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# Exact results for non-integrable systems

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**Abstract.** Quantum mechanical many-body systems described by an arbitrary Hamiltonian ( $\hat{H}$ ) are analyzed. It is shown how positive semidefinite operator ( $\hat{P}$ ) properties are able to lead in this case to exact results related to the ground state and the low lying part of the excitation spectrum. This is done independent on dimensionality and integrability. The technique first casts the Hamiltonian in a positive semidefinite form in exact terms ( $\hat{H} = \hat{P} + C$ , where  $C$  is a scalar). Second, the ground state is deduced by constructing the most general Hilbert space vector, on which applying  $\hat{P}$ , one obtains zero as a result. It is underlined, that the procedure, if applied for variable total number of particles  $N$ , allows to obtain information also related to the low lying part of the excitation spectrum. The uniqueness of the ground states can be demonstrated via the study of the kernel of  $\hat{H}' = \hat{H} - C$ . The physical properties of the obtained phases are deduced based on ground state expectation values calculated in terms of the constructed ground states. Since for a fixed structure of  $\hat{P}$ , usually the transformation  $\hat{H} = \hat{P} + C$  is exact only in a restricted parameter space domain ( $\mathcal{D}$ ), the deduced ground states are present only in  $\mathcal{D}$ . A global view on the phase diagram is obtained by different transformations of  $\hat{H}$  in positive semidefinite form.

## 1. Introduction

A positive semidefinite operator  $\hat{P}$  is defined as the operator which has only non-negative expectation values with all components  $|\chi\rangle \in \mathcal{H}$  of the Hilbert space  $\mathcal{H}$ , i.e.  $\langle\chi|\hat{P}|\chi\rangle \geq 0$ . From this relation automatically results that all eigenvalues  $p$  of  $\hat{P}$ ,  $\hat{P}|\psi\rangle = p|\psi\rangle$ , are non-negative scalars, that is,  $p \geq 0$ . This information seems trivial, but can be directly connected to the system Hamiltonian notion as follows: The spectrum of an arbitrary Hamiltonian ( $\hat{H}$ ) describing a physical system is always bounded below, the lower bound being the ground state energy  $E_g$ . Consequently  $\hat{H} - E_g = \hat{H}'$  is a positive semidefinite operator. This means that always, independent on integrability or dimensionality, an arbitrary  $\hat{H}$  can be written as a positive semidefinite operator  $\hat{P}$  plus a scalar  $C$ , i.e.

$$\hat{H} = \hat{P} + C. \quad (1)$$

Based on (1), the ground state can be deduced by constructing the most general wave vector  $|\Psi_g\rangle$  holding the property

$$\hat{P}|\Psi_g\rangle = 0. \quad (2)$$

If  $|\Psi_g\rangle$  as a solution of (2) exists, it will be the ground state, while the corresponding ground state energy becomes  $E_g = C$ . The procedure merits attention since several techniques have been worked out [1-13] for deducing (1) and solving (2).

The basic ideas serving as the background of the method are those presented above. Starting from these, Sect. 2 presents in details the steps of the procedure. Finally, Sect. 3 containing a short summary closes the presentation. The exemplifications are given in the fermionic case, but similar strategies are applicable also for bosonic systems as well.

## 2. Basic steps of the method

### 2.1. Transformation of $\hat{H}$ in a positive semidefinite form

The first step of the procedure represents an exact transcription of the Hamiltonian in a positive semidefinite form. For this reason, for example block operators can be used which are a linear combination of creation operators acting on the sites of a given block. In order to emphasize the aspects of this transformation, I present below an example in the case of the simplest two dimensional Hubbard model taken with periodic boundary conditions on a square lattice with Bravais vectors  $\mathbf{x}, \mathbf{y}$ . The Hamiltonian becomes of the form

$$\hat{H} = \sum_{\mathbf{i}, \sigma} (t_x \hat{c}_{\mathbf{i}+\mathbf{x}, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma} + t_y \hat{c}_{\mathbf{i}+\mathbf{y}, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma} + H.c.) + \hat{H}_U, \quad \hat{H}_U = U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}, \sigma} \hat{n}_{\mathbf{i}, -\sigma}, \quad (3)$$

where  $\hat{c}_{\mathbf{j}, \sigma}^\dagger$  creates an electron at the site  $\mathbf{j}$  with spin projection  $\sigma$ ,  $\hat{n}_{\mathbf{j}, \sigma} = \hat{c}_{\mathbf{j}, \sigma}^\dagger \hat{c}_{\mathbf{j}, \sigma}$  represents the particle number operator,  $t_x$  and  $t_y$  are the hopping matrix elements connecting nearest neighbors in  $x$  and  $y$  directions, while  $U > 0$  represents the strength of the on-site Coulomb repulsion. Now for each cell defined at the arbitrary site  $\mathbf{i}$  one introduces two block operators

$$\hat{A}_{\mathbf{i}, \sigma} = a_2 \hat{c}_{\mathbf{i}+\mathbf{x}, \sigma} + a_3 \hat{c}_{\mathbf{i}+\mathbf{x}+\mathbf{y}, \sigma} + a_4 \hat{c}_{\mathbf{i}+\mathbf{y}, \sigma}, \quad \hat{B}_{\mathbf{i}, \sigma} = b_1 \hat{c}_{\mathbf{i}, \sigma} + b_2 \hat{c}_{\mathbf{i}+\mathbf{x}, \sigma} + b_4 \hat{c}_{\mathbf{i}+\mathbf{y}, \sigma}, \quad (4)$$

where  $a_2, a_3, a_4$  and  $b_1, b_2, b_4$  are at the moment unknown block operator parameters, and the in-cell notation of sites by  $n = 1, 2, 3, 4$  follows in order the sites  $\mathbf{i}, \mathbf{i}+\mathbf{x}, \mathbf{i}+\mathbf{x}+\mathbf{y}, \mathbf{i}+\mathbf{y}$ . Considering the total number of electrons  $N$  fixed, from (3,4), on the line of (1), one obtains

$$\hat{H}_{AB} = \sum_{\mathbf{i}, \sigma} (\hat{A}_{\mathbf{i}, \sigma}^\dagger \hat{A}_{\mathbf{i}, \sigma} + \hat{B}_{\mathbf{i}, \sigma}^\dagger \hat{B}_{\mathbf{i}, \sigma}) = \hat{H} - \hat{H}_U + q\hat{N}, \quad \hat{P} = \hat{H}_{AB} + \hat{H}_U, \quad C = -qN, \quad (5)$$

where both  $\hat{H}_{AB}$  and  $\hat{H}_U$  are positive semidefinite operators, and the unknown block operator parameters are related to the known Hamilton operator parameters by

$$t_x = b_2^* b_1 + a_3^* a_4, \quad t_y = b_4^* b_1 + a_3^* a_2, \quad t_{y+x} = t_{y-x} = b_4^* b_2 + a_4^* a_2 = 0, \\ q = |b_1|^2 + |b_2|^2 + |b_4|^2 + |a_2|^2 + |a_3|^2 + |a_4|^2. \quad (6)$$

The system of equations (6) represents the *matching conditions*. This system is obtained by effectuating the calculations present in  $\hat{H}_{AB}$ , and equating term by term the obtained result with the similar components present in  $\hat{H}$ . For example, in  $\hat{H}$  one has  $t_x \hat{c}_{\mathbf{i}+\mathbf{x}, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma}$ , while from  $\hat{H}_{AB}$  one obtains  $(b_2^* b_1 + a_3^* a_4) \hat{c}_{\mathbf{i}+\mathbf{x}, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma}$ , consequently  $t_x = b_2^* b_1 + a_3^* a_4$  holds, etc.

Three observations have to be underlined at this stage: i) The matching conditions are representing usually coupled, complex algebraic non-linear equations. The solutions of this system of equations are present usually in a restricted  $\hat{H}$  parameter space region  $\mathcal{D}$  (in the present case, for example  $t_{y+x} = t_{y-x} = 0$ ). Consequently, the deduced results will be valid only in a restricted region  $\mathcal{D}$ . ii) As can be seen from (5,6), the constant  $C$  in (1) is not a given number, but usually a scalar with a complicated and implicit structure, depending on  $\hat{H}$  parameters. Consequently, the explicit expression of  $C$  becomes known only at the end of the calculation. iii) The number of unknown parameters and the number of equations in matching conditions [here Eqs.(6)] are usually different. Depending on the studied case, this difference

leads to: a) interdependences between  $\hat{H}$  parameters which determine  $\mathcal{D}$ , b) arbitrary parameters in the solutions of (6) which can be tuned during the process of solving (2) or deduction of  $E_g$ , and c) a combination of both a) and b).

Several other decompositions in positive semidefinite operators of the same  $\hat{H}$  can be effectuated, each of these placing the results in different regions  $\mathcal{D}$ . For example (5) usually works in the below system half filling region. Above half-filling, expressions as  $\sum_{\mathbf{i},\sigma} (\hat{A}_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger + \hat{B}_{\mathbf{i},\sigma} \hat{B}_{\mathbf{i},\sigma}^\dagger)$  must be used (the structure of the corresponding ground states demands that). Furthermore,  $\hat{P}$  can mix kinetic and interaction terms from  $\hat{H}$ . For example, this can be achieved by using instead of  $\hat{H}_U$  in the transformed  $\hat{H}$ , the positive semidefinite operator  $\hat{P}_{\mathbf{i}} = \hat{n}_{\mathbf{i},\sigma} \hat{n}_{\mathbf{i},-\sigma} - (\hat{n}_{\mathbf{i},\sigma} + \hat{n}_{\mathbf{i},-\sigma}) + 1$ . This last requires for its minimum eigenvalue zero at least one electron on the site  $\mathbf{i}$ . Similar mixing can be obtained by introducing in the block operators non-linear contributions, e.g. of the form  $a_{\mathbf{i}} \hat{c}_{\mathbf{i},\sigma} + b_{\mathbf{i}} \hat{c}_{\mathbf{i},\sigma} \hat{n}_{\mathbf{i},-\sigma}$ . I also note that the block operator coefficients can be considered cell variables (see [6,8]), which is useful in the study and description of random systems [6], or textures [8]. For multi-band systems, also the mixing of spin indices inside the same block operator can occur (see [7]). I further note that the number of block operators used in the positive semidefinite transcription of the Hamiltonian does not depend on dimensionality, but rather it is connected to the number and variety of terms present in  $\hat{H}$ .

## 2.2. Deduction of the ground states

Now one considers (1) given, and concentrates on solving (2) for  $|\Psi_g\rangle$ . The solution depends on the structure of  $\hat{P}$ , hence one analyzes below two of most often emerging cases, considering the block operators (as  $\hat{A}_{\mathbf{i},\sigma}$  and  $\hat{B}_{\mathbf{i},\sigma}$ ) linear combinations of fermionic operators.

*2.2.1. The  $\hat{P}$  operator contains terms of the form  $\sum_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma}$ ,  $\sum_{\mathbf{i},\sigma} \hat{B}_{\mathbf{i},\sigma}^\dagger \hat{B}_{\mathbf{i},\sigma}$ .* In this case the ground state is constructed by looking for a block operator  $\hat{C}_{\mathbf{i},\sigma}^\dagger$  which satisfies the anti-commutation relation

$$\{\hat{A}_{\mathbf{i},\sigma}, \hat{C}_{\mathbf{j},\sigma'}^\dagger\} = \{\hat{B}_{\mathbf{i},\sigma}, \hat{C}_{\mathbf{j},\sigma'}^\dagger\} = 0, \quad (7)$$

for all possible values of all indices. The reason for this strategy is that defining  $|\chi\rangle = \prod_{\mathbf{i},\sigma} \hat{C}_{\mathbf{i},\sigma}^\dagger |0\rangle$  where  $|0\rangle$  is the bare vacuum, starting from (7), one finds  $\hat{H}_{AB}|\chi\rangle = 0$ . The reason for this last equality is that based on (7), all  $\hat{A}_{\mathbf{i},\sigma}$ ,  $\hat{B}_{\mathbf{i},\sigma}$  operators present in  $\hat{H}_{AB}$  can be anti-commuted with all  $\hat{C}_{\mathbf{j},\sigma'}^\dagger$  present in  $|\chi\rangle$  and pushed in the right side of the expression  $\hat{H}_{AB}|\chi\rangle$  just in front of the vacuum state. Then, since  $\hat{A}_{\mathbf{i},\sigma}$ ,  $\hat{B}_{\mathbf{i},\sigma}$  contain only annihilation operators,  $\hat{A}_{\mathbf{i},\sigma}|0\rangle = \hat{B}_{\mathbf{i},\sigma}|0\rangle = 0$  holds, consequently  $\hat{H}_{AB}|\chi\rangle = 0$  is indeed satisfied. After this stage, usually a restriction  $(\mathbf{i},\sigma) \in \mathcal{M}$  introduces  $|\chi\rangle$  also in the kernel [14] of the other positive semidefinite operators present in  $\hat{P}$ , hence the ground state becomes  $|\Psi_g\rangle = \prod_{(\mathbf{i},\sigma) \in \mathcal{M}} \hat{C}_{\mathbf{i},\sigma}^\dagger |0\rangle$ . I note that often, the  $\hat{C}_{\mathbf{i},\sigma}^\dagger$  operators extend along the whole system (see [7]).

*2.2.2. The  $\hat{P}$  operator contains terms of the form  $\sum_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger$ ,  $\sum_{\mathbf{i},\sigma} \hat{B}_{\mathbf{i},\sigma} \hat{B}_{\mathbf{i},\sigma}^\dagger$ .* In this case one uses the property valid for all linear combination of fermionic operators

$$\hat{A}_{\mathbf{i},\sigma}^\dagger \hat{A}_{\mathbf{i},\sigma}^\dagger = 0, \quad \hat{B}_{\mathbf{i},\sigma}^\dagger \hat{B}_{\mathbf{i},\sigma}^\dagger = 0, \quad (8)$$

and starts the construction of the ground state by  $|\chi'\rangle = \prod_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^\dagger \hat{B}_{\mathbf{i},\sigma}^\dagger |0\rangle$ . Indeed, using (8), one obtains  $\hat{H}_{AB}|\chi'\rangle = 0$ . Now in most cases (see [9,10]), the introduction of a supplementary  $\hat{F}^\dagger$  operator in the constructed wave vector pushes  $\hat{F}^\dagger|\chi'\rangle$  in the kernel of the other operators

present in  $\hat{P}$ , consequently the ground state becomes  $|\Psi'_g\rangle = \prod_{i,\sigma} \hat{A}_{i,\sigma}^\dagger \hat{B}_{i,\sigma}^\dagger \hat{F}^\dagger |0\rangle$ . I further note that the number of particles  $N$  present in the system is given by the number of multiplied creation operators present in the expression of the ground state. Since this is higher in the case of  $|\Psi'_g\rangle$ ,  $\sum_{i,\sigma} \hat{A}_{i,\sigma} \hat{A}_{i,\sigma}^\dagger$  and  $\sum_{i,\sigma} \hat{B}_{i,\sigma} \hat{B}_{i,\sigma}^\dagger$  type of positive semidefinite operators are used in the above system half filling concentration region. For the case of non-linear Fermi operator combinations in block operators, similar techniques apply [4].

*2.2.3. Information regarding the low lying part of the excitation spectrum.* If  $E_g(N)$  is deduced, the chemical potential  $\mu(N+1) = E_g(N+1) - E_g(N)$ ,  $\mu(N) = E_g(N) - E_g(N-1)$ , and  $\delta\mu = \mu(N+1) - \mu(N)$  can be obtained. Now  $\delta\mu \neq 0$ , ( $\delta\mu = 0$ ), signals the presence, (absence) of the charge gap, consequently insulating, (conducting) behavior can be tested.

### *2.3. Demonstration of the uniqueness of the ground states*

In demonstrating the uniqueness of the deduced ground states one concentrates on the kernel  $Ker(\hat{P})$  [14] of the operator  $\hat{H} - C = \hat{P}$ . For the most general case, when the deduced ground state  $|\Psi_g(m)\rangle$  is  $M$  fold degenerate (i.e.  $m = 1, 2, \dots, M$ ), the proof of the uniqueness must be done in two steps: i) First one shows that for all possible  $m$  values  $|\Psi_g(m)\rangle \in Ker(\hat{P})$  holds. ii) Second, one demonstrates that an arbitrary wave vector  $|\nu\rangle \in Ker(\hat{P})$  can be expressed as a linear combination of the  $|\Psi_g(m)\rangle$  terms (see for exemplification [9,13]). In the non-degenerate case the demonstration is the same, but only the  $m = 1$  ground state component exists. As seen, at this step, the uniqueness and non-degenerate notions should be taken distinct: uniqueness means that non-deduced (i.e. unknown) vectors  $|\nu\rangle$ , satisfying  $\hat{P}|\nu\rangle = 0$  are not present.

### *2.4. Study of the physical properties of the deduced ground states*

The ground state being deduced, its physical properties are not visible at first view. In order to deduce them, different ground state expectation values must be calculated.

## **3. Summary and conclusions**

It was shown how positive semidefinite operator properties allow the deduction of exact ground states for many-body quantum systems independent on integrability or dimensionality.

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- [13] Gulácsi Z, Kampf A and Vollhardt D 2008 *Prog. Theor. Phys. Suppl.* **105** 1
- [14] The kernel  $Ker(\hat{O})$ , of an arbitrary operator  $\hat{O}$ , is a Hilbert subspace containing all wave vectors  $|\phi\rangle$  with the property  $\hat{O}|\phi\rangle = 0$ .