of wavelets (15) is

$$|F, k, J, J_z\rangle = \frac{1}{\sqrt{|F|}} \sum_{g \in (SU(2) \times I)} \Gamma(g) g |k, f^i, F\rangle, \quad (17)$$

and will be called *spin basis*, where $\Gamma(g)$ marks the irreducible representation of the group $SU(2)$ [25], and $|F|$ denotes the cardinality of the set F . The physical meaning of this symmetry is the decoupling of the spin and charge degrees of freedom related with the elementary excitations of the Luttinger liquid [27] called spinons and holons, respectively. The matrix (16) after the appropriate change of basis (17) transforms into

$$\check{H} = \begin{bmatrix} U & -\sqrt{3}t & 0 & 0 & 0 \\ -\sqrt{3}t & U & 0 & 0 & 0 \\ 0 & 0 & U & 0 & -\sqrt{2}\sqrt{3}t \\ 0 & 0 & 0 & U & -\sqrt{3}t \\ 0 & 0 & -\sqrt{2}\sqrt{3}t & -\sqrt{3}t & U \end{bmatrix}. \quad (18)$$

The diagonalization procedure for even $N < 7$ within the blocks with fixed k , J , J_z provides the eigenstates given as the irreducible basis of another $SU(2)$ group, possible to obtain by the Kostka matrices at the level of basis for $n = 2$, and $\mu = \{\mu_1, \mu_2\} = \{N - 1, 1\}$ [28]. This kind of symmetry ends the process of exact diagonalization. For the case of $N = 6$, $k = 1$, the representation of the Hamiltonian takes the form

$$\check{H} = \begin{bmatrix} U - \sqrt{3}t & 0 & 0 & 0 & 0 \\ 0 & U + \sqrt{3}t & 0 & 0 & 0 \\ 0 & 0 & U - 3t & 0 & 0 \\ 0 & 0 & 0 & U + 3t & 0 \\ 0 & 0 & 0 & 0 & U \end{bmatrix}. \quad (19)$$

4. Conclusions

In the present paper, we gave the description of the one-dimensional Hubbard model for the chains with N atoms, the same number of electrons, and $N - 1$ of them with the spin projection equal to $\frac{1}{2}$. After the decomposition of the set of electron configurations into orbits $\mathcal{O}_{f_i}$ of the cyclic symmetry group C_6 , we presented the quasidiagonal form of the Hubbard Hamiltonian on the example of $N = 6$, $N_e = 6$, $N_+ = 5$, $k = 1$ using the irreducible basis, adapted to the assumed translational symmetry. The appropriate gauge transformation removes the complex elements from the representation of the Hamiltonian. Next, we present, on the example of $N = 6$, the double action of the unitary group $SU(2)$ ending the process of the exact diagonalization. Rotational symmetry within the spinless part of the magnetic ring provides the quantum numbers J and J_z , whereas $S = M = 2$ for all cases. The group $SU(2)$ manifests itself for even $N < 7$ for the second time within each of $SU(2) \times I$ symmetrized parts of the wave function and leads to the appropriate transformation of amplitudes (17). The eigenstates are simply identified as given by the Kostka matrices at the level of basis for $n = 2$, and $\mu = \{\mu_1, \mu_2\} = \{N - 1, 1\}$. Adjusting the appropriate irreducible representations of $SU(2)$ for any N , as well as the physical meaning of the last transformation and its possible applications in more general cases are still the open questions.

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