Deducing exact ground states for many-body non-integrable systems

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Abstract—I describe in details the method which uses positive semidefinite operator properties in deducing non-approximated results for quantum mechanical many-body non-integrable systems. The steps of the procedure, namely i) the transcription of the Hamiltonian in a positive semidefinite form $\mathbf{H}=\mathbf{O}+\mathbf{C}$, where $\mathbf{O}$ is a positive semidefinite operator while C is a scalar, ii) the deduction of the total particle number dependent ground state by constructing the most general solution of the equation $\mathbf{O}\ |\Psi> = 0$, iii) the demonstration of the uniqueness by concentrating on the kernel of the operator $\mathbf{O}$, and iv) the study of the physical properties of the deduced phase by calculating elevated ground state expectation values and the analysis of the low lying part of the excitation spectrum, are described in extreme details.

Keywords—Exact ground states, Hamiltonian in positive semidefinite form, Non-integrable systems, Quantum mechanical many-body systems.

I. INTRODUCTION

THIS paper describes a procedure which can be used for deducing exact ground states for non-integrable quantum mechanical many-body systems. I start by recapitulating some basic concepts needed in the description process of physical systems.

A. A B. bout Description of Physical Systems

Let us fix first the notations which will be often used below. The lower bound of a spectrum LB($\mathbf{A}$) of an operator $\mathbf{A}$ is defined as follows: If $\mathbf{A}$ is an arbitrary self-adjoint operator, all its eigenvalues a(i) give together the spectrum of $\mathbf{A}$, namely Spec($\mathbf{A}$)={a(1),a(2),a(3),...}. The value LB($\mathbf{A}$) is defined as the minimum component of Spec($\mathbf{A}$).

In principle LB($\mathbf{A}$) must not be finite, but a Hamiltonian $\mathbf{H}$(S), describing a real physical system S, has always a spectrum which is bounded below by a finite bound because S exists. The lower bound of the spectrum LB($\mathbf{H}$(S)) is the ground state energy $E_{S,g}$, hence

$$H(S) - E_{S,g} = \mathbf{O}(S), \qquad (1)$$

holds, where $\mathbf{O}$(S) represents an operator which besides

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the fact that it is intimately connected to the system S, supplementary possesses the property that do not has negative eigenvalues. Please note that (1) is valid independent on dimensionality or integrability. This is the reason why this simple relation represents one of the main starting points in the non-approximated study of non-integrable many-body systems.

Studying S, if one has the possibility to know and hence to work with $\mathbf{O}$(S) instead of $\mathbf{H}$(S), this has several advantages. First, $\mathbf{O}$(S), as the starting $\mathbf{H}$(S), has the spectrum bounded below by a finite value. But contrary to the Hamiltonian – whose LB($\mathbf{H}$(S)) is usually unknown -, $\mathbf{O}$(S) has a known (i.e. zero) spectrum's lower bound, namely LB($\mathbf{O}$(S))=0. Second, given by the above mentioned property, the ground state of S at total number of particles N, namely $|\Psi_{S,N,g}>$, can be obtained simply by deducing the most general solution of the equation

$$\mathbf{O}(S)|\Psi_{S,N,g}>=0. \qquad (2)$$

Since several techniques [1]-[6] have been worked out for solving an equation of the type (2), the observations presented above suggest a procedure. This, via (2), can lead to the deduction possibility of the N-dependent, and non-approximated ground states. I further note that because of the N-dependence, such results also provide non-approximated information relating the low laying part of the excitation spectrum. Indeed, if $E_{S,N,g}$ is the eigenvalue corresponding to $|\Psi_{S,N,g}>$, the particle number dependent chemical potential μ(S,N+1)= $E_{S,N+1,g}$ - $E_{S,N,g}$, and for example the charge gap can be expressed as $\Delta = \mu$(S,N+1)-μ(S,N). Consequently, Δ=0 signals metallic characteristics, otherwise if $\Delta \neq 0$, the system is insulating. The spin gap can be similarly expressed. Σ_i

C. B. Positive Semidefinite Operators

Let us analyze below the connection of the properties presented above to the system Hamiltonians. The positive semidefinite operators emerge in this technique via (1). In fact, the operator $\mathbf{O}$(S) in (1) is a positive semidefinite operator $\mathbf{O}$. In fact, from mathematical point of view, the definition of $\mathbf{O}$ is more complicated, namely: For a Hilbert space H, if for all $|\varphi>$ components of H the expectation value $<\varphi\ |\mathbf{O}|\varphi>$ is non-negative, i.e.

$$<\varphi\ |\mathbf{O}|\varphi> \geq 0, \qquad (3)$$

than $\mathbf{O}$ is called to be a positive semidefinite operator. Now based on (3), a simple Lemma arrises, (Lemma 1): The non-negative eigenvalues requirement is a necessary and sufficient condition for $\mathbf{O}$ to be a positive semidefinite operator. The Proof of this statement is quite simple. Indeed,

from (3) it results that all eigenvalues λ_i of **O** are non-negative, i.e. $\lambda_i \geq 0$ holds. Furthermore, easily can be checked that if one negative eigenvalue, say λ', exists corresponding to the eigenfunction $|x'>$, than (3) calculated with $|x'>$ is no more satisfied. Consequently, the non-negative eigenvalues requirement is indeed a necessary and sufficient condition for **O** to be a positive semidefinite operator.

It results that **O**(S) from (1) is indeed a positive semidefinite operator, and since $E_{S,g}$ is a scalar C, the following theorem applies:

Theorem 1. All Hamiltonians **H**(S) describing real physical systems S can be written in the form

$$\mathbf{H}(S)= \mathbf{O} + C \qquad\qquad (4)$$

where **O** is a positive semidefinite operator and C a scalar. In this case, the equation for the ground state becomes of the form $\mathbf{O}|\Psi >=0$.

The Proof of the theorem is relatively simple. Indeed, based on (1), the scalar nature of $E_{S,g}$, and Lemma 1, the equality (4) automatically holds. Furthermore, since the lowest possible eigenvalue of a positive semidefinite operator is zero, see also (2), the presented equation for the ground state arrises. Q.E.D.

Note that Theorem 1. is independent on integrability and dimensionality. Hence, we can use it as a starting point in the exact study of non-integrable quantum mechanical many-body systems. This paper is devoted to the detailed presentation of this procedure.

C. The Matching Equations

In what will follows, I show that (4) has a direct algebraic consequence. This results as follows. When one transforms the Hamiltonian in positive semidefinite form as requested by (4), one uses some positive semidefinite operators, which have their own numerical parameters (coefficients) denoted hereafter by v_i. Besides, in the left side of (4), the Hamiltonian has its own physical parameters (i.e. coupling constants), as for example hopping matrix elements $t_{i,}$, on-site one particle potentials ϵ_i, and interaction strenghts $U_{i.}$ In these conditions it is easy to understand that (4) holds only if a given relationship exists in between the positive semidefinite operator parameters $\{v_i\}$, and Hamiltonian parameters hereafter denoted by $\Lambda[\mathbf{H}(S)]= \Lambda(\{t_{i,}\},\{\epsilon_i\},\{U_i\})$.

Consequently, one can state that the transformation relation (4) holds only if a relation exists between $\Lambda(\{t_{i,}\},\{\epsilon_i\},\{U_i\})$ and the parameters $P(\{v_i\},C)$, where C is the scalar in (4). This relationship (let denote it by F) which formally can be written as

$$\Lambda(\{t_{i,}\},\{\epsilon_i\},\{U_i\})=F[P(\{v_i\},C)] \qquad (5)$$

is called to be the matching system of equations. The matching equations usually represent a non-linear, coupled and complex algebraic system of equations. The non-linearity emerges because $\{v_i\}$ are usually numerical parameters of an operator **A**, from which, in the majority of cases $\mathbf{A}^+\mathbf{A}$ provides the positive semidefinite form. The complex algebraic nature

arises simply from the fact that there is no reason to restrict the variation domain of the parameters $\{v_i\}$ to a real manyfold.

Consequently, a given transformation of a Hamiltonian in positive semidefinite form (4) has its own matching equations (5), and the transformation of **H**(S) via (4) is valid only if the matching equations are satisfied, i.e. allow solutions. This information provides two main aspects which need to be underlined below, namely:

I) When the transformation of the Hamiltonian via (4) is done, the explicit expression of the scalar C need not be known, and in fact is not known explicitly. One has only the matching equations for it. This is important to be underlined, because as originating from (2) and mentioned below (4), the $\mathbf{O}|\Psi>=0$ will provide the N-dependent ground state wave vector $| \Psi_{S,N,g} >$, and the corresponding ground state energy becomes $E_{S,N,g} = C$ at the end of the calculations. At this stage it is important to stress that contrary to what (1) suggests at first view, the ground state energy is not known when the transformation in positive semidefinite form (4) is performed.

II) The non-linear system of equations (5) allows usually solutions only in a restricted parameter space region Λ_α of $\Lambda[\mathbf{H}(S)]$. This means that the transformation in positive semidefinite form of the Hamiltonian as shown in (4), can be performed in several different ways. Each transformation of this kind places us in a restricted parameter space region, where and only where, the deduced ground state wave vector together with its eigenvalue will be valid. In order to reach another parameter space region, another transformation in positive semidefinite form must be done, or another solution of the matching equations must be obtained. This motivates the difference in notations of the positive semidefinite operator in (1) – i.e. **O**(S) -, and (4) – i.e. **O** -. As a consequence the following property (Lemma 2) holds: The functional form of **O**(S) can change in different parameter space regions of the Hamiltonian. Namely, if Λ_α represents a given restricted Hamiltonian parameter space domain where the matching equations (5) present an individual solution, and if besides $\Lambda_\alpha \cap \Lambda_\beta = \emptyset$ at $\alpha \neq \beta$, one has $\Lambda[\mathbf{H}(S)] = \Lambda_1 \cup \Lambda_2 \cup \Lambda_3 \cup \Lambda_4 \cup ..... \cup \Lambda_n$, than

$$\mathbf{O}(S)=\mathbf{O}_\alpha \text{ in } \Lambda_\alpha , \alpha=1,2,3,.....,n. \qquad (6)$$

The Proof of this lemma is obvious. Indeed, a given individual solution of the matching equations, since fixes the expression of the positive semidefinite operator parameters, provides an individual $\mathbf{O}_\alpha$. Consequently, if the solution of (5) changes, also the positive semidefinite operators from (4) changes. In these conditions, for $\Lambda_\alpha \cap \Lambda_\beta = \emptyset$ at $\alpha \neq \beta$ and $\Lambda[\mathbf{H}(S)] = \Lambda_1 \cup \Lambda_2 \cup \Lambda_3 \cup \Lambda_4 \cup ..... \cup \Lambda_n$, the relation (6) automatically arises. Q.E.D.

This result shows that contrary to integrable cases where the whole solution and spectrum can be deduced in a single mathematical frame, in non-integrable cases, the ground state characteristics can be obtained only as a collection of different solutions valid in different restricted parameter space regions.

D. Non-integrable Systems

The introductory part of this material must also specify why it is important to analyze in a non-approximated manner non-integrable systems. I start by mentioning that contrary to what this name suggests, the notion *non-integrable* has nothing to do with the possibility to write a solution. Integrability in fact represents a supplementary constraint imposed to many-body systems. In a simplified view it requires an equal number of constants of motion (N_{CM}) and degrees of freedom (N_{DF}). As it is known, in many-body case N_{DF} has the order of magnitude of Avogadro's number, while usually in nature, N_{CM} = O(10). This means that integrability occurs only in quite special, and mostly one dimensional cases, and in fact in nature, 99% of real systems are non- integrable. This motivates the need to analyze non-integrable
systems.

The non-approximated nature refers to an exact model solution. Besides the situations where often poor approximations fail (e.g. the interaction value is high or strong correlation effects are present), its importance is underlined by the fact that exact results are important bench-marks of a given field. This is because they provide testing,, checking and developing possibilities for model descriptions, numerical procedures, and approximation schemes as well.

On the mentioned frame one must observe that the field of exact results for quantum mechanical many-body systems has a huge literature [7],[8]. But this literature is almost entirely connected to integrable systems. For non-integrable systems the exact results are extremely rare, and deduction techniques are practically missing. This is why the development of methods able to provide non-approximated results for such systems is of extreme importance. This demand is also underlined by the following aspect: Based on the till today published exact results relating integrable systems, one has an extended good quality picture about how these systems indeed behave. Now generated by these state of facts, the following question arises: Based on this image do we see properly how the systems in nature behave ? The studies which show tha the integrable systems evolve in time and thermalize [9]-[12] in a specific way given by the extensive amount of conserved quantities induced by integrability [13]-[16], and hence have non-ergodic characteristics in their behavior [17], [18] underline a negative answer to this question. Consequently, non-approximated results for non-integrable system cannot be avoided or substituted with something else in our aim to understand the nature.

The remaining part of the paper in Section 2 describes in details the deduction technique leading to non-approximated ground states for non-integrable systems originating from the background described above, and finally Section 3 containing a short summary and conclusions closes the presentation.

II. THE DEDUCTION METHOD

I describe below in details a deduction procedure of exact total particle number dependent ground states for non-

integrable quantum mechanical many-body systems. The aim of this presentation is to underline indeed the *method* character of the technique, i.e. to provide as much as possible know-how information at each step of the procedure. This requirement is motivated by the fact that otherwise, one remains only at the level of potential *gedanken* eventuality, placed far away from application possibilities.

A. The First Step: the Transformation of the Hamiltonian

We consider for exemplifications below Hamiltonians defined on a lattice or a graph.

1. The first topic which will be analyzed below is connected to the question: How we cast the Hamiltonian in positive semidefinite form ?

As it was mentioned before in the Introduction, the first step of the procedure transforms in exact terms the system Hamiltonian $\mathbf{H}(S)$ into a positive semidefinite form as required by (4). For this transformation one uses usually two type of operators, namely:

i) Positive semidefinite operators of the type

$\mathbf{I}_{1,i} = \Sigma_\gamma \mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$, where $\mathbf{A}_{i,\gamma}$ is an operator constructed on a finite block surrounding the site i, hence it represents in fact a *block operator*. At the level of a definition, the block operator $\mathbf{A}_{i,\gamma}$ is an algebraic sum over different operators $\mathbf{a}(i_n)$ acting on the site i_n placed in the block $B_{i,\gamma}$ connected to the site i. Based on this definition one has

$$\mathbf{A}_{i,\gamma} = \Sigma_j \ \alpha_{j,\gamma} \ \mathbf{a}(j,\gamma) \qquad\qquad (7)$$

where the sum over the j index covers all the sites $\{i_n\}$ from the block $B_{i,\gamma}$ constructed around the site i, the coefficients $\alpha_{j,\gamma}$ are numerical prefactors. I note that these numerical prefactors have been denoted in a condensed form as ν_i in (5), because via $\mathbf{I}_{1,i}$ they become positive semidefinite operator parameters. The γ index preserves the possibility to construct b different blocks connected to the site i, γ=1,2,...,b.

The positive semidefinite nature in this case is automatically provided by the $\mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$ construction. Please note that the sum of positive semidefinite operators is also a positive semidefinite operator, hence $\mathbf{O}$ is often expressed as a sum over several positive semidefinite contributions (i.e. sum over i in $\mathbf{I}_{1,i}$ is usually present).

ii) Positive semidefinite operators $\mathbf{I}_{2,i}$ which do not have the form $\mathbf{A}^+ \mathbf{A}$, where $\mathbf{A}$ is an arbitrary operator and $\mathbf{A}^+$ its adjoint. In order to exemplify, I note that for example in the fermionic case which is taken as example in this paper, the construction $\mathbf{P}_i = \mathbf{n}_{i,\uparrow} \ \mathbf{n}_{i,\downarrow} - (\mathbf{n}_{i,\uparrow} + \mathbf{n}_{i,\downarrow}) + 1$, where $\mathbf{n}_{i,\sigma} = \mathbf{c}^+_{i,\sigma} \mathbf{c}_{i,\sigma}$ is the particle number operator and $\mathbf{c}^+_{i,\sigma}$, $\mathbf{c}_{i,\sigma}$ are canonical Fermi operators (with σ being the spin index), is a positive semidefinite operator which attains its minimum eigenvalue zero when at least one fermion is present on the site i. Furthermore, the operator $\mathbf{D}_i = \mathbf{n}_{i,\uparrow} \ \mathbf{n}_{i,\downarrow}$ is also a positive semidefinite operator with minimum eigenvalue zero when there is no double occupancy present on the site i, etc.

From the above presented information the following

straightforward theorem arises:

Theorem 2. The positive semidefinite operator **O** from the right side of (4) has always the following form

$$\mathbf{O} = \mathbf{I}_1 + \mathbf{I}_2 , \quad \mathbf{I}_1 = \Sigma_\gamma \mathbf{I}_{1,\gamma}, \quad \mathbf{I}_2 = \Sigma_\gamma \mathbf{I}_{2,\gamma}, \qquad (8)$$

where $\mathbf{I}_{1,\gamma}$ and $\mathbf{I}_{2,\gamma}$ are specified at points i) and ii) above.

The Proof is quite simple. Indeed, a positive semidefinite operator or has the form $\mathbf{A}^+ \mathbf{A}$, or not, from where (8) arises. Q.E.D.

Several examples illustrating (8) in concrete cases can be seen in published results [1]-[6], [19]-[24] describing cases of real interest [25],[26].

At this level several questions arise, for example: What is the shape of $B_{i,\gamma}$?, How big should it be ? What is the number b of different blocks that must be chosen at a given lattice site ? The answers to these questions depend on the Hamiltonian. But there are several useful observation which drive the transformation of the Hamiltonian as follows:

a) For a fixed γ index, $B_{i,\gamma}$, hence $\mathbf{A}_{i,\gamma}$ is such chosen

to obtain an $\mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$ expression which reproduces as much as possible terms of the starting Hamiltonian **H**(S). For example if **H**(S) has only short range hopping terms, the block $B_{i,\gamma}$ must be small, since otherwise, the product $\mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$ introduces long range hopping contributions which are not present in the starting Hamiltonian. But independent of how many care and precaution is taken, at fixed γ and $B_{i,\gamma}$, usually $\mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$ introduces operator terms which are not present in **H**(S). These must be canceled out. This is the reason why connected to the same site i, another block $B_{i,\gamma'}$, $\gamma \neq \gamma'$, or even other blocks have to be introduced.

Let us have an example on this line. For this reason let consider the system S=S_1 a square Bravais lattice with Bravais vectors $\bar{a}_x$, $\bar{a}_y$. At the lattice site i one defines the first block, say $B_{i,\gamma=1}$, to be an elementary plaquette containing four sites, namely (i, i+ $\bar{a}_x$, i+ $\bar{a}_y$, i+$\bar{a}_x$+ $\bar{a}_y$). Furthermore one considers (for simplicity in a spinless fermion case, and only linear combination of fermionic operators in the block operator),

$$\mathbf{A}_{i,\gamma=1} = a_1 \mathbf{c}_i + a_2 \mathbf{c}_{i+\bar{a}x} + a_3 \mathbf{c}_{i+\bar{a}y} + a_4 \mathbf{c}_{i+\bar{a}x+\bar{a}y}, \qquad (9)$$

where a_1, a_2, a_3, a_4 are numerical scalar prefactors. In these conditions, the product $\mathbf{A}^+_{i,\gamma=1}\mathbf{A}i,\gamma=1$ creates terms of the form $a^*_1 a_4 \mathbf{c}^+_i \mathbf{c}_{i+\bar{a}x+\bar{a}y} + a^*_3 a_2 \mathbf{c}^+_{i+\bar{a}x} \mathbf{c}_{i+\bar{a}y}$ + H.c. (here H.c. represents the Hermitic conjugate), which represent next-nearest neighbor hopping terms. If such hoppings are not present in the starting Hamiltonian **H**(S), they must be canceled out. This can be done by introducing two more block operators at the same lattice site I. These are defined on two new blocks, namely $B_{i,\gamma=2}$ containing the sites (i, i+ $\bar{a}_x$, i+ $\bar{a}_x$ + $\bar{a}_y$), and $B_{i,\gamma=3}$ containing the sites (i, i+ $\bar{a}_x$, i+ $\bar{a}_y$). These triangular blocks will have the block operators

$$\mathbf{A}_{i,\gamma=2} = e_1 \mathbf{c}_i + e_2 \mathbf{c}_{i+\bar{a}x} + e_4 \mathbf{c}_{i+\bar{a}x+\bar{a}y},$$

$$\mathbf{A}_{i,\gamma=3} = f_1 \mathbf{c}_i + f_2 \mathbf{c}_{i+\bar{a}x} + f_3 \mathbf{c}_{i+\bar{a}y}, \qquad (10)$$

where e_α, $\alpha=1,2,4$ and f_β, $\beta=1,2,3$ are new numerical scalar prefactors. The products $\mathbf{A}^+_{i,\gamma=2} \mathbf{A}_{i,\gamma=2}$ and $\mathbf{A}^+_{i,\gamma=3} \mathbf{A}_{i,\gamma=3}$ will create the next-nearest neighbor hoppings obtained also previously, but now in the form $e^*_1 e_4 \mathbf{c}^+_i \mathbf{c}_{i+\bar{a}x+\bar{a}y} + f^*_3 f_2 \mathbf{c}^+_{i+\bar{a}x} \mathbf{c}_{i+\bar{a}y}$ + H.c. Hence taking

$$a^*_1 a_{4+} e^*_1 e_4 =0, \quad a^*_3 a_2 + f^*_3 f_2 = 0, \qquad (11)$$

we cancel out the not desired terms of **O**. Similarly, other type of cancellations also can be done.

We further note that the $\mathbf{I}_2$ contributions, see (8), are taken into account in order to introduce specific Hamiltonian contributions in **O**, and the transformation (4) is performed usually by taking periodic boundary conditions into consideration. The coefficients $\alpha_{j,\gamma}$ in (7) are considered the same in similar blocks defined at different lattice sites, given by the presence of the Bravais translational symmetry in the regular lattice cases. But such coefficients can be different and even plaquette dependent when a random disordered system is analyzed (see for example [1]). I also underline that in some cases, it is advantageous to achieve the positive semidefinite structure in $\mathbf{I}_1$ via a construction of the type $\mathbf{A}_{i,\gamma} \mathbf{A}^+_{i,\gamma}$. The reason will be visible in the Sectio II.2.

2. The second topic which must be analyzed here is connected to the matching equations. These represent relationships in which the positive semidefinite operator parameters and/or Hamiltonian parameters are present and preserve the validity of the transformation (4). As such, for the system S_1 presented previously, the equalities from (11) are part of the matching equations.

In general, the matching equations (5) are obtained by calculating in a first stage, effectively and explicitly, the right side of (8). One obtains a sum of different operators holding prefactors dependent on positive semidefinite operator coefficients v_i entering in P from (5) [in the previously presented example relating S_1, the v_i parameters are the coefficients a_α, e_α, and f_α present in (9)-(11)]. The same operators are present in **H**(S), but in the Hamiltonian, the numerical prefactors are the Hamiltonian parameters entering in Λ[**H**(S)] used in (5). Finally, the matching equations are obtained by taking equal the coefficients of the same operator in the left and right (4). For example, using the blocks $B_{i,\gamma}$, $\gamma=1,2,3$ introduced previously in the study of S_1, taking in **O** the sum contribution $\mathbf{I}_1 = \Sigma_i \Sigma_{\gamma=1,2,3} \mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$, the hopping matrix element t_y of the Hamiltonian $t_y \mathbf{c}^+_i \mathbf{c}_{i+\bar{a}y}$ becomes

$$t_y = a^*_1 a_3 + f^*_1 f_3 + e^*_2 e_4. \qquad (12)$$

This is because the operator $\mathbf{c}^+_i \mathbf{c}_{i+\bar{a}y}$ is obtained from $\mathbf{I}_1$ only in three places, namely with coefficient $a^*_1 a_3$ from $\mathbf{A}^+_{i,\gamma=1}\mathbf{A}i,\gamma=1$, with coefficient $f^*_1 f_3$ from $\mathbf{A}^+_{i,\gamma=3} \mathbf{A}_{i,\gamma=3}$, and finally with coefficient $e^*_2 e_4$ from $\mathbf{A}^+_{i,\gamma=2} \mathbf{A}_{i,\gamma=2}$. In the same way, for the Hamiltonian hopping term $t_x \mathbf{c}^+_i \mathbf{c}_{i+\bar{a}x}$ one finds

$$t_x = a^*_1 a_2 + e^*_1 e_2 + f^*_1 f_2 , \qquad (13)$$

where in order, the added terms in t_x appear in $\mathbf{I}_1$ from $\mathbf{A}^+_{i,\gamma}$ $\mathbf{A}_{i,\gamma}$ at $\gamma=1,2,3$. Similarly, all equations of (5) can be obtained, which means that all Hamiltonian parameters and the scalar C from (4) become to be expressed as a function of positive semidefinite operator parameters. Turning back to (11) and compairing it to (12),(13), I mention that the equations (11) have zero in the right side simply because plaquette diagonal (i.e. next-nearest neighbor) hopping terms as t_{y+x} , t_{y-x} , are missing from $\mathbf{H}(S)$, i.e. $t_{y+x} = t_{y-x} =0$ holds.

Consequently, for exemplifying how the matching equations are obtained, we presented the deduction of 4 of such equations in (11)-(13) connected to the system S_1 . Several complete examples you can find in published results, see e.g. [1]-[6], [19]-[24].

I further note that the resulting matching equations are nonlinear in the unknown positive semidefinite operator parameters. These equations in several cases can be analytically solved (see for example [3] for exemplification). For solutions in complicated situations stochastic methods can be used [27].

B. The Second Step: the Construction of the Ground State Wave Function

In constructing the ground state wave vector we already know explicitly the $\mathbf{O}$ structure from (8). Based on it, as explained below (4), we are looking for the most general wave vector $|\Psi\rangle$ which satisfies $\mathbf{O}$ $|\Psi\rangle =0$. If we find this wave function, we have the ground state $|\Psi_g\rangle$ in our hands, the corresponding ground state energy being $E_g =C$, where C is the scalar from (4). Insights about how this job effectively can be done, are presented in this subsection. We will analyze here three different cases in three different concentration regions, and for simplicity one considers the block operators as linear combinations of the starting canonical Fermi operators $c_{i,\sigma}$.

1. First case: low concentration of carriers
In this case $\mathbf{I}_1$ is constructed as shown in Section II.A. at point I), namely as $\mathbf{I}_1 = \Sigma_i \Sigma_\gamma \mathbf{A}^+_{i,\gamma} \mathbf{A}_{i,\gamma}$. Why this case is connected to the low concentration limit, will be clarified further on.

In the presented case the construction of the ground state begins with the construction of the wave vector $|\Psi_1\rangle$ satisfying the condition $\mathbf{I}_1 |\Psi_1\rangle =0$. Since $|\Psi_1\rangle$ contains particles, it must has the form

$$|\Psi_1\rangle = \prod_{\beta \in X} \mathbf{B}^+_\beta |0\rangle , \qquad (14)$$

where the index β covers a manifold X and denotes different (i.e. linearly independent) operators $\mathbf{B}^+$, $|0\rangle$ denotes the bare Fock vacuum with no fermions present [i.e. for the operator $\mathbf{A}_{i,\gamma}$ containing only annihilation terms, one has $\mathbf{A}_{i,\gamma} |0\rangle =0$ independent on indices (i,γ)]. Finally, $\mathbf{B}^+_\beta$ is an algebraic sum of creation operators, i.e. in a general spinfull case

$$\mathbf{B}^+_{i,\sigma,\delta} \quad = \quad \Sigma_j \quad b_{j,\sigma,\delta} \quad c^+_{j,\sigma} \quad .$$

(15)

Comparing to (7), one observes that $\mathbf{B}^+_{i,\sigma,\delta}$ is in fact a block operator where the index δ plays the role of γ in (7). As observed, the β index in (14) represents in fact a collection of indices $\beta =(j,\sigma, \delta)$, and b_β are numerical coefficients. The site index j from (15) covers a block $C_{i,\delta}$ on which the block operator $\mathbf{B}^+_{i,\sigma,\delta}$ defined. But I underline that the block $C_{i,\delta}$ is usually completely different from the block $B_{i,\gamma}$ present in (7).

In these conditions, the needed

$$\mathbf{I}_1 |\Psi_1\rangle =0 \qquad (16)$$

condition is satisfied, if we have the possibility to push the $\mathbf{A}_{i,\gamma}$ operators placed in the right side of $\mathbf{I}_1$, in front of the $\mathbf{B}^+_\beta$ operators present in (14). If this can be done, one pushes in fact the $\mathbf{A}_{i,\gamma}$ operators in front of the vacuum state obtaining by this shift $\mathbf{A}_{i,\gamma} |0\rangle$, which by definition is zero. But this to be possible (note that we are in the fermionic case), one must has the anti-commutation relation

$$\{\mathbf{A}_{i,\gamma}, \ \mathbf{B}^+_{i,',\sigma,\delta} \} =0 \qquad (17)$$

satisfied for all values of all indices. This is the prescription under which the operators $\mathbf{B}^+_\beta$ can be deduced. This means that based on (17) one can deduce the sites of the block $C_{i,\delta}$ on which the operator $\mathbf{B}^+_{i,\sigma,\delta}$ is defined, and in the same time one can deduce the numerical prefactors $b_{j,\sigma,\delta}$ present in (15). Based on this strategy, once one has the explicit $\mathbf{B}^+_{i,\sigma,\delta}$ operators, the half of the job to solve the $\mathbf{O}$ $|\Psi\rangle=0$ equation has been effectuated. This is because with (8) and (16), one has by $|\Psi_1\rangle$ a good starting point for $|\Psi\rangle$. After this result, the second half of the job follows, namely to modify $|\Psi_1\rangle$ in the wave vector $|\Psi_2\rangle$ (i.e. perform $|\Psi_1\rangle \to |\Psi_2\rangle$), such to not alter the relation $\mathbf{I}_1 |\Psi_2\rangle =0$, and supplementary to have besides it also the equality $\mathbf{I}_2|\Psi_2\rangle =0$ satisfied. In other words, in mathematical terms , we have to push $|\Psi_1\rangle$ (which at the moment is placed only in the kernel of $\mathbf{I}_1$) also in the kernel of $\mathbf{I}_2$. In order to do this job one observes that given by (17), all individual components β from $|\Psi_1\rangle$ in (14) satisfy individually the equality $\mathbf{I}_1 \mathbf{B}^+_\beta |0\rangle=0$. This means that by a restriction of the manifold X (see (14)) to a subset $Y\epsilon X$, we not alter the relation (16), but we modify $|\Psi_1\rangle \to |\Psi_2\rangle$ maintaining $\mathbf{I}_1 |\Psi_2\rangle =0$. Using this procedure, by a restriction of the manifold X to the manifold Y, we obtain

$$|\Psi_2\rangle = \prod_{\beta \in Y} \mathbf{B}^+_\beta |0\rangle , \qquad (18)$$

where now β covers the manifold Y, and $|\Psi_2\rangle$ from (18), besides $\mathbf{I}_1 |\Psi_2\rangle =0$, satisfies also $\mathbf{I}_2 |\Psi_2\rangle =0$. Consequently, taking into account (8), $\mathbf{O} |\Psi_2\rangle=0$ holds, hence the ground state becomes

$$|\Psi_{S,N,g}\rangle = |\Psi_2\rangle = \prod_{\beta \in Y} \mathbf{B}^+_\beta |0\rangle . \qquad (19)$$

At this stage we have to provide information about N, the total number of particles entering in the ground state (19). On this line I mention that, since $\mathbf{B}^{+}_{\beta}$ is a linear combination of canonical creation operators, one $\mathbf{B}^{+}_{\beta}$ operator introduces one particle into the system, consequently N represents the number of components of the manifold Y. Different β contributions in (14), for example in space periodic systems, are obtained by the translation of $\mathbf{B}^{+}_{\beta=1}$ to other sites. This means that in this case, the number of different β indices usually cannot exceed the number of lattice sites, and their number in (18) is further decreased by the reduction X → Y. As a consequence, the concentration of particles for the here treated 1. ``first case" is placed below system half filling, which means in fact low concentration.

Examples of deduced ground states of the presented kind can be found e.g. in [3], [19]-[23].

2. Second case: high concentration of carriers

In this situation, $\mathbf{I}_1$ is constructed (in the spinfull case) as $\mathbf{I}_1 = \Sigma_{i,\sigma,\gamma} \mathbf{A}_{i,\sigma,\gamma} \mathbf{A}^{+}_{i,\sigma,\gamma}$. Why this case is connected to the high concentration limit will be visible only at the end of this subsection.

The construction of the ground states in this situation differs considerably from the construction procedure used in the previous subsection 1. But the strategy is similar, namely we first obtain a wave vector $|\Psi_3\rangle$ such to satisfy $\mathbf{I}_1 |\Psi_3\rangle = 0$, and after this stage, by $|\Psi_3\rangle \rightarrow |\Psi_4\rangle$, we introduce the deduced wave vector also into the kernel of $\mathbf{I}_2$ such to obtain besides $\mathbf{I}_1 |\Psi_4\rangle = 0$, also the relation $\mathbf{I}_2 |\Psi_4\rangle = 0$, satisfying in this manner $\mathbf{O} |\Psi_4\rangle = 0$.

Taking into account again in block operators only linear combination of fermionic operators as in the low concentration limit, now the starting form of the constructed wave function becomes

$$|\Psi_3\rangle = \prod_{\eta} \mathbf{A}^{+}_{\eta} |0\rangle \ , \qquad (20)$$

where the index η is a combined index of all indices present on the $\mathbf{A}$ operators, i.e. $\eta = (i,\sigma,\gamma)$. The motivation for the structure of (20) is that now, because $\mathbf{A}^{+}_{\eta} \mathbf{A}^{+}_{\eta} = 0$ holds for all values of all indices, based on (20), the relations

$$\mathbf{I}_1 |\Psi_3\rangle = 0, \qquad (21)$$

is automatically satisfied. The second novelty which appears here is that now a reduction of indices in (20) is no more possible, because eliminating at least one term from the product in (20), the requested relation (21) will be not satisfied. So in the present situation, the modification of $|\Psi_3\rangle$ such to not alter (21) cannot be done by index reduction. But, since only creation operators are acting on the vacuum state in (20), and these anticommute in between them by definition, adding creation operators to (20) (these must be linearly independent on all $\mathbf{A}^{+}_{\eta}$ operators present in $|\Psi_3\rangle$), the equation (21) remains non-altered. Consequently, the

transformation $|\Psi_3\rangle \rightarrow |\Psi_4\rangle$ in the present case must be done as follows

$$|\Psi_4\rangle = (\prod_{\eta} \mathbf{A}^{+}_{\eta}) \mathbf{G}^{+} |0\rangle \ . \qquad (22)$$

Here $\mathbf{G}^{+}$ contains only creation operators such that the norm of $|\Psi_4\rangle$ remains finite. I underline that as explained previously, besides (21), the relation $\mathbf{I}_1 |\Psi_4\rangle = 0$ is also satisfied. The advantage of new vector presented in (22) is that it gives the possibility to modify $|\Psi_3\rangle$ in such a way to introduce it (besides the kernel of $\mathbf{I}_1$) also in the kernel of $\mathbf{I}_2$. In this manner, by properly choosing $\mathbf{G}^{+}$, one obtains as well the equality $\mathbf{I}_2 |\Psi_4\rangle = 0$, i.e. $\mathbf{O} |\Psi_4\rangle = 0$. Consequently, the ground state wave function becomes

$$|\Psi'_{S,N',g}\rangle = |\Psi_4\rangle = (\prod_{\eta} \mathbf{A}^{+}_{\eta}) \mathbf{G}^{+} |0\rangle. \qquad (23)$$

How the operator $\mathbf{G}^{+}$ looks like, depends on the system S. For $\mathbf{G}^{+}$ explicit expressions several examples are present in the published literature e.g. [3],[5],[19],[20],[22],[23].

Concerning N', the total number of particles in (23), one uses first the observation that $\mathbf{A}^{+}_{\eta}$ (being in the present case a linear combination of creation canonical Fermi operators) introduces one fermion into the system. Furthermore, since $\eta = (i,\sigma,\gamma)$ contains the lattice site index i, the number of $\mathbf{A}^{+}_{\eta}$ operators in (23) is usually higher than the number of lattice sites. Besides, $\mathbf{G}^{+}$ also introduces fermions into the system, so certainly, the number of particles in (22) is placed well above the system half filling value. Hence N' corresponds to high concentrations.

Deduced ground states of the presented kind can be seen e.g. in [3],[5],[19],[20],[22],[23],[28].

3. Third case: system half filling

When the system is half filled, the correlation effects are accentuated, hence the construction of the ground state wave vector needs supplementary attention. The construction procedure in this situation usually follows the first part of the strategy used in the low concentration case, point 1. Namely, with $\mathbf{I}_1 = \Sigma_i \Sigma_\gamma \mathbf{A}^{+}_{i,\gamma} \mathbf{A}_{i,\gamma}$, the starting wave function uses the operators $\mathbf{B}^{+}_{\beta}$ deduced from the anti-commutation relation (17). Hence, the starting form of the constructed ground state becomes $|\Psi_1\rangle$ from (14), consequently (16) will be satisfied. But now, contrary to the usual case encountered at point 1., where $\mathbf{B}^{+}_{\beta}$ was defined on a finite block, the solutions of (17) are mostly extended operators i.e. the blocks on which these operators are defined extend along the whole system (however, these blocks usually contain only a percentage of the total number of lattice sites). Further novelty appears in the procedure, since at the presented concentration value the index reduction [as given in (18)] usually is not possible to be applied. This is because the index reduction decreases the number of carriers from the wave function, consequently it pushes the ground state in the below half filling concentration region. In this conditions, the $|\Psi_1\rangle \rightarrow |\Psi_2\rangle$ step, i.e. the

introduction of the constructed wave vector also in the kernel of $\mathbf{I_2}$, is given by the technique

$$|\Psi_2> = \Sigma_\beta \; \Sigma_{\beta'} \; a_{\beta,\beta'} \; \Pi_\beta \; \Pi_{\beta'} \; \mathbf{B^+}_\beta \; \mathbf{B^+}_{\beta'} \; |0>, \qquad (24)$$

where $a_{\beta,\beta'}$ are numerical coefficients, β covers the manifold X_β and β' the manifold $X_{\beta'}$, furthermore the number of operators in each additive term from (24) is maintained at a constant value corresponding to half filling. The $a_{\beta,\beta'}$ numerical pre-factors are deduced from the $\mathbf{I_2} |\Psi_2>=0$ condition. Please note that since each individual $\mathbf{B^+}_\beta$ operator satisfies (17), the condition $\mathbf{I_1} |\Psi_2>=0$ automatically holds.

Consequently, the deduced ground state will have the form presented in (24). A pedagogical example of a such type of solution is presented [24].

However extended operators in the ground state wave vector appear also outside of half filling (see e.g. [32],[34],[39]-[41]), the main difficulty in treating the system half filling case is connected to the treatment possibilities of the extended operators that one has at disposal. Developments in handling such operators is badly needed.

C. The Third Step: The Proof of the Uniqueness

The proof of the uniqueness in the case of exact solutions is an important task, which often, even in integrable cases, is difficult to be effectuated. For example one knows integrable cases, were it turns out that not all solutions have Bethe ansatz form [29] (i.e. are not given by Bethe Ansatz), or in other cases, as for example the case of the integrable spin-1/2 XXZ chain, almost ten years passed from the written Bethe ansatz equations [30], and the proof of the uniqueness [31] of their solutions.

In the case of the method based on positive semidefinite operators described in details here, the proof of the uniqueness can be usually effectuated, and requires the study of the kernel of the operator $\mathbf{O}$.

At the level of a definition for the kernel: For an arbitrary operator $\mathbf{O}$, the kernel $Ker(\mathbf{O})$ is a Hilbert subspace H_K of the full Hilbert space H whose all components $|\varphi> \epsilon \; H_K$ have the property $\mathbf{O} |\varphi> = 0$.

Once the kernel notion is fixed, the uniqueness proof can be done on the line of the following Theorem:

Theorem 3. A deduced ground state wave vector $|\Psi_g>$ obtained from the equation $\mathbf{O} |\Psi_g>=0$ is unique if spans the kernel of $\mathbf{O}$, $Ker(\mathbf{O})$.

The Proof goes on the following line: Indeed, if $|\Psi_g>$ is i) inside $Ker(\mathbf{O})$, and ii) forms a base for $Ker(\mathbf{O})$, there is not present a $|\Psi'_g>$ vector which is linearly independent on $|\Psi_g>$, and satisfies $\mathbf{O} |\Psi'_g>=0$. Q.E.D.

In the light of the above Theorem, the proof of the uniqueness of a deduced ground state wave function $|\Psi_g>$ from mathematical point of view requires the proof of the following two steps, namely:
A.i) the ground state is inside the kernel, i. e. $|\Psi_g> \epsilon \; H_K$, and
A.ii) all components of the kernel can be written in term of the deduced ground state wave function, i.e. if $|\varphi> \epsilon \; H_K$, then $|\varphi> = \lambda \; |\Psi_g>$, where λ is a scalar. This uniqueness notion can be extended also in the degenerate case. In this situation, by uniqueness one understands that besides the linearly independent ground state components $|\Psi_g(m)>$, m=1,2,...,M, which together describe an M-fold degenerate ground state (i.e. m is the degeneracy index), other linearly independent $|\Psi_g(m>M)>$ wave vectors do not exist. In this case, in order to prove the uniqueness, we must demonstrate that B.i) all m components of the ground state are placed inside the kernel, i.e. $|\Psi_g(m)> \epsilon \; H_K$ for all m=1,...,M, and B.ii) all vectors of the kernel H_K can be expressed as a linear combination of the $|\Psi_g(m)>$, m=1,2,...,M, components, i.e. if $|\varphi> \epsilon \; H_K$, then $|\varphi> = \Sigma_m \; \lambda_m \; |\Psi_g(m)>$, where λ_m are scalar numerical coefficients.

Concerning the uniqueness proof, I mention that given by (2), which must be satisfied during the ground state deduction process, the points A.i) and B.i) are already demonstrated when the ground state is deduced and becomes to be known. Consequently, the uniqueness proof requires only the demonstration of the point A.ii) [or B.ii) in the degenerate case]. For demonstrating A.ii), usually one writes an arbitrary component of the kernel, and shows that it can be written in the form of the deduced ground state wave vector. In the degenerate case this technique can be such supplemented that we demonstrate that $|\Psi_g(m)>$ being inside the kernel, the transformation from $|\Psi_g(m)>$ to $|\Psi_g(m+1)>$ not moves the wave vector outside of kernel H_K, and together, all $|\Psi_g(m)>$ components span the kernel (i.e. represent a base in H_K).
Examples for the uniqueness proof can be seen e.g. in [3],[20],[23].

D. The Fourth Step: The Study of the Physical Properties

Since the ground state has been deduced without preconceptions, often it happens that its physical properties are not visible at the first view. Since the ground state at this stage is explicitly known, different ground state expectation values can be calculated with it. In this process different physical quantities and correlation functions can be deduced in a non-approximated manner (see e.g. [3]) which shed light on the physical characteristics of the studied system. As mentioned at the end of Section I.A., the deduced physical properties describe not only the ground state, but also the low lying part of the excitation spectrum.

III. SUMMARY AND CONCLUSIONS

In conditions in which non-integrable systems are attracting main interest today [5],[25],[37],[38], the presented paper describes in details the technique which allows the deduction of exact results for quantum mechanical many-body non-integrable systems. The method is based on the transcription of the Hamiltonian in positive semidefinite form, and the cons-truction of a wave vector on which we apply the obtained positive semidefinite operator and obtain zero as a result. This

technique is independent on dimensionality and integrability for Hamiltonians which describe physical systems. This is the reason why the procedure is applicable in non-integrable cases as well. The consecutive steps of the technique have been presented together with detailed know-how information, which have been exemplified with the broad spectrum of results published in the literature.

At the end of the presentation I would like to underline that the method based on positive semidefinite operators has lead to exact results for non-integrable many-body quantum systems in circumstances unimaginable before, as: disordered systems in 2D [1], stripes and droplets in 2D [21], 2D Hubbard model in the low concentration limit with consequences to nano-grains [32], multiband systems in 2D [28], delocalization effects of the interactions in 2D [4], periodic Anderson model in 3D [19],[20], non-approximated non Fermi-liquid behavior of interacting Fermi systems in 3D [20], band flattening effect of the interaction [33], non-integrable chain structures [22],[23],[39]-[42], or conducting polymers [3],[5],[34]-[36]. This new technique successfully extends the possibilities of other methods [43]-[47] used especially in the study of strongly correlated systems.
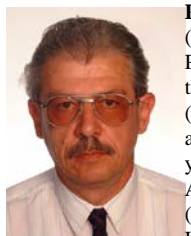
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