

Exact Ground States for Quasi 1D Systems with Hubbard Interaction

E. Kovács^{1*}, Zs. Gulácsi²

¹ University of Miskolc, Egyetemváros, Department of Physics, 3515 Miskolc, Hungary

² University of Debrecen, Department of Theoretical Physics, Bemtér 18/b, 4026 Debrecen, Hungary

(Received 26 September 2011; revised manuscript received 23 February 2012; published online 14 March 2012)

Using a positive semidefinite operator technique we deduced exact ground states for a modified diamond chain described by a non-integrable Hubbard model with on-site repulsion. Our results are valid for arbitrary length of the chain and strength of the Hubbard interaction. For the analyzed parameter space region of the quasi 1D chain structure we found that two flat bands are present in the bare band structure of the system, both for zero and for a fixed value of magnetic field. We obtained ground states of nonmagnetic and ferromagnetic insulator type and studied their physical properties.

Keywords: Strongly interacting systems, Hubbard model, Nanowires, Ferromagnetism, Exact solutions, Chain structures, Diamond chains.

PACS numbers: 68.65.–k, 75.10.Jm

1. INTRODUCTION

The investigation of nanostructure objects with itinerant electrons is one of the most quickly progressing fields in the modern material science. These systems present a drastic change of physical properties under given conditions, e.g. fixed external magnetic field or given site-selective gate potential [1, 2]. As specific nanostructures, quasi 1D structures have been intensively studied in the last years. Among these, the non-integrable systems (the number of degrees of freedom is much higher than the number of constants of motion) become to be more and more investigated since these are closely placed to real systems encountered in nature. Among these systems, ladder structures [3], or chain structures [4] are special in view, from which, we concentrate here on the last group. The chains, considered periodic structures holding a closed polygon type of base as a repeat unit, have been gradually studied following mainly the increasing number of atoms in the base. On this line triangular [5, 6], quadrilateral [1, 7, 8], pentagonal [9-12], and hexagonal [13, 14] chains have been investigated. In this frame, we analyze below chains with quadrilateral base as electron systems where the interaction between the electrons is the Hubbard on-site interaction originating from the Coulomb repulsion.

Our goal is to find exact ground-state wave functions for arbitrary strength of the interaction, thus we do not use perturbation theory or any other approximations. It is worth to mention that the full exact solution of the Hubbard model is still unknown for dimensions larger than 1. In the paper [1] a new method was developed and applied for the diamond Hubbard chain. In this paper we use the same method to investigate a similar, but modified system. The modifications consist in the introduction of external links, which pushes the system more closely to experimental realizations, and as shown by us, actually shift the emergence regions of different possible phases in the parameter space.

The remaining part of the paper is constructed in the following way. Section 2 contains the description of

the studied system, more concretely the chain structure and the Hamiltonian. In Section 3 we deal with the noninteracting band-structure, then explain the essence of the positive semidefinite operator method and perform the transformation. In Section 4 we construct the ground state wave functions and analyze the physical properties of them. We summarize the essence of the paper in Section 5.

2. THE STUDIED SYSTEM

Fig. 1 shows the modified Hubbard diamond chain we analyzed. The sites of the chain for the i th cell are denoted by $i + r_s$, where $s = 1, 2, 3$ denoting in-cell positions represents also the sublattice index.

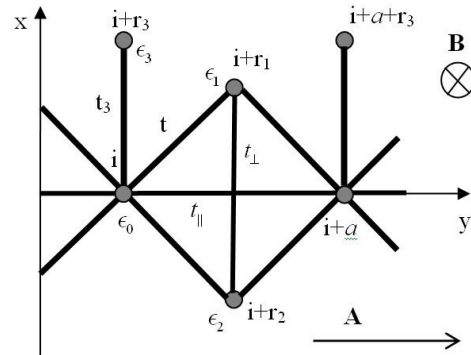


Fig. 1 – The diamond Hubbard chain with external links. The cell defined at the site i contains 4 sites placed at $i, i + r_1, i + r_2$ and $i + r_3$. The Bravais vector is denoted by a . t, t_1, t_2, t_3 are in order the nearest-neighbor (t, t_3), the next nearest-neighbor hopping matrix element – parallel and perpendicular to the line of the chain. $\epsilon_0, \epsilon_1, \epsilon_2$ and ϵ_3 are on-site potentials, at the sites $i, i + r_1, i + r_2$ and $i + r_3$, respectively. B is the external magnetic field perpendicular to the line of the chain, while A represents the corresponding vector potential

The Bravais vector of the lattice is a , horizontal in Fig. 1 N_C is the number of unit cells, N is the number of electrons, N_S is the number of sites, and one has $N_S = 4N_C$. The Hamiltonian of the system is the following:

* fizendre@uni-miskolc.hu

$$\begin{aligned}
H = \sum_{\sigma} \sum_{i=1}^{N_c} & \left([t e^{i\delta/2} (c_{i+r_1,\sigma}^{\dagger} c_{i,\sigma} + c_{i+a,\sigma}^{\dagger} c_{i+r_1,\sigma}) \right. \\
& + c_{i+r_2,\sigma}^{\dagger} c_{i+a,\sigma} + c_{i,\sigma}^{\dagger} c_{i+r_2,\sigma}) \\
& + t_3 c_{i+r_3,\sigma}^{\dagger} c_{i,\sigma} + t_{\perp} c_{i+r_1,\sigma}^{\dagger} c_{i+r_2,\sigma} + t_{\parallel} c_{i+a,\sigma}^{\dagger} c_{i,\sigma}] + H.c. \\
& \left. + \epsilon_0 n_{i,\sigma} + \epsilon_1 n_{i+r_1,\sigma} + \epsilon_2 n_{i+r_2,\sigma} + \epsilon_3 n_{i+r_3,\sigma} \right) + H_U
\end{aligned}$$

The operator $c_{i,\sigma}^{\dagger}$ creates an electron with spin σ in at site i , $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ is the particle number operator, while

$$H_U = \sum_{i=1}^{N_s} n_{i,\uparrow} n_{i,\downarrow}$$

is the operator of the on-site Coulomb repulsion, $U > 0$. The movements of the electrons from site to site are described by the hopping matrix elements t , t_{\parallel} , t_{\perp} , and t_3 . The first characterizes the nearest-neighbor hoppings (except for sites $i + r_3$) while t_{\parallel} and t_{\perp} the second nearest neighbor terms parallel and perpendicular to a , respectively. The last hopping term t_3 refers to movements along the external leg, and the epsilons are one-site one particle potentials. The system is placed in an external magnetic field perpendicular to the plane of the chain and described by the Peierls phase factor δ . During the calculations arbitrary but fixed N and periodic boundary conditions are taken into account along the chain.

We note that the presence of the external legs into the system allows the use of external site selective gate potentials in order to modify and easily manipulate the potential ϵ_3 and therefore the physical behavior of the system.

3. ABOUT THE METHOD

First we calculate the non-interacting band-structure of the system. For this we have to write the Hamiltonian without the H_U term into the k -space by Fourier transformation.

$$\begin{aligned}
H_0 = \sum_{k,\sigma} & \left[(t_1 c_{1,k,\sigma}^{\dagger} c_{2,k,\sigma} + t_3 c_{0,k,\sigma}^{\dagger} c_{3,k,\sigma} \right. \\
& + 2t \cos \frac{ak + \delta}{2} c_{0,k,\sigma}^{\dagger} c_{1,k,\sigma} + 2t \cos \frac{ak - \delta}{2} c_{0,k,\sigma}^{\dagger} c_{2,k,\sigma} \\
& + H.c.) + (\epsilon_0 + 2t_{\parallel} \cos ak) c_{0,k,\sigma}^{\dagger} c_{0,k,\sigma} \\
& \left. + \epsilon_1 c_{1,k,\sigma}^{\dagger} c_{1,k,\sigma} + \epsilon_2 c_{2,k,\sigma}^{\dagger} c_{2,k,\sigma} + \epsilon_3 c_{3,k,\sigma}^{\dagger} c_{3,k,\sigma} \right]
\end{aligned}$$

Then, by diagonalizing via the secular equation, we derive an algebraic equation. This contains the four unknown energies, as we have four sites in the primitive cell. The solutions of this equation as a function of k give the four bands of the bare band structure. After solving the secular equation by a commercial computer program we obtained that the lowest two bands are always flat. In Fig. 2 one can see an example for the noninteracting band-structure of the system. At 0.7 there are two coincident flat bands, indicated with green and black colors in Fig. 2

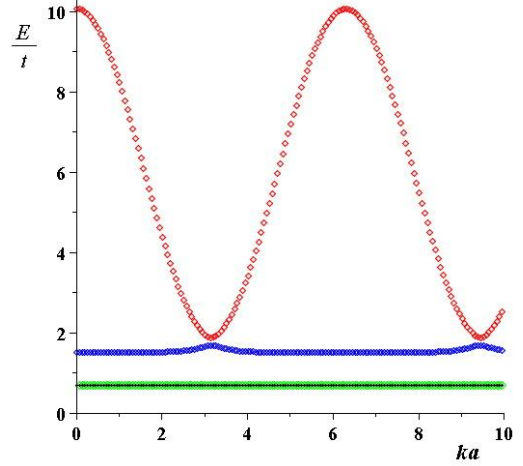


Fig. 2 – An example for the noninteracting band-structure at $\delta = 0$. Only the positive values of ka is shown along the horizontal axis because of symmetry. The border of the first Brillouin zone is at $ka = \pi$. On the vertical axis the energy E is normalized by t

To find the GS of the interacting system, we use the method of positive semidefinite operators. A Hermitian operator is called positive semidefinite if its spectrum is nonnegative, i.e. its lowest eigenvalue is zero or positive. Therefore if H_+ is a positive semidefinite Hamiltonian and we have an eigenvector of H_+ with zero eigenvalue, then this vector belongs to the ground-state (GS) subspace of H_+ . Suppose that we manage to write the H Hamiltonian of the interacting system in the form

$$H = H_+ + C, \quad (1)$$

where H_+ is positive semidefinite and C is a constant which depends on the parameters of the Hamiltonian. Now if $|\psi_g\rangle$ is the most general element of the kernel of H_+ , then $|\psi_g\rangle$ is the GS vector of H and the corresponding GS energy is C . Thus in our method we transform the Hamiltonian into the form (1) and calculate the kernel of H_+ .

In order to perform the transformation first we define new operators

$$\begin{aligned}
A_{i,\sigma} &= a_1 c_{i,\sigma} + a_2 c_{i+r_1,\sigma} + a_3 c_{i+a,\sigma} + a_4 c_{i+r_2,\sigma} \\
A_{i,\sigma}^{\dagger} &= a_1^* c_{i,\sigma}^{\dagger} + a_2^* c_{i+r_1,\sigma}^{\dagger} + a_3^* c_{i+a,\sigma}^{\dagger} + a_4^* c_{i+r_2,\sigma}^{\dagger}
\end{aligned}$$

and

$$\begin{aligned}
B_{i,\sigma} &= b_1 c_{i,\sigma} + b_2 c_{i+r_3,\sigma} \\
B_{i,\sigma}^{\dagger} &= b_1^* c_{i,\sigma}^{\dagger} + b_2^* c_{i+r_3,\sigma}^{\dagger}
\end{aligned}$$

where the a_i and b_i numerical coefficients are unknown at this stage and must be calculated during the transformation. In Fig. 3 we illustrate which lattice sites are covered by the block-operators A_i and B_i .

We can calculate the product of these operators

$$\begin{aligned}
 A_{i,\sigma}^\dagger A_{i,\sigma} = & |a_1|^2 c_{i,\sigma}^\dagger c_{i,\sigma} + a_1^* a_2 c_{i,\sigma}^\dagger c_{i+r_1,\sigma} + a_1^* a_3 c_{i,\sigma}^\dagger c_{i+a,\sigma} + a_1^* a_4 c_{i,\sigma}^\dagger c_{i+r_2,\sigma} \\
 & a_2^* a_1 c_{i+r_1,\sigma} c_{i,\sigma} + |a_2|^2 c_{i+r_1,\sigma}^\dagger c_{i+r_1,\sigma} + a_2^* a_3 c_{i+r_1,\sigma}^\dagger c_{i+a,\sigma} + a_2^* a_4 c_{i+r_1,\sigma}^\dagger c_{i+r_2,\sigma} \\
 & a_3^* a_1 c_{i+a,\sigma}^\dagger c_{i,\sigma} + a_3^* a_2 c_{i+a,\sigma}^\dagger c_{i+r_1,\sigma} + |a_3|^2 c_{i+a,\sigma}^\dagger c_{i+a,\sigma} + a_3^* a_4 c_{i+a,\sigma}^\dagger c_{i+r_2,\sigma} \\
 & a_4^* a_1 c_{i+r_2,\sigma}^\dagger c_{i,\sigma} + a_4^* a_2 c_{i+r_2,\sigma}^\dagger c_{i+r_1,\sigma} + a_4^* a_3 c_{i+r_2,\sigma}^\dagger c_{i+a,\sigma} + |a_4|^2 c_{i+r_2,\sigma}^\dagger c_{i+r_2,\sigma}
 \end{aligned}$$

and it is easy to calculate $B_{i,\sigma}^\dagger B_{i,\sigma}$ similarly. These products are obviously positive semidefinite and consist of a sum of products of creation and annihilation operators $c_\alpha^\dagger c_\beta$, which are present in the Hamiltonian as well. It is possible to produce the H_+ operator as a sum of operator-products:

$$H_+ = \sum_{\sigma} \sum_{i=1}^N (A_{i,\sigma}^\dagger A_{i,\sigma} + B_{i,\sigma}^\dagger B_{i,\sigma})$$

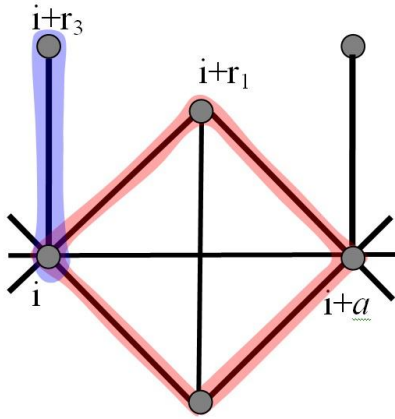


Fig. 3 – Illustration of the A_i and B_i block operators. The pink square containing sites i , $i+r_1$, $i+r_2$, $i+a$, represents the A_i operator, while the thick blue vertical line connecting sites i , $i+r_3$ represents the B_i operator

The transformation of the noninteracting part of the starting H in the form (1) using the H_+ presented above is valid if the coefficient of each $c_\alpha^\dagger c_\beta$ operator-product is the same in the original Hamiltonian and in the expression $\sum_{\sigma} \sum_{i=1}^N (A_{i,\sigma}^\dagger A_{i,\sigma} + B_{i,\sigma}^\dagger B_{i,\sigma})$. This provides us matching equations which must be solved, and which in the present case have the form:

$$\begin{aligned}
 |a_1|^2 + |a_3|^2 + |b_1|^2 &= \epsilon_0 - K \\
 |a_2|^2 &= \epsilon_1 - K \\
 |a_4|^2 &= \epsilon_2 - K \\
 |b_2|^2 &= \epsilon_3 - K \\
 a_1 a_2^* &= t e^{i\delta/2} \\
 a_2 a_3^* &= t e^{i\delta/2} \\
 a_3 a_4^* &= t e^{i\delta/2} \\
 a_4 a_1^* &= t e^{i\delta/2} \\
 b_1 b_2^* &= t_3 \\
 a_1 a_3^* &= t_{\parallel} \\
 a_2 a_4^* &= t_{\perp}
 \end{aligned}$$

We have found two families of solutions for this system of equations, one with $\delta = 0$ and the other with $\delta = \pi$.

The first family is valid for zero external magnetic field and gives the following conditions for the parameters:

$$\begin{aligned}
 \delta &= 0 \\
 \epsilon_0, \epsilon_3 &> \lambda, \quad \epsilon_1 = \epsilon_2 > \lambda \\
 t_{\perp}, t_{\parallel} &> 0, \\
 t^2 &= t_{\parallel} t_{\perp} \\
 t_{\perp} &= \epsilon_2 - \lambda \\
 2t^2 / t_{\perp} + t_{\parallel}^2 / (\epsilon_3 - \epsilon_2 + t_{\perp}) &= \epsilon_0 - \epsilon_2 + t_{\perp}
 \end{aligned} \tag{2}$$

The solution itself for a_i and b_i prefactors has the form:

$$\begin{aligned}
 a_2 &= a_4 = \sqrt{t_{\perp}} e^{i\phi} \\
 a_1 &= a_3 = (t / \sqrt{t_{\perp}}) e^{i\phi} \\
 b_2 &= \sqrt{\epsilon_3 - K} e^{i\chi} \\
 b_1 &= \frac{t_3}{\sqrt{\epsilon_3 - K}} e^{i\chi} \\
 K &= \lambda \\
 \lambda, \phi, \chi &\text{ arbitrary}
 \end{aligned} \tag{3}$$

The ground state energy is $E_g = -(\epsilon_2 - t_{\perp})N$.

The second family is valid in the case of nonzero external magnetic field, in the following regime of the parameter-space:

$$\begin{aligned}
 \delta &= \pi \\
 \epsilon_0, \epsilon_3 &> \lambda, \quad \epsilon_1 = \epsilon_2 > \lambda \\
 t_{\perp}, t_{\parallel} &< 0 \\
 t^2 &= t_{\parallel} t_{\perp} \\
 t_{\perp} &= -(\epsilon_2 - \lambda) \\
 2t^2 / (-t_{\perp}) + t_{\parallel}^2 / (\epsilon_3 - \epsilon_2 - t_{\perp}) &= \epsilon_0 - \epsilon_2 - t_{\perp}
 \end{aligned} \tag{4}$$

The solution in this case becomes:

$$\begin{aligned}
 a_2 &= -a_4 = \sqrt{-t_{\perp}} e^{i\phi} \\
 a_1 &= -a_3 = i(t / \sqrt{-t_{\perp}}) e^{i\phi} \\
 b_2 &= \sqrt{\epsilon_3 - K} e^{i\chi} \\
 b_1 &= (t_3 / \sqrt{\epsilon_3 - K}) e^{i\chi} \\
 K &= \lambda \\
 \lambda, \phi, \chi &\text{ arbitrary}
 \end{aligned} \tag{5}$$

On this line we managed to transform the Hamiltonian into the form

$$H = \sum_{\sigma} \sum_{i=1}^N (A_{i,\sigma}^\dagger A_{i,\sigma} + B_{i,\sigma}^\dagger B_{i,\sigma}) + H_U - KN, \tag{6}$$

where the terms $A_{i,\sigma}$ and $B_{i,\sigma}$ are block operators which represent a linear combination of fermionic operators defined on a finite domain of the system, see Fig. 3. One can easily see that the terms in the bracket are positive semidefinite. On the other hand, the Hubbard-term is positive semidefinite as well, and provides its smallest possible zero eigenvalue if there are no doubly occupied sites in the system. Furthermore, $C = -KN$, where N is the operator of the total number of particles in the system, which is a constant of motion.

4. THE OBTAINED GROUND STATES

4.1 The expression of the ground states

We obtained the GS wave vector in the form

$$|\Psi_g\rangle = \prod_i G_{i,\sigma_i}^\dagger |0\rangle,$$

where $|0\rangle$ is the vacuum state. We consider the G_{i,σ_i}^\dagger operators as the most general linear combination of creation operators acting on each lattice site of the system. Furthermore, because of the positive semidefinite Hubbard term, we take into consideration that the lowest energy value must be provided by a state without doubly occupied sites. We found the following two families of G_{i,σ_i}^\dagger operators at $\delta = 0$, denoted hereafter by D^\dagger and E^\dagger :

$$D_{i+a,\sigma}^\dagger = \frac{t}{t_\perp} c_{i+r_1,\sigma}^\dagger - c_{i+a,\sigma}^\dagger + \frac{t_3}{\alpha} c_{i+a+r_3,\sigma}^\dagger + \frac{t}{t_\perp} c_{i+a+r_2,\sigma}^\dagger$$

$$E_{i,\sigma}^\dagger = c_{i+r_1,\sigma}^\dagger - c_{i+r_2,\sigma}^\dagger$$

where $\alpha = \epsilon_3 - \epsilon_2 + t_\perp$. The GS energy of this wavefunction is $E_g = -(\epsilon_2 - t_\perp)N$. This solution is valid in phase diagram region described by (2).

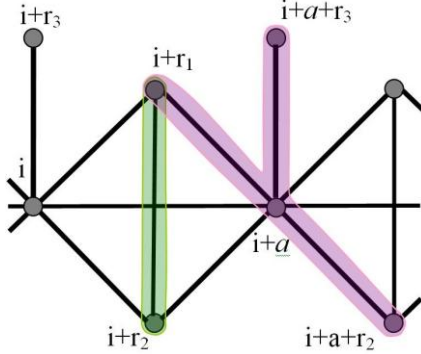


Fig. 4 – Illustration of the ground state wave functions. The sites $i + r_1$, $i + a$, $i + a + r_2$, $i + a + r_3$ which are present in D_{i+a} , are denoted with purple, while sites $i + r_1$ and $i + r_2$ present in E_i are denoted by green.

For $\delta = \pi$ we obtained a similar expression for the GS wave function, however, the coefficients of the creation operators in D and E is slightly different:

$$D_{i+a,\sigma}^\dagger = i \frac{t}{t_\perp} c_{i+r_1,\sigma}^\dagger - c_{i+a,\sigma}^\dagger + \frac{t_3}{\beta} c_{i+a+r_3,\sigma}^\dagger + i \frac{t}{t_\perp} c_{i+a+r_2,\sigma}^\dagger$$

$$E_{i,\sigma}^\dagger = c_{i+r_1,\sigma}^\dagger + c_{i+r_2,\sigma}^\dagger$$

where $\beta = \epsilon_3 + \epsilon_2 + t_\perp$. The GS energy is $E_g = -\epsilon_2 - t_\perp N$. The phase diagram region is the one determined by equations (4). We emphasize that this region is disjoint from the (2) region.

4.2 The magnetic properties of the GS

Now we have two sets of operators, namely D_{i,σ_i}^\dagger and E_{i,σ_i}^\dagger which can appear in the GS vectors, each with

N_C terms for both up and down spins. Every vector from the kernel of the transformed Hamiltonian can be written as a product of these operators. The number of the operators in the product specifies the number of electrons in the system. The most general GS vector is obtained as a linear combination of these vectors. As D_{i,σ_i}^\dagger and E_{i,σ_i}^\dagger have no common lattice-points for different i (except for D_{i,σ_i}^\dagger and E_{i,σ_i}^\dagger), the spin indices σ_i of them for different cells are usually independent. For the same cell, the D_{i,σ_i}^\dagger and E_{i,σ_i}^\dagger operators must have the same spin index in order to avoid the double occupancy. Physically this means that the solution is globally a non-magnetic (paramagnetic) phase up to the electron number $N < 2N_C - 1$. For the case when in the same cell both operators D and E are present, the cell itself is ferromagnetic and behaves as a ferromagnetic cluster. However, different cells are magnetically not correlated. This is the reason why the system globally is non-magnetic if $N < 2N_C - 1$. At $N = 2N_C - 1$ or $N = 2N_C$ all the D and E operators touch each other, the connectivity condition is satisfied and the system becomes ferromagnetic.

4.3 The electric properties of the GS

The long range hopping ground state expectation value (to the y direction, horizontal in Fig. 1.) can be defined as

$$\Gamma(r) = \frac{\langle \Psi_g | c_{i+r_1+ra,\sigma}^\dagger c_{i+r_1,\sigma} + H.c. | \Psi_g \rangle}{\langle \Psi_g | \Psi_g \rangle}. \quad (7)$$

We calculated Γ as a function of r (the distance of the hopping of the electron), more precisely the logarithm of the absolute value of this function: $\ln|\Gamma(r)|$, for the $\delta = 0$ GS wave function by a computer program written by us (see Fig. 5). We considered the maximum number of electron, $N = 2N_C$, which can be constructed as the product of N_C D_{i,σ_i}^\dagger operators and N_C E_{i,σ_i}^\dagger operators. We obtained that the $\ln|\Gamma(r)|$ function is close to

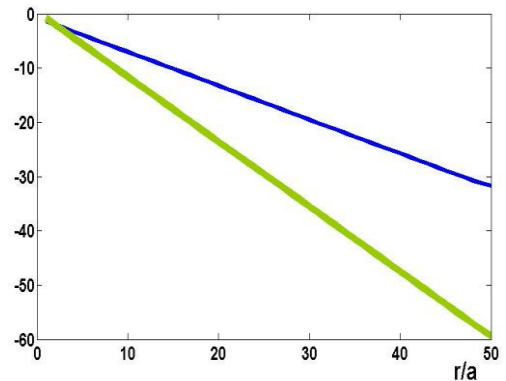


Fig. 5 – Logarithm of the absolute value of the $\Gamma(r)$ function (see (5)), for $\delta = 0$. The variable r/a is plotted along the horizontal axis, where a is the absolute value of the Bravais vector, while $\ln|\Gamma(r)|$ is plotted along the vertical axis. The upper thin blue line is for $t_\perp/t = 0.4$ while the lower thick green line is for $t_\perp/t = 0.8$

a straight curve, which means that the long range hopping ground state expectation value is exponentially decreasing. We can express it as

$$\Gamma(r) = Ae^{-r/\lambda},$$

where A is a constant and λ is the one particle localization length. This λ is strongly depend on Hamiltonian parameter t_{\perp}/t , for example if $t_{\perp}/t = 0.4$, then $\lambda \approx 1.57a$, while if $t_{\perp}/t = 0.8$ then $\lambda \approx 0.84a$, where a is the absolute value of the Bravais vector.

Thus we can conclude that the ground state electrons are localized, although not exactly to one lattice site. Therefore the GS is an insulator, albeit not a band insulator. As this system is insulating because of the interaction between the electrons, thus it is a Mott insulator [20]. Further investigation of the GS is in progress and will be published elsewhere [19].

5. SUMMARY

An itinerant diamond chain with external link is analyzed in the presence of a perpendicular external magnetic field in the frame of a non-integrable Hubbard model. For this chain exact ground states are deduced by a method using positive semidefinite operator properties. The ground states turn out to be nonmagnetic and ferromagnetic in character, the latter is localized in the thermodynamic limit.

The method we use has a large spectrum of applicability which not depends on dimensionality or integrability, working well even in conditions completely unfamiliar for the traditional view about exact solutions, as three dimensions [15], two dimensions [16] or textures as stripes in 2D [17], or disordered systems [18]. Extreme details regarding the application of the method for chain structures have been presented in [8]. The method transforms first the Hamiltonian (H) in a positive semidefinite form (H_+) plus an additive constant (C) and after this step deduces the ground state $|\Psi_g\rangle$ by constructing the most general wave vector which provides the minimum possible energy (i. e. zero) for H_+ . If this becomes possible, one finds the ground state energy $E_g = C$ and the ground state $|\Psi_g\rangle$ in the parameter space region P_s where the exact transformation from H to H_+ has been done. This transformation is not unique, can be performed in several different ways leading to different regions of the parameter space with separately existing ground states. One notes that the transformation in a positive semidefinite form of the Hamiltonian can always be done since the spectrum of a real system is always bounded from below, hence the relation $H = H_+ + C$, where H_+ is positive semidefinite, always holds (but usually, it is not easy to find H_+). In deducing H_+ in the present case one applies block operators (see A^+ and B^+ in Sec. 3) which are linear combinations of creation operators acting on the

sites of a block. The such constructed positive semidefinite operator H_+ must exactly reproduce $H_+ - C$, and this obligatory matching provides the equations from where the unknown numerical coefficients of the block operators can be deduced, and also the parameter space domain P_s arises. One notes however that the use of linear combination of creation operators in building up the block operators is not obligatory, and also other type of expressions can be used, as bilinear combinations for example [4, 19].

After obtaining H_+ containing the

$$P_{i,\sigma} = A_{i,\sigma}^\dagger A_{i,\sigma} + B_{i,\sigma}^\dagger B_{i,\sigma}$$

expressions, in the present case the deduction of the ground state in the first step, reduces to the job to find the most general G^+ operator which anticommutes with all block operators (here A^+ , B^+) for all possible value of all indices. This is necessary since in this case the A and B operators of H can be pushed in front of the G^+ operators from $|\Psi_g\rangle$, and because of $A|0\rangle = B|0\rangle = 0$, where $|0\rangle$ is the bare vacuum, the ground state can be deduced.

In this way one finds the kernel of $\sum_i \sum_\sigma P_{i,\sigma} = H - C$, from where, paying attention to the possible presence of the double occupancy, the kernel of the whole Hamiltonian can be obtained. This procedure of deducing the ground state works well for the concentration region described in Section 4, where the deduced solutions exist. For other concentration regions, often other procedures are suitable, see for example [1, 19].

In the presented paper, using the above described method in the case of the chain structures, our aim was to analyze the action of external links or side groups in the development of different ground states. We used here for this purpose external links which do not connect different cells of the chain. Comparing our deductions to known results relating the diamond Hubbard chain without external links [1], one finds that in the present case, the external links mainly shift different phases in the parameter space of the model. We note that more drastic effects can be obtained in the case of external links which connect different cells of the chain. The study of this last case is at the moment in development, and will be published elsewhere [19].

ACKNOWLEDGEMENTS

For E.K. (Z.G.), this work was carried out as part of the TAMOP-4.2.1.B-10/2/KONV-2010-0001, (TAMOP-4.2.1/B-09/1/KONV-2010-0007) project in the framework of the New Hungarian Development and for Z.G. also OTKA-K-100288. The realization of this project is supported by the European Union, co-financed by the European Social Fund.

REFERENCES

1. Z. Gulacsi, A. Kampf, D. Vollhardt, *Phys. Rev. Lett.* **99**, 026404 (2007).
2. A.S. Dhoot, G.M. Wang, D. Moses, A.J. Heeger, *Phys. Rev. Lett.* **96**, 246403 (2006).
3. E. Kovacs, Z. Gulacsi, *J. Phys. A* **38**, 10273 (2005).
4. I. Chalupa, Z. Gulacsi, *J. Phys.:Condens. Matter* **19**, 386209 (2007).
5. H.K. Kono, Y. Kuramoto, *Journ. Phys. Soc. Jpn.* **75**, 084706

- (2006).
6. O. Derzhko, A. Honecker, J. Richter, *Phys. Rev. B* **76**, 220402R (2007).
 7. J. Vidal, B. Douçot, R. Mosseri, P. Butaud, *Phys. Rev. Lett.* **85**, 3906 (2000).
 8. Z. Gulacsi, A. Kampf, D. Vollhardt, *Progr. Theor. Phys. Suppl.* **176**, 1 (2008).
 9. R. Arita, Y. Suwa, K. Kuroki, H. Aoki, *Phys. Rev. B* **68**, 140403R (2003).
 10. Y. Suwa, R. Arita, K. Kuroki, H. Aoki, *Phys. Rev. B* **68**, 174419 (2003).
 11. O.R. Nascimento, A.J.A. de Oliveira, A.A. Correa, L.O.S. Bulhões, E.C. Pereira, V.M. Souza, L. Walmsley, *Phys. Rev. B* **67**, 144422 (2003).
 12. Z. Gulacsi, A. Kampf, D. Vollhardt, *Phys. Rev. Lett.* **105**, 266403 (2010).
 13. R. Trencsenyi, E. Kovacs, Z. Gulacsi, *Phil. Mag.* **89**, 1953 (2009).
 14. R. Trencsenyi, K. Gulacsi, E. Kovacs, Z. Gulacsi, *Annalen der Physik*, **523**, 741 (2011).
 15. Z. Gulacsi, D. Vollhardt, *Phys. Rev. Lett.* **91**, 186401 (2003).
 16. Z. Gulacsi, *Phys. Rev. B* **77**, 245113 (2008).
 17. Z. Gulacsi, M. Gulacsi, *Phys. Rev. B* **73**, 014524 (2006).
 18. Z. Gulacsi, *Phys. Rev. B* **69**, 054204 (2004).
 19. E. Kovacs, Z. Gulacsi, under preparation.
 20. In the case of a band insulator, a conducting band becomes full and the insulating behavior is given by the action of the periodic potential. In the present case the conduction band is not full, and the insulating behavior emerges because of the inter-electronic interactions.