THE EXACT RESULTS IN THE ONE-DIMENSIONAL 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 - 1of them have the same spin projection. The exact diagonalization was performed for any number N of atoms. The eigenvectors and eigenvalues in some cases are constructed based on the Golden Number.

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1. Introduction

The Hubbard model derived in [1], and independently by Gutzwiller [2, 3] and Kanamori [4], is one of the simplest approximate models used for describing the main aspects of the fundamental many-body systems in condensed matter physics, as an improvement on the tight-binding model, which includes only the hopping term. One such example is strongly correlated quantum system of interacting electrons in narrow energy bands, where the electrons occupying the atoms can move between them by hopping during conduction. The Hubbard model produces both a metallic and an insulating state, depending on the value of U. 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, including 1D conductors [5, 6]. The Hubbard model has been applied to problems as diverse as ferromagnetism, antiferromagnetism, the Mott transition, high-temperature superconductivity, the Bose–Einstein condensate in cold optical lattice [7–9]. The exact solution of the Hubbard Hamiltonian exists only for one spatial dimension, given in year 1968 by Lieb and Wu [10], by using the method of Yang [11],

and [12] 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 [13–15] which is of much importance for its possible generalizations to higher dimensions, and as the exactly solvable model [16, 17]. In addition, the one-dimensional case may become more important due to its possible applications in intensively studied carbon nanotubes [18], one-dimensional organic superconductors [19], or one-dimensional organic ferromagnet [20]. There is also possibility of modelling the one-dimensional Hubbard model of fermionic quantum gas loaded into an optical lattice [21], which is a promising candidate for quantum information processing. Ultracold atomic physics offers numerous possibilities to study strongly correlated many-body systems in lower dimensions.

In a previous paper [15], we discussed translational and unitary symmetries of the one-dimensional attractive Hubbard model providing the exact diagonalization of the Hamiltonian only for even N < 7 via various applications of the unitary group. In this article, we provide a thorough analysis of the eigenproblem resulting in obtaining the general analytical formulas for the eigenvalues and the eigenvectors, for any number N.

2. The symmetries of the system

The most simple way to get insight into the dynamics of a finite system of interacting electrons occupying the one-dimensional chain consisting of N atoms, provides the Hubbard Hamiltonian in the following form

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

where $\tilde{N} = \{j = 1, 2, ..., N\}$ 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 anihilation operators of electron of spin *i*, on the site *j*. 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 [22]. In general, U can be any value, with U < 0 ($U \ll 0$ — the case presented in this article) and U > 0 ($U \gg 0$ [23, 24]) responsible for attraction and repulsion, respectively, while U = 0 stands 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
$$h_j = n = 4$$
, $h_j = lc_{\mathbb{C}} \{\pm, \emptyset, +, -\}$, (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} . The final Hilbert space \mathcal{H} of all quantum states of the system has the form

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

where \mathcal{H}^{N_e} denotes the space with fixed number of electrons N_e . The initial, orthonormal basis of the Hilbert space \mathcal{H} consists of all linearly independent vectors called *electron configurations* [25], defined by the following mapping

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

$$(4)$$

and constitute the N-sequences of the elements from the set 4

$$|f\rangle = |f(1)f(2)\dots f(N)\rangle = |i_1i_2\dots i_N\rangle, \qquad i_j \in \tilde{4}, \qquad j \in \tilde{N}$$
(5)

with

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

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

The symmetries of the one-dimensional Hubbard model has been studied by many researchers, starting from Lieb and Wu [10], Yang [11] and continued in, *inter alia*, Refs. [22, 26, 27], with the book of Essler *et al.* being the eminent summary and supplement of their work [28]. Since the periodic boundary condition are assumed, the Hamiltonian (1) has the obvious translational symmetry $(\hat{a}_{N+1i} = \hat{a}_{1i})$, this mean 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 [28, 29], that is SU(2)×SU(2), in spin and pseudospin space [30]. 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

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

$$\hat{J}_{z} = \frac{1}{2} \sum_{j \in \tilde{N}} \left(\hat{a}_{j+}^{\dagger} \hat{a}_{j+} + \hat{a}_{j-}^{\dagger} \hat{a}_{j-} - 1 \right), \qquad \hat{J}_{+} = \sum_{j \in \tilde{N}} (-1)^{j} \hat{a}_{j+}^{\dagger} \hat{a}_{j-}^{\dagger}, \\
\hat{J}_{-} = \sum_{j \in \tilde{N}} (-1)^{j} \hat{a}_{j+} \hat{a}_{j-} \qquad (9)$$

and the transfer between these two sets is known as the Shiba transformation [10, 28, 31]. The eigenvalues of the operators \hat{S}_z and \hat{J}_z are labelled by M and J_z , whereas the eigenvalues of the operators

$$\hat{S}^2 = \frac{1}{2} \left(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+ \right) + \hat{S}_z^2 \tag{10}$$

and

$$\hat{J}^2 = \frac{1}{2} \left(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ \right) + \hat{J}_z^2 \tag{11}$$

are labelled by S(S + 1) and J(J + 1), respectively, due to the quantum algebra of the angular momentum.

3. The exact results of the diagonalization

From now on, we confine our considerations only to the case of $U \ll 0$, and to the half-filling magnetic rings with N nodes occupied by $N_e = N$ electrons, including N - 1 electrons with the same spin projection. The set of electron configurations for $U \ll 0$ does not contain the elements with two atoms singly occupied by opposite spin projection (unpaired spins). Since the numbers of up- and down-spin electrons are separately conserved — the matrix representation of the Hamiltonian (1) gets reduced to the sectors characterized by elements of the subset

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

of the Cartesian product $N_+ \times N_-$, where N_+ and N_- denotes 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 set of the electron configurations. As we consider the case of $U \ll 0$ — the nodes with the "-" alone will never appear.

The first step in the process of exact diagonalization of the system Hamiltonian is application of the so-called basis of wavelets [32] *i.e.* a Fourier transform on the orbits \mathcal{O}_{f^t} of the translational symmetry group C_N , as the aftermath of the translational symmetry of the magnetic ring. Each orbit \mathcal{O}_{f^t} is marked by the *initial electron configuration* f^t [15], *i.e.* the first electron configuration in the orbit \mathcal{O}_{f^t} , with the most left positions of \pm and \emptyset within the first N/2 + 1 and (N + 1)/2 nodes for even and odd N, respectively. For example, Table I constitutes the orbit $\mathcal{O}_{f^{t=2}}$ of the translation group C_6 with the initial electron configuration given by the second column of this table. The number $t \in T$ denotes the distance between the elements \pm and \emptyset in the initial electron configuration f^t , and is equal to the number of singly occupied nodes between them plus 1, t is positive when \pm is at the

TABLE I

$\mathcal{O}_{f^{t=2}}$	$f^{t=2}$
$ \begin{array}{c} \pm + \emptyset + + + \rangle \\ + \pm + \emptyset + + \rangle \\ + + \pm + \emptyset + \rangle \\ + + \pm + \psi \rangle \\ \theta + + + \pm + \rangle \\ \theta + + + \pm + \rangle \end{array} $	$ \pm + \emptyset + + + \rangle$

left of the \emptyset , and negative in the opposite case, that is the set of all t has the form

$$T = \left\{ t = 1, -1, 2, -2, \dots, \frac{+N/2}{\pm (N-1)/2} \text{ for } N \text{ even} \right\}.$$
 (13)

The j^{th} electron configuration of the orbit \mathcal{O}_{f^t} is denoted by $|f_j, f^t\rangle$, with $|f_1, f^t\rangle \equiv f^t$, and $|f_j, f^t\rangle = (c_N)^j f^t$, where

$$c_N = \begin{pmatrix} i_1 & i_2 & i_3 & \dots & i_N \\ i_N & i_1 & i_2 & \dots & i_{N-1} \end{pmatrix} \in C_N.$$
(14)

Each element of the basis of wavelets has the form [15]

$$|k,t\rangle = \frac{1}{\sqrt{N}} \sum_{j \in \tilde{N}} e^{i2\pi k j/N} \left| f_j, f^t \right\rangle \,, \tag{15}$$

where the quasi-momentum $k \in B$, with

$$B = \left\{ k = 0, \pm 1, \pm 2, \dots, \begin{array}{l} \pm (N/2 - 1), N/2 & \text{for } N \text{ even} \\ \pm (N - 1)/2 & \text{for } N \text{ odd} \end{array} \right\}.$$
 (16)

To get rid of the complex elements of the Hamiltonian, one can introduce the local gauge field dependent on the quasi-momentum k and the absolute value of t due to (13), by adding to the amplitude (15) the additional phase as follows [15]

$$|k,t\rangle' = \frac{1}{\sqrt{N}} e^{i\pi k|t|/N} \sum_{j\in\tilde{N}} e^{i2\pi kj/N} \left| f_j, f^t \right\rangle \,. \tag{17}$$

The next step in the exact 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 (17) has the following form [15]

$$|k,|t|,J\rangle = \frac{1}{\sqrt{2}} \sum_{g \in (\mathrm{SU}(2) \times I)} \Gamma(g) \, g \, |k,t\rangle' \,, \tag{18}$$

where $J_z = 0$, $\Gamma(g)$ marks the irreducible representation of the group SU(2) [30], and the absolute value |t|, according to (13), is given as follows

$$|t| = 1, 2, \dots, \begin{cases} N/2 & \text{for } N \text{ even, } k \text{ even and } J = 1, \\ & \text{or for } N \text{ even, } k \text{ odd and } J = 0, \\ (N-2)/2 & \text{for } N \text{ even, } k \text{ odd and } J = 1, \\ & \text{or for } N \text{ even, } k \text{ even and } J = 0, \\ (N-1)/2 & \text{for } N \text{ odd.} \end{cases}$$
(19)

The basis (18) is called *pseudo-spin basis*. 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 [33] called spinons and holons, respectively. For example, the pseudo-spin states for |t| = 1 take the following forms

$$|k, |t| = 1, J = 0$$
 $\rangle = \frac{1}{\sqrt{2}} \left(|k, t = 1\rangle' - |k, t = -1\rangle' \right)$ (20)

and

$$|k, |t| = 1, J = 1$$
 $\rangle = \frac{1}{\sqrt{2}} \left(|k, t = 1\rangle' + |k, t = -1\rangle' \right)$. (21)

The representation of the system Hamiltonian in the basis (18) takes the form dependent on the parity of the number of electrons N (or nodes in the considered half-filling case) and the parity of the quasi-momentum k.

At the very beginning, we present the case of any even N and any even k — the representation of the Hamiltonian has the quasi-diagonal form with two blocks for J = 1 and J = 0, respectively as follows

and

where $a = 2t \cos\left(\frac{k\pi}{N}\right)$. The energies given as the eigenvalues of the matrix (22) are given by the formula ,

$$E = U + 2\cos\left(\frac{l\pi}{N}\right)a, \ l \in \{1, 3, 5, \dots, N-1\}.$$
 (24)

The eigenvectors of the matrix (22) have the form

$$|k,J,l\rangle = \sqrt{\frac{4}{N}} \left[\sum_{|t|=1}^{\frac{N}{2}-1} \cos\left(\frac{\left(\frac{N}{2}-|t|\right)l\pi}{N}\right) |k,|t|,J\rangle + \cos\left(\frac{\pi}{4}\right) |k,|t| = N/2, J\rangle \right],\tag{25}$$

with $l \in \{1, 3, 5, \dots, N-1\}$. An exemplary eigenvector for N = 10, any $k \in \{0, \pm 2, \pm 4\}, J = 1$, and l = 5 takes the form

$$|l = 5\rangle = \sqrt{4/10} \left[\cos \left(20\pi/10 \right) ||t| = 1 \right] + \cos \left(15\pi/10 \right) |2\rangle + \cos \left(10\pi/10 \right) |3\rangle + \cos \left(5\pi/10 \right) |4\rangle + \cos \left(2\pi/8 \right) |5\rangle \right].$$
(26)

The eigenvalues of the matrix (23) are given by the formula

$$E = U + 2\cos\left(\frac{l\pi}{N}\right)a, \ l \in \{2, 4, 6, \dots, N-2\}.$$
 (27)

The form of the eigenvectors of the matrix (23) is as follows

$$|k, J, l\rangle = \sqrt{\frac{4}{N}} \sum_{|t|=1}^{N-2} \cos\left(\frac{((l-N)|t|+N/2)\pi}{N}\right) |k, |t|, J\rangle, \qquad (28)$$

with $l \in \{2, 4, \ldots, N-2\}$. An exemplary eigenvector for N = 14, any $k \in \{0, \pm 2, \pm 4, \pm 6\}, J = 0$, and l = 4 takes the form

$$|l = 4\rangle = \sqrt{4/14} \left[\cos\left(-3\pi/14\right) ||t| = 1 \right] + \cos\left(-13\pi/14\right) |2\rangle + + \cos\left(-23\pi/14\right) |3\rangle + \cos\left(-33\pi/14\right) |4\rangle + \cos\left(-43\pi/14\right) |5\rangle + \cos\left(-53\pi/14\right) |6\rangle.$$
(29)

Next, we present the case of any even N and any odd k — the representation of the Hamiltonian has the quasi-diagonal form with two blocks for J = 1 and J = 0, respectively. The first matrix is exactly the same as (23), while the case for J = 0 provides

The eigenvalues of the matrix (30) have the following form

$$E = U + 2\cos\left(\frac{l\pi}{N}\right)a, \ l = \{1, 3, 5, \dots, N-1\}.$$
 (31)

The eigenvectors of the matrix (30) are given by (25) after cyclic shift to the right as follows

$$|k, J, l\rangle = \sqrt{\frac{4}{N}} \left[\cos\left(\frac{\pi}{4}\right) |k, |t| = 1, J \right] + \sum_{|t|=2}^{\frac{N}{2}} \cos\left(\frac{\left(l + \left(\frac{N}{2} - |t|\right)l\right)\pi}{N}\right) |k, |t|, J \right], \quad (32)$$

where $l = \{1, 3, 5..., N - 1\}$. An exemplary eigenvector for N = 6, any $k \in \{\pm 1\}, J = 0$, and l = 3 takes the form

$$|l = 3\rangle = \sqrt{2/3} \left[\cos(2\pi/8) \, ||t| = 1 \right\} + \cos(6\pi/6) \, |2\rangle + \cos(3\pi/6) \, |3\rangle \right] \,. \tag{33}$$

The eigenvalues of the matrix (23) exhibits very interesting fact for the case of N = 10 — they are built based on the Golden Number $\phi = \frac{\sqrt{5}+1}{2}$ and provide the following set

$$\{\phi a + U, (\phi - 1) a + U, -(\phi - 1) a + U, -\phi a + U\}.$$
 (34)

The appropriate eigenvectors are given by equations (28), and before normalization can be presented in the form of rows of Table II for any $k \in \{0, \pm 1, \pm 2, \pm 3, \pm 4, 5\}$ and J = 0. The Golden Number is closely related to the Fibonacci sequence which is defined recursively by $F_n = F_{n-1} + F_{n-2}$ for $n \ge 2$ with the initial terms $F_0 = F_1 = 1$. Some new interesting properties and applications of the Fibonacci sequence were studied in [34, 35].

TABLE II

	$ t = 1\rangle$	$ 2\rangle$	3 angle	$ 4\rangle$
$ l=2\rangle$	-1	ϕ	$-\phi$	1
$ l=4\rangle$	1	$-(\phi - 1)$	$-(\phi - 1)$	1
$ l=6\rangle$	-1	$-(\phi - 1)$	$(\phi - 1)$	1
$ l=8\rangle$	1	ϕ	ϕ	1

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The representation of the system Hamiltonian for odd N has the general form as follows

U	-a	0	0	0		0	0	0	0	0 -	
-a	U	-a	0	0		0	0	0	0	0	
0	-a	U	-a	0		0	0	0	0	0	
:	÷	÷	÷	÷	÷	÷	÷	:	:	÷	(35)
0	0	0	0	0		0	-a	U	-a	0	
0	0	0	0	0		0	0	-a	U	-a	
0	0	0	0	0		0	0	0	-a	$U \mp a$	

The last diagonal element is equal to U - a for even k and J = 1 or odd k and J = 0. Other cases, that is for even k and J = 0 or odd k and J = 1 provide the last diagonal element in the form U + a. The eigenvalues and eigenvectors of the matrix (35) are given by the formulas

$$E = U + 2\cos\left(\frac{l\pi}{N}\right)a\tag{36}$$

and

$$|k, J, l\rangle = \sqrt{\frac{4}{N}} \sum_{|t|=1}^{\frac{N-1}{2}} \cos\left(\frac{(2(l-N)|t|+N)\pi}{2N}\right) |k, |t|, J\rangle, \qquad (37)$$

where $l \in \{2, 4, 6, \ldots, N-1\}$ and $l \in \{1, 3, 5, \ldots, N-2\}$ for the last diagonal element of the matrix (35) equal to U - a and U + a, respectively. An exemplary eigenvector for N = 9, any $k \in \{0, \pm 2\}$, J = 1, and l = 5 takes the form

$$|l = 5\rangle = \sqrt{4/9} \left[\cos(\pi/18) ||t| = 1 \right] + \cos(-7\pi/18) |2\rangle$$
(38)

$$+\cos\left(-15\pi/18\right)|3\rangle + \cos\left(-23\pi/18\right)|4\rangle].$$
 (39)

The eigenvalues and eigenvectors of the matrix (35) for N = 5 are built based on the Golden Number by analogy to (34) due to (37).

4. Summary and conclusions

In the present paper, we gave a thorough analysis of the one-dimensional attractive Hubbard model for the chains with N atoms, the same number of electrons, and N-1 of them with the same spin projection. The translational symmetry of the system provides the basis of wavelets, and appropriate

gauge transformation removes the complex elements from the representation of the Hamiltonian. The rotational symmetry within the spinless part of the magnetic ring provides the quantum number J, whereas J_z , the total spin Sand the total magnetization M are fixed. We provide the general forms of the representation of the system Hamiltonian in assumed translational and unitary symmetry with respect to the parity of the total number of nodes N, and quasi-momentum k. Next, we derived the appropriate energies and the eigenvalues. The eigenvalues for all cases are obtained by the formula $E = U + 2\cos(\frac{l\pi}{N})a, \ l \in \tilde{N}$, with even number l providing the energies for the cases with even number k + J, and with odd number l providing the energies for odd number k + J — for even number N, and contrariwise for odd number N. The set $\{k, J, l\}$ of quantum numbers provides all exact solutions for the case of one-dimensional attractive Hubbard model for the chains with N atoms, the same number of electrons, and N-1 of them with the same spin projection. The eigenvalues and eigenvectors in some cases are built based on the Golden Number $\phi = \frac{\sqrt{5}+1}{2}$.

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