Mathematical properties and algorithm for fast calculation of full Wick's contractions in quantum many-body fermion systems

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Abstract

Wick's contractions, also related to Wick's theorem, represent important mathematical technique used in quantum many-body theory to simplify calculations involving creation and annihilation operators. In this work we study the properties of full Wick's contractions and discuss in details corresponding graph and group theory aspects. We observed isomorphism between graph-like objects which are in fact contained in the full Wick's contractions and some geometrical objects, such as circle or regular rectangle with internal structure. We also found isomorphism between two induced groups, one which is related to permutations of one end of Wick's lines and the second which corresponds to rotations of directed lines inside geometrical object. We present fast and efficient algorithm for calculation of the expectation value of large number of creation and annihilation particle and hole operators in order to achieve different particle-hole or particle-particle terms in many-body theories, from nuclear to solid state physics or quantum chemistry. The algorithm is based on observed isomorphisms. It simplifies full Wick's contractions to simple adjacency and geometrical relations, which are also used for sign determination. Also, we presented several illustrative examples of computation, such as calculation of the two-body particle-hole terms in Hartree-Fock's theory and the Random phase approximation.

Keywords: *Wick's theorem, Wick's contractions, group theory, graph theory, quantum mechanics, quantum many-body theory, Hartree-Fock, Random phase approximation*

1. Introduction

In the many-body theories we must often calculate expectation values of particle-particle (hole-hole) or particle-hole, transition or density matrix elements which may contain large number of creation and annihilation operators. This particular task is usually done by hand, which can be rather tedious, especially if the total number of operators is larger than . In order to reduce the amount of time needed for this task and possibility for human errors, we present simple and fast algorithm which calculates quantum mechanical expectation values using full Wick's contractions, based on geometrical mapping of operators on vertices of regular polygon or equidistant points of unit circle and Wick's lines on directed lines (edges) between vertices, i.e., simple adjacency and geometrical conditions and relations. For illustration, here we will use unit circle representation.

Wick's contractions are a set of mathematical rules that describe the simplification of complex many body interactions in quantum mechanical systems. They provide a systematic way of eliminating redundant terms in a quantum many-body wave function, leading to a more compact and manageable description of the system. The contractions are named after the physicist Gian Carlo Wick, who introduced them in 1950 in his work as a tool for analyzing quantum field theory (Wick, 1950). In other words, Wick's contractions are a way grouping, i.e., combining creation and annihilation operators in a quantum mechanical bracket. For example, see refs.: (Shankar, 1994; Sakurai & Napolitano, 2014). These operators represent the creation and annihilation of particles (holes) in the system, and their combinations determine the total number of particles or holes present in the wave function in particle-hole many-body picture (Suhonen, 2007).

Although Wick's theorem is originally proposed to simplify problem of bringing products of field operators into a normal form and to give clear derivation of Feynman's diagrammatic rules of perturbation theory (Wick, 1950), it is still widely used in quantum field theory for systematical calculation of higher-point correlation functions since they can be expressed in terms of lower-point propagators. See for example refs.: (Weinberg, 1995; Mandl, 2010). Wick's theorem and contractions have been used extensively in many other areas of physics, including condensed matter physics, nuclear, atomic physics, and cosmology. In condensed matter physics, for example, they have been used to study the behavior of electrons in solids (Altland & Simons, 2010) and the properties of superconductors (Baym & Pethick, 2004). In atomic physics, they have been used to understand the behavior of atomic systems, including the spectroscopy of atoms and the behavior of atoms in magnetic fields (Avron et al., 1987). In nuclear physics Wick's contractions can be used to calculate ground state properties of nuclei, transition amplitudes and other quantities related to nuclear reactions and decays (Suhonen, 2007). In cosmology, they have been used to study the properties of the early universe and the behavior of cosmic radiation (Baumann, 2016). The theorem has also been extended in the quantum gravity due to additional degrees of freedom and extra dimensions (see for example: (Rovelli, 2004)).

In this work we are focused on Wick's contractions in fermionic systems only, which are important for most practical reasons in theoretical physics and chemistry. In the Section 2. we present novel perspective on mathematical properties of Wick's contractions as graph-like objects and properties from the group theory perspective. In the Section 3. we describe our computational algorithm for full Wick's contractions in quantum many-body fermion systems (FWC-QMBFS) based on these properties, while in the Section 4. we show few illustrative computational results for applications in the Hartree-Fock and Random phase approximation.

2. Mathematical properties of Wick's contractions

Observables in the formalism of second quantization are proportional to a product of creation and annihilation particle (or hole) operators. Although observables may have nonzero expectation value in the vacuum state, when one constructs them by arranging creation operators to the left of annihilation operators, which is so called normal order of operators, their expectation values become zero. First it is necessary to define Wick's contraction as mathematical objects and its relation to the normal ordered product of the operators (Mattuck, 1976; Suhonen 2007). We are focused here only on the time independent case.

Definition 1. The contraction of two arbitrary quantum mechanical operators A_1 and A_2 regardless of its fermionic or boson nature, is defined as:

$$\overset{\sqcap}{A_1 A_2} \equiv A_1 A_2 - N\left[A_1 A_2\right], \tag{1}$$

where N stands for normal ordered product of operators.

Definition 2. Sums of normally ordered products of n arbitrary operators for fixed number of contractions are defined as:

$$
\begin{aligned}
N_{n,1} &= \sum_{(i_1 i_1')} \mathrm{N}\left[A_1 \dots \overbracket{A_{i_1} \dots A_{i_1'}} \dots A_n\right], \\
N_{n,2} &= \sum_{(i_1 i_1')(i_2 i_2')} \mathrm{N}\left[A_1 \dots \overbracket{A_{i_1} \dots A_{i_1'}} \dots \overbracket{A_{i_2} \dots A_{i_2'}} \dots A_n\right], \\
&\vdots \\
N_{n,k} &= \sum_{(i_1 i_1')\dots(i_k i_k')} \mathrm{N}\left[A_{i_1} \dots A_{i_k} \dots A_{i_{k-1}} \dots A_{i_1'} \dots A_{i_{k-1}'} \dots A_{i_2} \dots A_{i_2'} \dots A_{i_k}\right]
\end{aligned}
\tag{2}
$$

where i_1 and i_1' are indices related to a pair of operators connected with corresponding Wick's contraction line and $k = \lfloor n/2 \rfloor$ in the last expression.

Explanation: In the first expression $k = 1$ and sum runs on single contractions of pairs (pair of indices i_1 and i_1', with a condition $i_1 \neq i_1'$). In the second one $k = 2$ and sum runs on double contractions (two pairs of indices i_1, i_1' and i_2, i_2', with a condition $i_1 \neq i_1'$, $i_2 \neq i_2'$, $i_1 \neq i_2'$, and $i_2 \neq i_1'$), while in the last summation runs over $\lfloor n/2 \rfloor$ index pairs, without repetition any of indices. If n is an even number, it contains terms (all possible permutations) which are products of contractions (c-numbers). If n is odd, the last sum has terms with a single unpaired operator.

Theorem 1. (Wick's theorem): For a given product of quantum mechanical operators $A_1 A_2 \cdots A_n$ we have:

$$
A_1 A_2 \cdots A_n = N\left[A_1\ A_2\ A_3 \cdots A_{n-1}\ A_n\right] + \sum_{k=1}^{\lfloor n \rfloor} N_{n,k}. \tag{3}
$$

Proof: The theorem is proven by the mathematical induction (see ref. (Molinari, 2017)). When $n=2$ operators, it is true (see Definition 1.). Suppose that the statement is true for a product of creation/annihilation operators $A_1 \cdots A_n$, then we need to show that is also true for the product of $A_1 \cdots A_n A_{n+1}$ operators. By hypothesis of the induction for n operators we have:

$$
A_1 A_2 \cdots A_n = \sum_{k=0}^{\lfloor n \rfloor} N_{n,k}. \tag{4}
$$

Lets consider:

$$
N_{n,k} A_{n+1} = N\left[N_{n,k} A_{n+1}\right] + \sum_{k=1}^{\lfloor n \rfloor} N\left[\overbracket{N_{n,k} A}_{n+1}\right]. \tag{5}
$$

The contraction in last expression means the sum of all contractions of A_{n+1} with unpaired operators A_i in $N_{n,k}$. On the other hand, we have the following relation:

$$
N\left[\overbracket{N_{n,k} A}_{n+1}\right] + N\left[N_{n,k+1} A_{n+1}\right] = N_{n+1,k+1} \tag{6}
$$

Using identities (5) and (6) one obtains:

$$
\begin{aligned}
A_1 \cdots A_n A_{n+1} =& N_{n,0}A_{n+1} + N_{n,1}A_{n+1} + \ldots + N_{n,n}A_{n+1} \\
=& N\left[N_{n,0}A_{n+1}\right] + N\left[\overbracket{N_{n,0}A}_{n+1}\right] + N\left[N_{n,1}A_{n+1}\right] + \\
& N\left[\overbracket{N_{n,1}A}_{n+1}\right] + \ldots + N\left[N_{n,\lfloor n/2\rfloor}A_{n+1}\right] + N\left[\overbracket{N_{n,\lfloor n/2\rfloor}A}_{n+1}\right] \\
=& N_{n+1,0} \;+\; N_{n+1,1} \;+\; \ldots \;+\; N_{n+1,\lfloor n/2\rfloor},
\end{aligned}
\tag{7}
$$

which is Wick's theorem for *n+1* operator.

Corollary 1. If a state | *gs* ⟩ represents a ground state of a system of even number of particles and the action of the operators $A_1, A_2, \ldots, A_{2n}$ with respect to reference state | *gs* ⟩ is given by:

$$A_i^- |gs\rangle = 0 \text{ , and } \langle gs| A_i^+ = 0. \tag{8}$$

The expectation value of the operators is given by the expression (see refs. (Suhonen, 2007; Molinari, 2017).:

$$
\begin{aligned}
\langle gs\,|A_1 \cdots A_{2n}|\,gs\rangle \;=&\; \langle gs\,|N_{2n,n}|\,gs\rangle \\
\sum_{(i_1 i_1')\ldots(i_n i_n')} & A_{i_1} \ldots A_n \ldots A_{i_{n-1}} \ldots A_{i_1'} \ldots A_{i_{n-1}'} \ldots A_{i_2} \ldots A_{i_2'} \ldots A_n
\end{aligned}
\tag{9}
$$

Explanation: In the last equality we used the Definition 2. and the fact that each contraction is a complex number. The last summation runs over n index pairs, without repetition any of indices, which corresponds to a sum of all possible permutations P up to a $sign(P)$. For details about "constrained permutation" with respect to the nonvanishing Wick's contractions for a particular ordering of operators in the particle-hole quantum many-body picture see the Definition 6. below.

Corollary 1. is a direct consequence of the Wick's theorem. Wick's contractions represent the connected parts of the so-called correlation function, which describe the genuine interactions between the particles (Weinberg, 1995). In other words, we can use them to calculate one- and two-body matrix elements, transition amplitudes and density matrix, which is shown in Section 4. for few illustrative examples.

Proof: From the Theorem 1. one can always rewrite product of operators $A_1, A_2, \ldots, A_{2n}$ as sum of normal product of $2n$ operators without and with k contractions, where $1 \le k \le n$ from the Definition 2. The expectation value with respect to the reference state ¿ *gs* of the sum of normal product of operators is vanishing by its definition. On the other hand, each contracted pair of operators "can be moved outside" of the normal product (they are just c-numbers), which is again vanishing. Therefore, only full Wick's contractions, i.e., without any unpaired operators ($k = n$) will give nonvanishing contribution to the expectation value.

Corollary 2. Expectation value of the product of odd number of quantum mechanical operators $A_1 \cdots A_{2n+1}$ is given by:

$$\langle gs|A_1 \cdots A_{2n+1}|gs\rangle = 0 \tag{10}$$

Proof: If total number of operators is odd, there is one unpaired operator left for $k = n$ contractions in the normal product, which expectation value is by the definition 0, due to $A_i^- |gs\rangle = 0$ or $\langle gs| A_i^+ = 0$. The rest of the proof related to the sum of normal product of the operators without and with $0 \le k < n$ contractions is the same as in the Corollary 1.

Definition 3. The contraction of two arbitrary fermionic operators for the time independent case in the particle-hole quantum many-body picture (see for example refs. (Mattuck, 1976; Suhonen 2007)) is given by the following expressions:

$$
\begin{aligned}
c_\alpha c^{\dagger}_{\alpha}{}' &= \langle HF|c_\alpha c^{\dagger}_{\alpha}{}'|HF\rangle = \delta_{\alpha\alpha'} \qquad (\epsilon_\alpha, \epsilon'_\alpha > \epsilon_F),\\
h_\beta h^{\dagger}_{\beta}{}' &= \langle HF|h_\beta c^{\dagger}_{\beta}{}'|HF\rangle = \delta_{\beta\beta'} \qquad (\epsilon_\alpha, \epsilon'_\alpha \leq \epsilon_F),\\
\text{others} &= 0.
\end{aligned}
\tag{11}
$$

where $c^\dagger$ and c ($h^\dagger$ and h) denote creation and annihilation of particle (hole) respectively, with $c_\alpha\,|\,HF\,\rangle = 0$ and $h_\beta\,|\,HF\,\rangle = 0$, with condition $\epsilon_\alpha > \epsilon_F$, $\epsilon_\beta \leq \epsilon_F$ where ϵ_F stands for the Fermi level and $|\,HF\,\rangle$ for particle-hole (Hartree-Fock) vacuum.

Definition 4. Set of full Wick's contractions S is defined as a set of all nonvanishing arrangements of annihilation and creation operator pairs of the same kind connected with corresponding Wick's contraction lines related to specific ordering of operators.

Example 1: a) Set S related to two-body term in the Hartree-Fock approximation:

$$S = \{\langle HF|h_a h_b h^\dagger_c h^\dagger_d|HF\rangle,\ \langle HF|h_a h_b h^\dagger_c h^\dagger_d|HF\rangle\}. \tag{12}$$

b) Sets S_1, S_2, ..., S_5 are related to the A matrix in Random phase approximation (RPA):

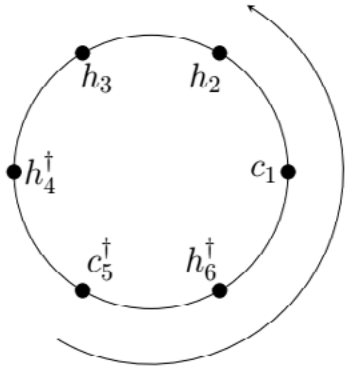
$$
\begin{aligned}
S_1 &= \{\langle HF|h_i c_m c^\dagger_a h_b c_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m c^\dagger_a h_b c_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle\},\\
S_2 &= \{\langle HF|h_i c_m c^\dagger_a h_b h^\dagger_c c_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m c^\dagger_a h_b h^\dagger_c c_d c^\dagger_o h^\dagger_k|HF\rangle\},\\
S_3 &= \{\langle HF|h_i c_m h_a c^\dagger_b c_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m h_a c^\dagger_b c_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle\},\\
S_4 &= \{\langle HF|h_i c_m h_a c^\dagger_b h^\dagger_c c_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m h_a c^\dagger_b h^\dagger_c c_d c^\dagger_o h^\dagger_k|HF\rangle\},\\
S_5 &= \{\langle HF|h_i c_m h_a h_b h^\dagger_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m h_a h_b h^\dagger_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\\
&\quad \langle HF|h_i c_m h_a h_b h^\dagger_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m h_a h_b h^\dagger_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\\
&\quad \langle HF|h_i c_m h_a h_b h^\dagger_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle,\ \langle HF|h_i c_m h_a h_b h^\dagger_c h^\dagger_d c^\dagger_o h^\dagger_k|HF\rangle\}.
\end{aligned}
\tag{13}
$$

Definition 5. Let us consider expectation value of n quantum mechanical creation and annihilation particle and hole operator pairs. There exists a map f from a set of full Wick's nonvanishing contractions S to a set W of $2n$ equidistant (special) points on unit circle interconnected with n straight directed lines, as follows:

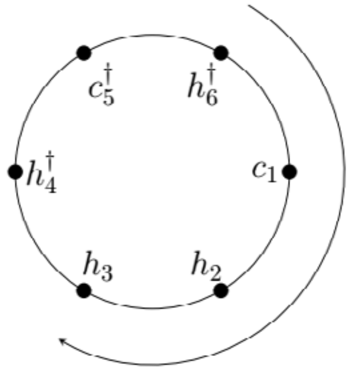
1. for every point on unit circle, there exists one and only one operator,
2. all points set on unit circle are following the same order of appearance as operators, with an arbitrary choice of the first point and an arbitrary choice of a direction (clockwise or counterclockwise, see Fig. 1.),
3. each point related to annihilation operator is connected using directed straight line exactly to one point related to creation operator of the same kind, i.e., particle (hole) annihilation operator to particle (hole) creation operator, obeying the same direction (clockwise or counterclockwise) as points in point 2) of the definition,

4. each directed line that connects pair of points on unit circle from point 3) of this definition corresponds to a Wick's contraction line that connects pair of operators,
5. sign of the result of the Wick's contraction of operators corresponds to the number of intersections of directed lines inside unit circle I, i.e., the sign is -1 if I is an odd number and 1 if it is an even number or zero.

Fig.1. Counter-clockwise and clockwise choice of direction.



(a) *Counter-clockwise direction.*



(b) *Clockwise direction.*

Theorem 2. Let S and W be two sets of graph-like objects described above. Set S is isomorphic to set W.

Proof: If two sets contain graph-like objects, which have an internal structure, as elements of sets, it is possible to define properties such as homomorphism and isomorphism which one typically relates to group properties. However, it is necessary to follow general steps in order to prove that there is an isomorphism between two sets. First, we need to examine the structure of two sets S and W. From Definitions 4. and 5. follows directly that sets S and W must always contain the same number of elements.

Second, we need to prove that the mapping f from the Definition 5. is bijection. Any two different operators regardless of their kind are mapped into two different points on unit circle. Similarly, any two different Wick's lines are mapped into two different directed lines that connect distinct pairs of points on unit circle. Therefore, it is injection. From the points 1) – 4) of the Definition 5. it is ensured that there is no free element in the set of all realizations of circles, i.e., codomain, and there are eliminated all unimportant rotations of the unit circle (point 2) of the same definition). In other words, from the point 1) one can never add more or have less points than the number of operators in the specific arrangement. From points 3) and 4) each directed line corresponds to specific pair of points, therefore there are no extra, nor less directed lines then corresponding Wick's contraction lines. Thus, the mapping f between set S and W is surjection. When mapping is both injection and surjection, we say that the mapping is bijection, and we have proven the second part of the theorem.

In the third part we need to show that the mapping f is homomorphism. The same ordering of operators leads to the same ordering of corresponding (special) points on unit circle and the same arrangement of Wick's contraction lines that connects operators of the same kind leads to the same arrangement of directed lines between points on unit circle, which is ensured by the points 2) and 4) of the Definition 5. Mathematically speaking, let denote operators in the specific arrangement of operators as vertices V and Wick's lines as edges E and similarly (special) points on unit circle as vertices Λ and directed lines as edges Σ in the other set. In other words, let assume we have graph-like objects $G = (V, E)$, and $\Delta = (\Lambda, \Sigma)$. We also have intersections I, which exist in graph-like objects in both sets and here are treated independently. We can define adjacency operation $*$ between each vertex $a, b \in V$ as

$$a \divideontimes b = 1 \text{ if } (a, b) \in E, \quad a \divideontimes b = 0 \text{ otherwise.} \tag{14}$$

Similar definition may be found in ref.: (Hell & Nešetřil, 2004). In other words, the adjacency operation returns 1 if the vertices a and b are connected by an (directed) edge in the graph and returns 0 otherwise. Analogous operation one can define between each vertex $c, d \in \Lambda$ of the other graph-like object. The homomorphism between two graph-like objects, i.e., in our case elements of set S and set W, satisfies the following relation:

$$f(a \divideontimes b) = f(a) \divideontimes f(b). \tag{15}$$

The adjacency operation $\divideontimes$ is already explicitly includedin each Wick's contraction line which connects annihilation and creation operators of the same kind, but also in directed line which connects corresponding pair of points on unit circle, which follows directly from the Definition 5. Both result in Kronecker delta usually with an additional information about state which may be bellow or above the Fermi surface, due to difference between particles and holes. Therefore, the mapping f from the Definition 5. is a homomorphism. Note also that one can define adjacency matrix as in the graph theory, see for example ref.: (Veljan, 2001).

Adjacency operation is just a part of internal structure of graph-like objects, which also contain intersection points, which are treated separately through sign operation. The sign result is also preserved by the function f. From the point 5) of the Definition 5. for each $g \in S$ and some $w \in W$ follows that $sign(g) = sign(w)$. To see why, note that the minimal number of intersections of Wick's lines, if exist (otherwise is zero), regardless of operator arrangement inside quantum mechanical bra-ket is equal to the number of intersections of directed lines inside the unit circle, which may be obtained from simple geometrical relations, i.e., the position of lines with respect to each other. This corresponds to solving system of linear equations for each pair of lines. Furthermore, any additional intersections of Wick's lines inside bra-ket, which may come from the choice of an individual, always come in pairs, which means that the sign of Wick's contraction will remain unchanged regardless of individual calculation procedure. Therefore, we conclude that the sign is also conserved by homomorphism f. Every element $g \in S$ corresponds to some realization of non-vanishing full Wick's contractions for specific operator arrangement, which means that homomorphism f also preserves the total contraction result, i.e.,

$$\prod_{i=1}^{n} f\left(a_i \divideontimes b_i\right) = \prod_{i=1}^{n} f\left(a_i\right) \divideontimes f\left(b_i\right) \tag{16}$$

which follows directly from the previous step, where n is the number of operator pairs.

In the last step we need to prove that it is possible to construct inverse mapping f^{-1} which is also a homomorphism. The Definition 5. also describe the internal structure of arbitrary element $w \in W$, in particular point 2) of the same definition fixes point ordering up to irrelevant choice of the first point and a choice of direction and similarly point 4) fixes lines which connect pairs of points. Due to arrangement preservation in terms of points and directed lines on unit circle, it is always possible to map back to the arrangement of operators and Wick's lines inside a bra-ket. The proof is the same as in the third part of the proof, with only difference where points and directed lines are replaced by operators and Wick's lines, and opposite. Point 5) holds in both directions, what is proven in the previous step, which means also for mapping f^{-1}. Therefore, the mapping f^{-1} is also homomorphism. From previous steps we conclude that sets S and W are isomorphic.

Definition 6. Let indices $p_1, p_2, p_3, \dots, p_n$ ($h_1, h_2, h_3, \dots, h_m$) represent the order of appearance of n annihilation particle (m hole) operators corresponding to one end (left end) of the Wick's contraction lines, while indices $p_1', p_2', p_3', \dots, p_n'$ ($h_1', h_2', h_3', \dots, h_m'$) for the positions of n creation particle (m hole) operators which are connected to p_1-th,…, p_n-th, (h_1-th, …, h_m-th) Wick's line respectively. Permutation operation of the creation end (right end) of at most $(n+m)$ Wick's contraction lines, while keeping annihilation operator places fixed, is defined as (written in two-line notation):

$$P = \begin{pmatrix} p_1 - p_1' & p_2 - p_2' & \dots & p_n - p_n' & h_1 - h_1' & h_2 - h_2' & \dots & h_m - h_m' \\ p_1 - \tilde{p}_1' & p_2 - \tilde{p}_2' & \dots & p_n - \tilde{p}_n' & h_1 - \tilde{h}_1' & h_2 - \tilde{h}_2' & \dots & h_m - \tilde{h}_m' \end{pmatrix}, \tag{17}$$

where elements $p_k - p_k'$ ($h_k - h_k'$) in the first row represent k-th Wick's contraction line connecting fixed k-th annihilation and free creation operator of the same kind with corresponding indices and elements of the second row $p_k - \tilde{p}_k'$ ($h_k - \tilde{h}_k'$) after transformation, with the following conditions: $p_k < p_k' (h_k < h_k') \wedge p_k < \tilde{p}_k' (h_k < \tilde{h}_k')$ for every column $k \in P$. The action of P is defined as the change of the end of the k-th Wick's contraction line (in the k-th column), i.e., the ending creation operator, if $\tilde{p}_k' \neq p_k'$ ($\tilde{h}_k' \neq h_k'$), otherwise it is not changed. Indices $\tilde{p}_k$ ($\tilde{h}_k$) stand for new positions of the end of the line.

Claim 1. Any permutation of ends of Wick's contraction lines from the Definition 6. may be composed of a sequence of one-end swaps of two Wick's contraction lines.

Explanation: With a sequence of swaps of only one end of two Wick's contraction lines one can make all possible arrangements of Wick's lines, obeying standard rules defined by Wick (Wick, 1950). It corresponds to a well-known problem which states that from a sequence of swaps of arbitrary two elements of a set one can build all possible permutations of elements (creation operators of the same kind in our case), which is proven by and used as the computational algorithm by Heap, B. R., see ref. (Heap, 1963). We use this algorithm for construction of all permutations of Wick's lines in our computer code (see Section 4.)

Lemma 1. Set of permutations of one end of Wick's lines X described by the Definition 6. is a group with the respect to the composition of permutations as the group operation.

Explanation: The proof follows directly from the permutation group properties with additional constraints from the Definition 6. and will not be discussed further.

Example 2: Multiplication table for the permutations of ends of Wick's lines connecting operators in the Hartree-Fock approximation two body form is shown in Table 1. Let us define abbreviation for the following permutations in which Wick's lines stay the same:

$$E = P \begin{pmatrix} h_1 - h_1' & h_2 - h_2' \\ h_1 - h_1' & h_2 - h_2' \end{pmatrix}, \tag{18}$$

and the transposition of two lines

$$\tau = P \begin{pmatrix} h_1 - h_1' & h_2 - h_2' \\ h_1 - h_2' & h_2 - h_1' \end{pmatrix}. \tag{19}$$

where Wick's lines are changing one end between two hole creation operators, while keeping annihilation hole operators fixed. The multiplication table, i.e., the composition of permutations, one builds straight forward, except for the term:

$$\tau^2 = \tau \circ \tau = P \begin{pmatrix} h_1 - h_1' & h_2 - h_2' \\ h_1 - h_2' & h_2 - h_1' \end{pmatrix} P \begin{pmatrix} h_1 - h_1' & h_2 - h_2' \\ h_1 - h_2' & h_2 - h_1' \end{pmatrix} = E \tag{20}$$

Table 1. Multiplication table for the permutation group X **(**$hh\, h^\dagger\, h^\dagger$**).**

$\otimes$	E	τ
E	E	τ
τ	τ	E

Definition 7. Let X be a group of permutations of ends of Wick's lines described by the Definition 6 and let S be a non-empty set of nonvanishing Wick's contractions. Natural action of X on S is given by the function $\phi : X \times S \to S$ defined by (see for example ref. (Dummit, & Foote, 2004)):

$$\phi(P, g) = \phi_P(g) = P \circ g = P(g), \quad \text{for all } P \in X \text{ and all } g \in S \tag{21}$$

which satisfies the following conditions of a group actions:

i) for each $g \in S$ the identity element $E \in X$ fixes g, i.e., $E \circ g = E\,(g) = g$,
ii) for each $P, Q \in X$ and each $g \in S$ we have $(P \otimes Q) \circ x = P \circ (Q \circ x)$, where binary operation $\otimes$ stands for the composition of permutations from the Definition 6.

Explanation: Note that the action of X on S is always well behaved, i.e., from the Definition 6. directly follows that the action of each $p \in X$ on each $g_1 \in S$ is just $P(g_1)=g_2$, where $g_2 \in S$. The action always results in some element of S. Note also the difference between operations $\otimes$ and $\circ$, i.e., operation $\otimes$ is composition between two arbitrary permutations, while $\circ$ represents the action of arbitrary element of X i.e., permutation, to arbitrary element of S.

Lemma 2. The set of all bijections from S to itself from the Definition 7. that can be obtained by applying all elements of X to all elements of S, i.e., the set of functions ϕ_P, forms a group under composition of functions. This group is called the Wick's permutation group of X induced by the action of X on S and is denoted by X_S.

Proof: The proof naturally comes from the properties of the group action from the Definition 7. Let us assume that for each $g \in S$ and each bijection $\phi_P \wedge \phi_Q \in X_S$, the composition of the actions on element g is then $\phi_P \circ \phi_Q(g) = \phi_R(g)$, where $\phi_R(g)$ is another action on element g and $\phi_R \in X_S$. From the Definition 7. we have $\phi_P\,(g) = P(g)$ and $\phi_Q\,(g) = Q(g)$, where P and $Q \in X$. On the other hand, from the Lemma 2. the composition of permutations $P\,Q = R$ is just another permutation, i.e., $R \in X$, therefore $\phi_P \circ \phi_Q = \phi_R$, independent of choice of the element $g \in S$, so the group closure condition is satisfied.

In the second step we want to show the existence of the identity bijection . Let us assume that for each exists an identity bijection for which we have:

$$\phi_P \circ \phi_E(g) = \phi_E \circ \phi_P(g) = \phi_P(g) \tag{22}$$

In other words, for every $g \in S$ holds $\phi_E(g) = E(g) = g$ therefore $\phi_P \circ \phi_E(g) = \phi_P(g) = P(g)$. Similarly, from the second condition in the Definition 7. follows that $\phi_E \circ \phi_P(g) = E \circ (P \circ g) = (E\,P) \circ g$, while from Lemma 1. follows that $(E\,P) \circ g = (E\,P)(g) = P(g)$ from which $\phi_P \circ \phi_E = \phi_E \circ \phi_P = \phi_P$, independent of the choice of the element $g \in S$. Therefore, we have proven the existence of identity bijection $\phi_E \in X_S$.

Similarly, let us assume that for each $g \in S$ and each ϕ_P, ϕ_Q and $\phi_R \in X_S$:

$$\phi_P \circ (\phi_Q \circ \phi_R)(g) = (\phi_P \circ \phi_Q) \circ \phi_R(g) \tag{23}$$

The associativity of the composition of bijections follows directly from Lemma 1, i.e., the group closure and associativity of permutations, and the second group action condition from the Definition 7. In other words, from the first part of the proof, for every $g \in S$ the action of the composition of bijections $\phi_Q \circ \phi_R(g)$ is just another action $\phi_T(g)$, where bijection $\phi_T \in X_S$ i.e., $\phi_T(g) = T(g)$, for which from the Lemma 1. and Definition 7. follows $T(g) = Q \circ R(g)$. However, $\phi_P \circ \phi_T\,(g)$ is again another action $\phi_U\,(g)$, where bijection $\phi_U \in X_S$, for which analogously have $U(g)=P \otimes T(g)=P \otimes (Q \otimes R)\,(g)$. On the other hand, for every $g \in S$ let the action of the composition of bijections $\phi_P \circ \phi_Q(g)$ be equal to $\phi_W(g)$ where $\phi_W \in X_S$, i.e., $\phi_W(g) = W\,(g)$, for which $W(g)=P \otimes Q\,(g)$. Similarly, we have $\phi_W \circ \phi_R\,(g) = W \otimes R(g) = (P \otimes Q) \otimes R(g)$ From the Lemma 1., i.e., the associativity of permutations $P \otimes (Q \otimes R)= (P \otimes Q) \otimes R$ from which follows that $\phi_P \circ \phi_T = \phi_W \circ \phi_R$ therefore $\phi_P \circ (\phi_Q \circ \phi_R) = (\phi_P \circ \phi_Q) \circ \phi_R$, independently of the choice of the element $g \in S$ and we have proven the third part.

In the last part we need to show that for each bijection $\phi_P \in X_S$ exists a unique inverse bijection $\phi_P^{-1} \in X_S$. Let us assume they satisfy the following property for each $g \in X_S$:

$$\phi_P \circ \phi_P^{-1}(g) = \phi_P^{-1} \circ \phi_P(g) = \phi_E(g) \tag{24}$$

In other words, let assume that for each $\phi_P \in X_S$ exists unique ϕ_P for which $\phi_P \circ \phi_Q(g) = \phi_E(g)$, where and From the Definition 7. follows (P⊗Q)(g)=E(g), while from Lemma 2. follows P^{-1}=Q. Further, $\phi_Q(g) = \phi_{P^{-1}}(g)$ from which follows $\phi_P^{-1}(g) = \phi_{P^{-1}}(g)$. On the other hand, the same holds for $\phi_Q \circ \phi_P(g) = \phi_E(g)$. From the Definition 7. follows that (Q⊗P)(g)=E(g), while from Lemma 1. again follows P^{-1}=Q. The rest of the proof is the same as in previous step, which means that from (P⊗Q)= (Q⊗P)=E, follows that for each $\phi_P \in X_S$ exists a unique inverse bijection $\phi_{P^{-1}} \in X_S$, independent of any choice of the element $g \in S$. Therefore, we have proven that X_S satisfies all group properties, which correspond to the properties of the group X.

Definition 8. Let $(x_{p_1}, y_{p_1}), (x_{p_2}, y_{p_2}), \dots, (x_{p_n}, y_{p_n})$ are coordinates of points related to ends and $(X_{p_1}, Y_{p_1}), (X_{p_2}, Y_{p_2}), \dots, (X_{p_n}, Y_{p_n})$ of the beginning of n directed lines that corresponds to pairs of particle operators. Similarly, from m directed lines that connect pairs of points related to hole operators we have coordinates $(x_{h_1}, y_{h_1}), (x_{h_2}, y_{h_2}), \dots, (x_{h_m}, y_{h_m})$ and $(X_{h_1}, Y_{h_1}), (X_{h_2}, Y_{h_2}), \dots, (X_{h_m}, Y_{h_m})$. Rotation Υ of the beginning of direct lines which connect pairs of points of the same kind on unit circle is defined as:

$$\begin{pmatrix} \widetilde{X}_{p_1} \\ \widetilde{Y}_{p_1} \\ \widetilde{X}_{p_2} \\ \widetilde{Y}_{p_2} \\ \vdots \\ \widetilde{X}_{p_n} \\ \widetilde{Y}_{p_n} \\ \widetilde{X}_{h_1} \\ \widetilde{Y}_{h_1} \\ \widetilde{X}_{h_2} \\ \widetilde{Y}_{h_2} \\ \vdots \\ \widetilde{X}_{h_n} \\ \widetilde{Y}_{h_n} \end{pmatrix} = \begin{pmatrix} c_{p_1} & -s_{p_1} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ s_{p_1} & c_{p_1} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & c_{p_2} & -s_{p_2} & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & s_{p_2} & c_{p_2} & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & c_{p_n} & -s_{p_n} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & s_{p_n} & c_{p_n} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & c_{h_1} & -s_{h_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & s_{h_1} & c_{h_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & c_{h_2} & -s_{h_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & s_{h_2} & c_{h_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c_{h_n} & -s_{h_n} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{h_n} & c_{h_n} \end{pmatrix} \begin{pmatrix} X_{p_1} \\ Y_{p_1} \\ X_{p_2} \\ Y_{p_2} \\ \vdots \\ X_{p_n} \\ Y_{p_n} \\ X_{h_1} \\ Y_{h_1} \\ X_{h_2} \\ Y_{h_2} \\ \vdots \\ X_{h_n} \\ Y_{h_n} \end{pmatrix} \tag{25}$$

where $(X_{p_1}, Y_{p_1}), (X_{p_2}, Y_{p_2}), \dots, (X_{p_n}, Y_{p_n})$ and $(X_{h_1}, Y_{h_1}), (X_{h_2}, Y_{h_2}), \dots, (X_{h_m}, Y_{h_m})$ represent new coordinates of the beginning of lines after performed operation and $c_{p_1}, c_{p_2}, \dots, c_{p_n}$ $s_{p_1}, s_{p_2}, \dots, s_{p_n}$ stands for $c_{p_k} = \cos(\alpha_{p_k}), s_{p_k} = \sin(\alpha_{p_k})$, where we have operationally defined angles of rotation:

$$\alpha_{p_k} := \tilde{\theta}_{p_k} - \theta_{p_k}, \tag{26}$$

with

$$\alpha_{p_k} = \frac{2 r_k \pi}{2(n+m)} \tag{27}$$

and similarly, to hole operators, where $0 \leq r_k < 2(n+m)$. Regardless of the operator kind, for every k = 1, 2, 3, ..., $(n+m)$ must hold $\tilde{\theta}_k > \omega_k$ for counterclockwise, and $\tilde{\theta}_k < \omega_k$ for clockwise direction of setting points, where θ_k ($\tilde{\theta}_k$) represents old (new) angle between line connecting the center of unit circle S and a point related to the first operator (independent of operator kind) and a line connecting S and point related to the k-th creation operator, and similarly for ω_k for annihilation operator.

Lemma 3. Let W be a set of (special) equidistant points on unit circle connected with directed lines from the Definition 5. Set of all rotations Υ of points which are the beginning (or end) of directed lines from the Definition 5. is a group $\mathcal{R}$ with respect to the composition of rotations $\odot$ as a group operation.

Proof: Rotation of one end of each directed line is a subset of a discrete version of orthogonal group SO(2), the so called Z_n group, cyclic group of order n, which consists of rotations of the plane by an angle of $2\pi/n$ radians. Further, there exist additional constraint, i.e., new angles must satisfy $\tilde{\theta}_k > \omega_k$, for counterclockwise, and $\tilde{\theta}_k < \omega_k$ for clockwise choice of a direction for every k-th line (see the Definition 6.). Therefore, the group R corresponds to a subgroup of a group obtained by Cartesian product $Z_{n+m} \times Z_{n+m} \times \ldots \times Z_{n+m} = Z_{n+m} \oplus Z_{n+m} \oplus \ldots \oplus Z_{n+m}$ with additional constraints from the Definition 8., where $\oplus$ here denotes the direct sum.

First, we need to show that the group is closed with respect to rotation Υ, which means that applying any composition of operation performed on two arbitrary elements in the group always produces another element in the group. Second, note that angles in Υ are operatively defined, not with fixed values, therefore $\alpha_{p_1}, \ldots, \alpha_{p_n}, \alpha_{h_1}, \ldots, \alpha_{h_m}$ rather contain angle relations between pairs of corresponding points. In order to prove the closure property of the group, we need to show that additional condition from the Definition 8. also behave well for each $\Upsilon_1, \Upsilon_2 \in \mathcal{R}$ where $\Upsilon_1 = \Upsilon(\alpha_{p_1}, \ldots, \alpha_{p_n}, \alpha_{h_1}, \ldots, \alpha_{h_m})$ and $\Upsilon_2 = \Upsilon(\alpha_{p_1}, \ldots, \alpha_{p_n}, \alpha_{h_1}, \ldots, \alpha_{h_m})$ while the rest follow from the group properties of the $Z_{n+m} \oplus Z_{n+m} \oplus \ldots \oplus Z_{n+m}$ group. In other words, the composition of corresponding rotations is given by:

$$\Upsilon(\alpha_{p_1}, \ldots, \alpha_{p_n}, \alpha_{h_1}, \ldots, \alpha_{h_m}) \odot \Upsilon(\beta_{p_1}, \ldots, \beta_{p_n}, \beta_{h_1}, \ldots, \beta_{h_m}) = \Upsilon(\gamma_{p_1}, \ldots, \gamma_{p_n}, \gamma_{h_1}, \ldots, \gamma_{h_m}) \tag{28}$$

where from the properties of Z_{n+m} group we have: $(\alpha_k + \beta_k) \bmod 2\pi = \gamma_k$, for each k = 1, ... , $(n+m)$ regardless of kind, while from the Definition 8. we have:

$$\alpha_k = \frac{2\pi r_k}{2(n+m)}, \quad \beta_k = \frac{2\pi w_k}{2(n+m)}, \tag{29}$$

where $0 \leq r_k < 2(n+m)$, $0 \leq w_k < 2(n+m)$, from which

$$\frac{2\pi(r_k + w_k)}{2(n+m)} \bmod 2\pi = \frac{2\pi y_k}{2(n+m)} \tag{30}$$

where $0 \leq y_k < 2(n+m)$. By comparison must hold

$$\gamma_k = \frac{2\pi y_k}{2(n+m)} \tag{31}$$

which has the same form as for α_k and β_k. Condition $\tilde{\theta}_k > \omega_k$ must hold for each rotation for counterclockwise, and $\tilde{\theta}_k < \omega_k$ for clockwise direction of setting points on unit circle. In other words, composition of rotations of beginnings (or ends) of directed lines is another rotation $\Upsilon_3 = \Upsilon(\gamma_{p_1}, \ldots, \gamma_{p_n}, \gamma_{h_1}, \ldots, \gamma_{h_m})$, which satisfy the Definition 8., therefore the group $\mathcal{R}$ is closed.

Second, the existence of identity rotation $\Sigma \in \mathcal{R}$ follows directly from the properties of the Z_{n+m} group, where identity element is 0. In other words, in order to obtain $\alpha_k = 0$ the request is that for each line $r_k = 0$ ($k = 1, 2,...(n+m)$) regardless of operator species. Therefore, Σ must contain only rotation angles $\alpha_k = 0$ i.e., $\Sigma = \Upsilon(0,...,0)$, ie. for each $\Upsilon \in \mathcal{R}$ satisfies $\Sigma \odot \Upsilon = \Upsilon \odot \Sigma = \Upsilon$.

Third, for each Υ_1, Υ_2 and $\Upsilon_3 \in \mathcal{R}$, where $\Upsilon_1 = \Upsilon(\alpha_{p_1}, \dots, \alpha_{p_n}, \alpha_{h_1}, \dots, \alpha_{h_m})$, $\Upsilon_2 = \Upsilon(\beta_{p_1}, \dots, \beta_{p_n}, \beta_{h_1}, \dots, \beta_{h_m})$ and $\Upsilon_3 = \Upsilon(\gamma_{p_1}, \dots, \gamma_{p_n}, \gamma_{h_1}, \dots, \gamma_{h_m})$, we have:

$$(\Upsilon_1 \odot \Upsilon_2) \odot \Upsilon_3 = \Upsilon_1 \odot (\Upsilon_2 \odot \Upsilon_3), \tag{32}$$

which may be rewritten as in the previous step in the following form:

$$((\alpha_k + \beta_k) \bmod 2\pi + \gamma_k) \bmod 2\pi = (\alpha_k + (\beta_k + \gamma_k) \bmod 2\pi) \bmod 2\pi, \text{ for each } k = 1, \dots, (n+m) \text{ regardless of kind.} \tag{33}$$

The two expressions are equivalent because addition of angles is associative, i.e., the order in which we add three angles does not affect the result. From the previous step, the condition $\tilde{\theta}_k > \omega_k$ for counterclockwise, and $\tilde{\theta}_k < \omega_k$ for clockwise direction setting points on unit circle, must hold at each step of summation. Therefore, we can group the terms in either way and get the same result and we have proved the associativity.

Every element in a group has a unique inverse element. For any element $\Upsilon_1 \in \mathcal{R}$, there exists a unique element $\Upsilon_2 \in \mathcal{R}$ such that

$$\Upsilon_1 \odot \Upsilon_2 = \Upsilon_2 \odot \Upsilon_1 = \Sigma, \tag{34}$$

where the inverse element of Υ_1 is denoted by $\Upsilon_2 = \Upsilon_1^{-1}$.

$$\Upsilon(\alpha_{p_1}, \dots, \alpha_{p_n}, \alpha_{h_1}, \dots, \alpha_{h_m}) \odot \Upsilon(\beta_{p_1}, \dots, \beta_{p_n}, \beta_{h_1}, \dots, \beta_{h_m}) = \Upsilon(0, \dots, 0), \tag{35}$$

$$(\alpha_k + \beta_k) \bmod 2\pi = 0, \text{ for each } k = 1, \dots, (n+m) \text{ regardless of kind.} \tag{36}$$

from which we have the first case with $\alpha_k + \beta_k = 2\pi$ if both $\alpha_k \neq 0$ and $\beta_k \neq 0$, and the second case with $\alpha_k + \beta_k = 0$ if $\alpha_k = \beta_k = 0$. All other possibilities are excluded by the Definition 8. which put constraints on values of angles. Therefore, we have proven the last part and the group properties of $\mathcal{R}$.

Example 3.: Let us consider the multiplication table for the discrete rotation group $\mathcal{R}(hchhh^\dagger h^\dagger c^\dagger h^\dagger)$, where rotations Υ are defined operationally as: $e = \Upsilon(0,0,0,0)$, $\sigma_{13} = \sigma_{13} = \Upsilon(\theta_3 - \theta_1, 0, \theta_1 - \theta_3, 0)$, $\sigma_{14} = \Upsilon(\theta_4 - \theta_1, 0, 0, \theta_1 - \theta_4)$, $\sigma_{34} = \Upsilon(0, 0, \theta_4 - \theta_3, \theta_3 - \theta_4)$, $\tau_{413} = \Upsilon(\theta_4 - \theta_1, 0, \theta_1 - \theta_3, \theta_3 - \theta_4)$, $\tilde{\tau}_{341} = \Upsilon(\theta_3 - \theta_1, 0, \theta_4 - \theta_3, \theta_1 - \theta_4)$.

Table 2. Multiplication table for the discrete rotation group $\mathcal{R}(hchhh^\dagger h^\dagger c^\dagger h^\dagger)$.

$\odot$	e	σ_{13}	σ_{14}	σ_{34}	τ_{413}	$\tilde{\tau}_{341}$
e	e	σ_{13}	σ_{14}	σ_{34}	τ_{413}	$\tilde{\tau}_{341}$
σ_{13}	σ_{13}	e	$\tilde{\tau}_{341}$	τ_{413}	σ_{34}	σ_{14}
σ_{14}	σ_{14}	τ_{413}	e	$\tilde{\tau}_{341}$	σ_{13}	σ_{34}
σ_{34}	σ_{34}	$\tilde{\tau}_{341}$	τ_{413}	e	σ_{14}	σ_{13}
τ_{413}	τ_{413}	σ_{14}	σ_{34}	σ_{13}	$\tilde{\tau}_{341}$	e
$\tilde{\tau}_{341}$	$\tilde{\tau}_{341}$	σ_{34}	σ_{13}	σ_{14}	e	τ_{413}

Definition 9. Let $\mathcal{R}$ be a finite group of rotations and let W be a nonempty set from previous lemma and the Definition 5. respectively. The natural action of $\mathcal{R}$ on W is given by the function $\varphi : \mathcal{R} \times W \rightarrow W$ defined by:

$$\varphi(\Upsilon,w)=\varphi_{\Upsilon}(w)= \Upsilon \circ w = \Upsilon(w), \text{ for all } \Upsilon \in \mathcal{R} \text{ and all } w \in W \tag{37}$$

which satisfies the following conditions of a group actions:

i) for each $w \in W$ the identity element $\Sigma \in X$ fixes w, i.e., $\Sigma \circ w = \Sigma(w) = w$.
i) For each $\Upsilon_1, \Upsilon_2 \in \mathcal{R}$ and each $w \in W$ we have $(\Upsilon_2 \odot \Upsilon_1) \circ w = \Upsilon_2 \circ (\Upsilon_1 \circ w)$, where binary operation $\odot$ stands for the composition of rotations from the Definition 7.

Lemma 4. The set of all bijections from W to itself that can be obtained by applying elements of $\mathcal{R}$ to W, i.e., the set of functions φ_{Υ}, forms a group under composition of functions. This group is called the permutation group of $\mathcal{R}$ induced by the action of $\mathcal{R}$ on W and is denoted by $\mathcal{R}_W$.

Explanation: Steps of the proof are analogous to the ones of the proof of the Lemma 2. Therefore, it will not be discussed separately here.

Example 4.: For example, let $w_1,\ldots,w_6$ are the elements of the set W which corresponds to geometric interpretation of the full Wick's contractions shown on Fig. 5. with designations from *(15, 0), … , (15, 5)*. One can build all elements of the group starting from any of them by performing group action, i.e., rotations explained above. As an example, if we take w_2, we get:

$$\begin{gathered} e(w_2)=w_2,\ \sigma_{13}(w_2)=w_6,\ \sigma_{14}(w_2)=w_4, \\ \sigma_{34}(w_2)=w_1,\ \tau_{134}(w_2)=w_3,\ \tilde{\tau}_{134}(w_2)=w_5 \end{gathered} \tag{38}$$

Theorem 3. Let X_S and $\mathcal{R}_W$ be two groups described earlier. The induced group X_S is isomorphic to induced group $\mathcal{R}_W$.

Proof: First, we need to examine the structure of two groups X_S and $\mathcal{R}_W$. From Definitions 4. and 6. it follows directly that group X_S and $\mathcal{R}_W$ must always contain the same number of elements. They both satisfy group axioms, which is proven earlier in this work (see Lemmas 3. and 4.).

Second, let us assume that such mapping exists and is given by function h: $X_S \rightarrow \mathcal{R}_W$, defined as: $h(\phi_P)=\varphi_{\Upsilon}(w)$, for all $\phi_P \in X_S$ and all $\varphi_{\Upsilon} \in \mathcal{R}_W$. From the Definition 7., for every $\phi_P \in X_S$ and $g \in S$ we have $\phi_P(g) = g'$ where g' is just some element of the set S, and similarly from the Definition 9. for every $\varphi_{\Upsilon} \in \mathcal{R}_W$ and $w \in W$ we have $\varphi_{\Upsilon}(w) = w'$, where w' some element of set W. From the Theorem 2., which states that $g \xrightarrow{f} w$ for all $g \in S$ and all $w \in W$, in order to have group actions from Definitions 4. and 6., preserved, the function h must be both injection and surjection, i.e., bijection. To prove that we will assume the opposite situation, i.e., h is not surjection nor bijection. If h is not surjection, there exist some $\varphi_{\Upsilon'} \in \mathcal{R}_W$ which cannot be obtained by mapping h. But this is contradiction by the definition of function h, therefore the function must be surjection. On the other hand, let us assume that the function is not injection. Let $\phi_{P_1}, \phi_{P_2} \in X_S$ and $\varphi_{\Upsilon_1}, \varphi_{\Upsilon_2} \in \mathcal{R}_W$, if $\phi_{P_1} \xrightarrow{h} \varphi_{\Upsilon_1}$ and $\phi_{P_2} \xrightarrow{h} \varphi_{\Upsilon_2}$ then there must be some $\phi_{P_1} \neq \phi_{P_2}$ for which $\varphi_{\Upsilon_1} = \varphi_{\Upsilon_2}$. Therefore, for every $g \in S$ if $\phi_{P_1}(g) = g_1$ and $\phi_{P_2}(g) = g_2$, where both g_1 and g_2 are some elements of set S, from the Definition 7. follows that $g_1 \neq g_2$, while for every $w \in W$ from the Definition 9. follows that $\varphi_{\Upsilon}(w) = w'$, where $w' \in W$. However, from the Theorem 2. if $g_1 \xrightarrow{f} w'$ and $g_2 \xrightarrow{f} w'$, follows that $g_1 = g_2$ which is a contradiction. In other words, function h is an injection. When function is both injection and surjection, we conclude that h is a bijection.

In order to prove that mapping h is a homomorphism, we need to show that for each ϕ_{P_1} and $\phi_{P_2} \in X_S$ some φ_{Υ_1} and $\varphi_{\Upsilon_2} \in \mathcal{R}_W$ we have: $\phi_{P_1} \circ \phi_{P_2} \xrightarrow{h} \varphi_{\Upsilon_1} \star \varphi_{\Upsilon_2}$. Let us assume that there exists such homomorphism h. For each $g \in S$ and all $w \in W$, and for each P_1 and $P_2 \in S$ some Υ_1 and $\Upsilon_2 \in W$ if $P_1(g) \xrightarrow{f} \Upsilon_1(w)$ and $P_2(g) \xrightarrow{f} \Upsilon_2(w)$, follows that $P_1 \otimes P_2(g) \xrightarrow{f} \Upsilon_1 \odot \Upsilon_2(w)$. In order to prove previous statement, from the Lemma 1. follows that for each $P_1, P_2 \in X$ and $g \in S$ we have $P_1 \otimes P_2 = P_3$ where $P_3 \in X$, so $P_3(g) = g'$, where $g' \in S$ by the Definition 7. Similarly, from the Lemma 4. for each $\Upsilon_1, \Upsilon_2 \in \mathcal{R}$ and $w \in W$, we have $\Upsilon_1 \odot \Upsilon_2 (w) = \Upsilon_3 (w)$, from which $\Upsilon_3 (w) = w'$, where $w' \in W$ by the Definition 9. On the other hand, the Theorem 2. states that the mapping between graph-like objects from the Definition 5., i.e., $g' \xrightarrow{f} w'$ for all $g' \in S$ and $w' \in W$ is a homomorphism, therefore must hold $P_1 \otimes P_2(g) \xrightarrow{f} \Upsilon_1 \odot \Upsilon_2(w)$. From previous statements follows that $P_1 \otimes P_2(g) \xrightarrow{h} \Upsilon_1 \odot \Upsilon_2$, so $\phi_{P_3} \xrightarrow{h} \varphi_{\Upsilon_3}$. Therefore, such homomorphism h exists and we have proven the third part.

One can easily see how homomorphism h impose these conditions on the mapping, i.e., for identity bijection $\phi_E \in X_S$ we have: for each $\phi_P \in X_S$ must hold $\phi_P \circ \phi_E = \phi_P$. Since h is a homomorphism, $h(\phi_P \circ \phi_E)=h(\phi_P)\star h(\phi_E)$, so $h(\phi_P)=h(\phi_P)\star h(\phi_E)$. By cancelation laws for groups, this means that $h(\phi_E)= \varphi_\Sigma$, which is identity in the group $\mathcal{R}_W$. This is rather general property of the homomorphisms than this specific case, i.e., they always map unique identity element of one group to the unique identity element of another group. Similarly, inverse element of ϕ_P is also mapped to the inverse of the element $h(\phi_p)$.

From the point 5) of the Definition 5. for all $g \in S$ and $w \in W$ if $g \xrightarrow{f} w$ then $sign(g) = sign(w)$. Further, from the Definitions 7. and 9. for some $P \in \mathrm{X}$ and some $\Upsilon \in \mathcal{R}$ $sign(P(g))$ may be different than $sign(g)$ and similarly $sign(\Upsilon(w))$ may also be different from $sign(w)$, therefore it is not necessarily conserved by respective operations. However, for each $g \in S$ and $w \in W$ and for each $P \in \mathrm{X}$ and some $\Upsilon \in \mathcal{R}$ if $g \xrightarrow{f} w$ and $P(g) \xrightarrow{f} \Upsilon(w)$ follows that $sign(P(g)) = sign(\Upsilon(w))$. From the previous statement follows that for each $\phi_P \in X_S$ and some $\varphi_\Upsilon \in \mathcal{R}_W$ if $\phi_P \xrightarrow{h} \varphi_\Upsilon$ then $parity(\phi_P)=parity(\varphi_\Upsilon)$. Similarly, for each $g \in S$ and $w \in W$, and for each $P_1, P_2 \in \mathrm{X}$ and some $\Upsilon_1, \Upsilon_2 \in \mathcal{R}$ if $P_1(g) \xrightarrow{f} \Upsilon_1(w)$ and $P_2(g) \xrightarrow{f} \Upsilon_2(w)$, then $sign(P_1 \otimes P_2(g)) = sign(\Upsilon_1 \odot \Upsilon_2(w))$. Therefore, for each ϕ_{P_1} and $\phi_{P_2} \in X_S$ and some φ_{Υ_1} and $\varphi_{\Upsilon_2} \in \mathcal{R}_W$ if $\phi_{P_1} \circ \phi_{P_2} \xrightarrow{h} \varphi_{\Upsilon_1} \star \varphi_{\Upsilon_2}$ then $parity(\phi_{P_1} \circ \phi_{P_2})=parity(\varphi_{\Upsilon_1} \star \varphi_{\Upsilon_2})$ and we have proven this part. Consequently, we also have that for each $g \in S$ and $w \in W$ if $g \xrightarrow{f} w$ and E is identity in X and Σ is identity in $\mathcal{R}$, then $sign(E(g)) = sign(\Sigma(w))$, while for inverses $sign(P^{-1}(g)) = sign(\Upsilon^{-1}(w))$. Therefore, for the identity bijection ϕ_E in X_S and φ_Σ in $\mathcal{R}_W$ we have $parity(\phi_E)=parity(\varphi_\Sigma)$. On the other hand, for each $\phi_P \in X_S$ and some $\varphi_\Upsilon \in \mathcal{R}_W$, if ϕ_P^{-1} is an inverse of ϕ_P, φ_Υ^{-1} is an inverse of φ_Υ and $\phi_P \xrightarrow{h} \varphi_\Upsilon$, then $\phi_P^{-1} \xrightarrow{h} \varphi_\Upsilon^{-1}$ and $parity(\phi_P^{-1})=parity(\varphi_\Upsilon^{-1})$. Consequently, we also have $parity(\phi_P^{-1})=parity(\phi_P)$ and $parity(\varphi_\Upsilon^{-1})=parity(\varphi_\Upsilon)$.

One can easily prove bijection h^{-1} is also homomorphism by interchanging two induced groups. From the Theorem 2., the sign operation holds in both directions, therefore it must also hold for the mapping h^{-1}. All steps are the same as in the case of the function h. Therefore, the mapping h^{-1} is also homomorphism. From previous steps one finds that there is one-to-one correspondence between two induced groups, therefore there exist an isomorphism between them. From the mathematical side, we have proven all necessary parts needed to build our algorithm.

Example 5.: Let us take w_1 from previous example which has the contraction $sign(w_1)=-1$. Performing operations with negative parity, such as transpositions of one end of two lines, σ_{13}, σ_{14}, and σ_{34} respectively, one gets elements with opposite sign, i.e., 1. Identity and rotations of one end of three lines at the same time have the positive parity, which means they always lead to elements with the same sign result. Note, that the previous explanation is valid regardless of the choice of the element $w \in W$. Also, note that E, σ_{13}, σ_{14}, and σ_{34} have inverses which are in fact themselves and inverse of τ_{413} is just $\tilde{\tau}_{341}$ (and opposite). Because of the Definition 8. for every $w \in W$ the $sign(\tau_{413}(w)) = sign(\tilde{\tau}_{341}(w))$.

3. Description of the FWC-QMBFS Algorithm

The full code in C programming language may be found on the webpage with complete pseudocode description of the algorithm and examples, i.e., the link is: https://github.com/denivale/FWC-QMBFS.

The algorithm starts from reading data from input file using simple syntax, where data here represent creation and annihilation fermion operators that usually appears in calculation of quantum mechanical expectation values in particle-hole many-body picture. The canonical transformation to particle and hole operators is also provided in the first step of calculation if one uses general operators for one- or two-body terms, transition or density matrix elements.

After performing canonical transformation of general operators, we need to calculate full Wick's contraction of quantum mechanical operators. Previous step may be avoided if the calculation of the expectation value does not contain any operator of the general type. First it necessary to check whether we have an even number of operators. If that number is odd, the function immediately returns 0. While calculating full Wick's contraction for each combination, it is enough to check whether at any moment of counting we have different number of creation and annihilation hole (particles) operators. If there is an excess or deficiency of creation operators with respect to annihilation operators of each kind, the result for combination is 0. In other words, the failure to fulfill at least one of the conditions means the disappearance of the expected value for corresponding combination.

The next step includes mapping between a set of full Wick's contraction S (see the Definition 4.) and a set of equidistant points on unit circle W with rules described in the Definition 5. and an isomorphism between two sets S and W from the Theorem 2. Note that each element of the set S corresponds to the specific arrangement of pairs of operators connected with Wick's lines for each possible nonvanishing combination. If the conditions from previous step are fulfilled, the calculation of each contraction line is performed for each arrangement of operators. This corresponds to the creation of all permutations of one end of Wick's lines, i.e., the creation operator. Note that from any nonvanishing arrangement of Wick's contraction lines one can achieve every other nonvanishing realization, which is by Theorem 3. also true for rotations of one end of directed lines on the unit circle. The last geometric representation is particularly useful for the calculation number of intersection. The complete calculation takes place in several steps: i) Checking whether it is possible to realize a contraction line between each pair of operators. If there is a contraction line that cannot be realized, then the result is 0 for specific arrangement. ii) If all contraction lines between pairs of operators for a given permutation can be realized, we calculate the sign of Wick's contractions. iii) The contraction line is valid of two operators if the following conditions are met: a) The two operators must correspond to an annihilation and a creation operator of the same type, b) The annihilation operator must precede the creation operator. The procedure is repeated for each permutation of the Wick's lines, i.e., arrangement of Wick's contraction lines, but also for all non-vanishing combinations obtained after canonical transformation of operators to particle-hole picture. If the contraction is successfully performed, the contraction result is saved in the form of Kronecker type data which also contains information whether it is related to states above or below Fermi level. The sign calculation from point ii) corresponds to the calculation of the number of intersections of directed lines within the unit circle, which is -1 if the number of intersections is odd, or 1 if the number of intersections is even number or zero.

In the last step of the algorithm the result is printed on standard output. Complete mathematical procedure done by algorithm presented here may also be exported in latex output, converted to pdf and also shown in pdf viewer. Geometrical interpretation of Wick's contraction can be exported in various data types, such as pdf, eps or dvi, and viewed. It is stored with specific ordering, i.e., containing information of the order of combination used in calculation and permutation index (which are both just the matter of choice, i.e., the algorithm used).

4. Results

Averaged calculation times of expectation values of $N \lesssim 6$ quantum mechanical operators containing general or only particle (hole) type are $t_{calc} \lesssim 60$ ms (Intel i7 processor, 8 GB RAM), with calculation time difference between operators of general and particular type (holes or particles) which is less than 20 ms. The former can be explained by the necessary canonical transformations of general operators into particles or holes as intermediate step in calculation of expectation values, which in turn increases the number of combinations of particle and/or hole operators, i.e., corresponding bra-kets with non-vanishing Wick's contractions. The difference is even larger for $N>6$ operators, usually few times larger than only particle (hole) case, due to larger number of particle and/or hole nonvanishing combinations. The results of the computation time for different numbers of operators are shown in Fig. 2.

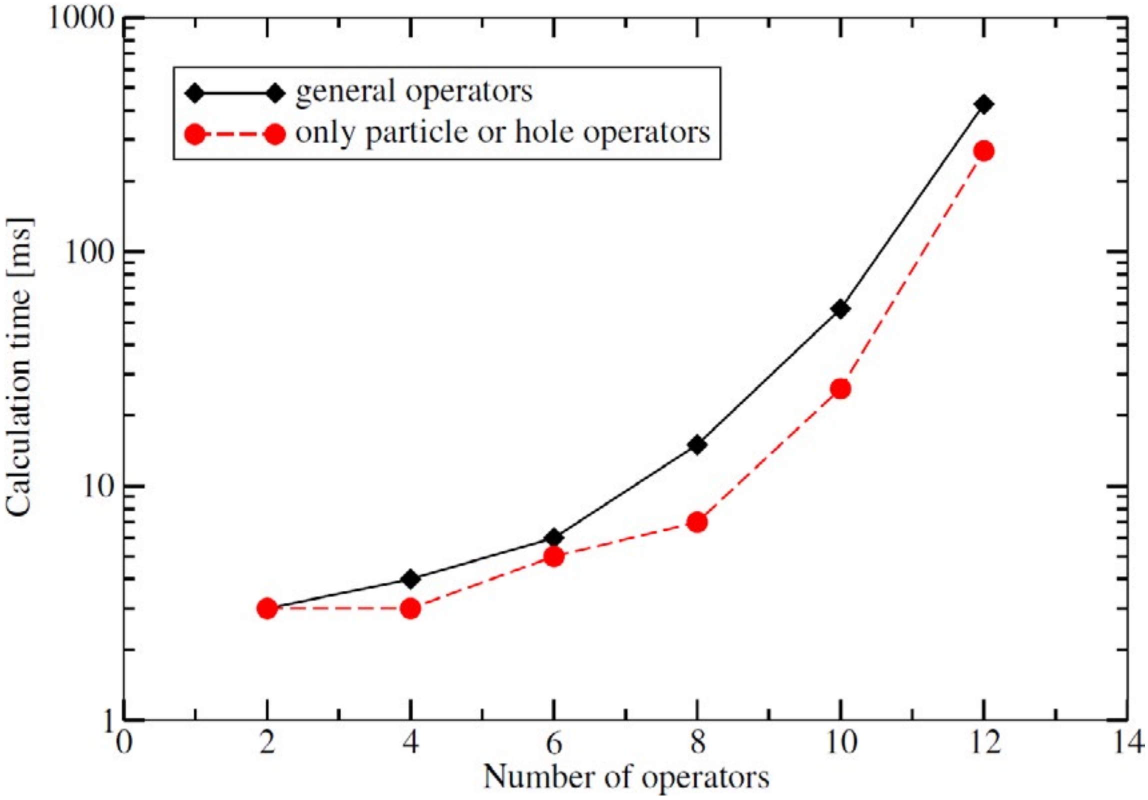


Fig. 2. Averaged calculation time for full Wick's contractions for various number of second quantization general and only particle (only hole) operators without latex or eps/dvi/ps geometrical interpretation output

In the following we demonstrate the importance of our algorithm by showing few calculations of specific arrangements of quantum operators used in many-body theories such as Hartree-Fock and RPA (see Example 1.). For both canonical transformation of operators to particles and hole type is done in the first step of the calculation, after which the operators are connected with the corresponding Wick's lines. In the next step each arrangement of the Wick's lines is mapped into the unit circle after which full Wick's contraction procedure is performed, as described in previous section, with the result written as the sum of Kronecker deltas and theta functions. The elements of the set W, which we will refer here as the geometrical interpretation of Wick's contraction, are obtained in the intermediate step.

The calculation of two body terms in Hartree-Fock approximation is related to the set S from the Example 1.a). Performed mathematical procedure is the output of our computational algorithm, which is shown in Fig. 3. The geometrical interpretation (the set W) is shown on the Fig. 4.

$$
\begin{aligned}
\langle HF|a_a^\dagger a_b^\dagger a_c a_d|HF\rangle &= \langle HF|h_a h_b h_c^\dagger h_d^\dagger|HF\rangle \\
&= \langle HF|h_a h_b h_c^\dagger h_d^\dagger|HF\rangle + \langle HF|h_a h_b h_c^\dagger h_d^\dagger|HF\rangle \\
&= (-1)\delta_{ac}\Theta_{Fa}\delta_{bd}\Theta_{Fb} + \delta_{ad}\Theta_{Fa}\delta_{bc}\Theta_{Fb}
\end{aligned}
$$

Fig. 3. Latex output of the calculation of the expectation value of the particle-hole contributions to Hartree-Fock two body term.

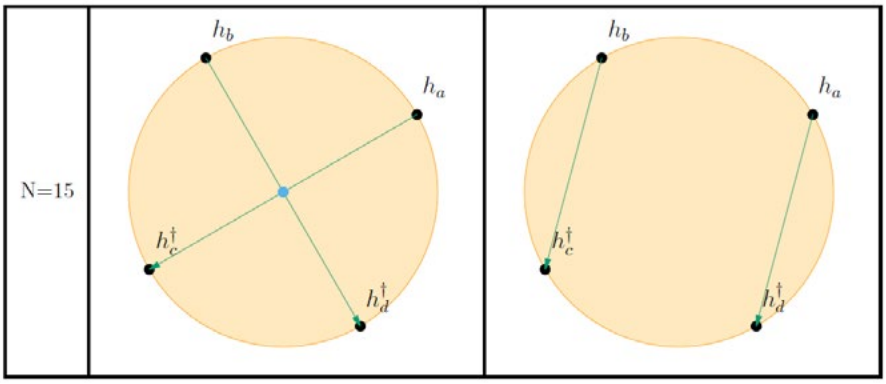


Fig. 4. Geometrical interpretation of full Wick's contractions related with calculation of the expectation value of the operators of the two-body particle-hole term in the Hartree-Fock approximation.

According to the Thouless theorem, it is possible to connect two arbitrary non-orthogonal states of the nucleus as $|\Psi\rangle = e^{\hat{S}}|\Phi\rangle$, where S is an operator that enables this by creating various combinations of particle-annihilation pairs or various complex configurations (Thouless, 1960). Usually, we are interested in the case where Slater determinant $|\Phi\rangle$ is describing the ground state. Therefore, for two-body element we have (Da Providência, 1965):

$$\langle\Psi|V|\Psi\rangle = \langle\Phi|\left(1+\hat{S}^\dagger+\frac{1}{2}(\hat{S}^2)^\dagger+\ldots\right)\frac{1}{4}\sum_{abcd}\hat{v}_{abdc}a_a^\dagger a_b^\dagger a_c a_d\left(1+\hat{S}+\frac{1}{2}\hat{S}^2+\ldots\right)|\Phi\rangle \quad (39)$$

In order to calculate expectation value of the two-body particle-hole term in the so-called random phase approximation (RPA) we need to investigate the following term:

$$\langle\Psi|V|\Psi\rangle^{(2,2)} = \frac{1}{4}\sum_{abcd}\hat{v}_{abdc}\langle\Phi|\hat{S}^\dagger a_a^\dagger a_b^\dagger a_c a_d\hat{S}|\Phi\rangle \quad (40)$$

The procedure for the calculation of expectation values of operators which are related to the two-body term of the RPA A matrix, which is the latex output of our computer program as in the first case and it is presented in Fig. 5. We are focused on the first order RPA only, therefore the operator $\hat{S}$ describes only particle-hole configurations, i.e., $\hat{S} = \sum C_{mi} C_m^\dagger h_i^\dagger$. Each contraction term corresponds to different physical process in the particle-hole many-body picture. The first six terms on the Fig. 5., which correspond to the 5th, 6th, 9th and 10th combination of the canonical transformation of operators, are presented in the Fig. 6., while the last six terms from the Fig. 5. are presented in the Fig. 7.

$$
\begin{aligned}
&\langle HF|h_i c_m a_a^\dagger a_b^\dagger a_c a_d c_o^\dagger h_k^\dagger|HF\rangle \;= \\
&= \langle HF|h_i c_m c_a^\dagger h_b c_c h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m c_a^\dagger h_b c_c h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle \\
&+ \langle HF|h_i c_m c_a^\dagger h_b h_c^\dagger c_d c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m c_a^\dagger h_b h_c^\dagger c_d c_o^\dagger h_k^\dagger|HF\rangle \\
&+ \langle HF|h_i c_m h_a c_b^\dagger c_c h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m h_a c_b^\dagger c_c h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle \\
&+ \langle HF|h_i c_m h_a c_b^\dagger h_c^\dagger c_d c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m h_a c_b^\dagger h_c^\dagger c_d c_o^\dagger h_k^\dagger|HF\rangle \\
&+ \langle HF|h_i c_m h_a h_b h_c^\dagger h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m h_a h_b h_c^\dagger h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle \\
&+ \langle HF|h_i c_m h_a h_b h_c^\dagger h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m h_a h_b h_c^\dagger h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle \\
&+ \langle HF|h_i c_m h_a h_b h_c^\dagger h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle + \langle HF|h_i c_m h_a h_b h_c^\dagger h_d^\dagger c_o^\dagger h_k^\dagger|HF\rangle \\
&= \delta_{id}\Theta_{Fi}\delta_{bk}\Theta_{Fb}\delta_{ma}\Theta_{mF}\delta_{co}\Theta_{cF} - \delta_{ik}\Theta_{Fi}\delta_{bd}\Theta_{Fb}\delta_{ma}\Theta_{mF}\delta_{co}\Theta_{cF} \\
&- \delta_{ic}\Theta_{Fi}\delta_{bk}\Theta_{Fb}\delta_{ma}\Theta_{mF}\delta_{do}\Theta_{dF} + \delta_{ik}\Theta_{Fi}\delta_{bc}\Theta_{Fb}\delta_{ma}\Theta_{mF}\delta_{do}\Theta_{dF} \\
&- \delta_{id}\Theta_{Fi}\delta_{ak}\Theta_{Fa}\delta_{mb}\Theta_{mF}\delta_{co}\Theta_{cF} + \delta_{ik}\Theta_{Fi}\delta_{ad}\Theta_{Fa}\delta_{mb}\Theta_{mF}\delta_{co}\Theta_{cF} \\
&+ \delta_{ic}\Theta_{Fi}\delta_{ak}\Theta_{Fa}\delta_{mb}\Theta_{mF}\delta_{do}\Theta_{dF} - \delta_{ik}\Theta_{Fi}\delta_{ac}\Theta_{Fa}\delta_{mb}\Theta_{mF}\delta_{do}\Theta_{dF} \\
&- \delta_{ic}\Theta_{Fi}\delta_{ad}\Theta_{Fa}\delta_{bk}\Theta_{Fb}\delta_{mo}\Theta_{mF} + \delta_{ic}\Theta_{Fi}\delta_{ak}\Theta_{Fa}\delta_{bd}\Theta_{Fb}\delta_{mo}\Theta_{mF} \\
&+ \delta_{id}\Theta_{Fi}\delta_{ac}\Theta_{Fa}\delta_{bk}\Theta_{Fb}\delta_{mo}\Theta_{mF} - \delta_{id}\Theta_{Fi}\delta_{ak}\Theta_{Fa}\delta_{bc}\Theta_{Fb}\delta_{mo}\Theta_{mF} \\
&+ \delta_{ik}\Theta_{Fi}\delta_{ad}\Theta_{Fa}\delta_{bc}\Theta_{Fb}\delta_{mo}\Theta_{mF} - \delta_{ik}\Theta_{Fi}\delta_{ac}\Theta_{Fa}\delta_{bd}\Theta_{Fb}\delta_{mo}\Theta_{mF}
\end{aligned}
$$

Fig. 5. Latex output of the calculation of the expectation value of the operators of the particle-hole contributions to the A matrix in RPA. The output of the canonical transformation of operators is omitted here in the first step of the calculation.

After inserting the result of full Wick's contraction back to the expression in eq. (29) we obtain:

$$
\begin{aligned}
\langle\Psi|V|\Psi\rangle_1^{(2,2)} &= \sum_{mnij} C_{mi}^* C_{nj}\hat{v}_{mjin} + \sum_{mnij} C_{mi}^* C_{ni}\hat{v}_{mjnj} - \sum_{mijk} C_{mi}^* C_{mj}\hat{v}_{kjki} \\
&+ \frac{1}{2}\sum_{mijk} C_{mi}^* C_{mi}\hat{v}_{jkjk}
\end{aligned}
\tag{41}
$$

In other words, when combined with asymmetric matrix element $\hat{v}_{abdc}$ and expansion coefficients C_{mi}^* and C_{nj}, each of them can be related to different physical processes described by 8 topologically distinct Goldstone-Providencia diagrams (Da Providência, 1963; Mattuck, 1967), which are shown in the Fig. 8. Second column in Fig. 8. corresponds to direct (Hartree) terms, while the third column corresponds to exchange (Fock) terms. As an example of the Hartree contribution let us focus on the first term in eq. (41):

$$
C_{m2}^* C_{n4} v_{m42n}\langle\Phi|h_2 c_m c_m^\dagger h_4 c_n h_2^\dagger c_n^\dagger h_4^\dagger|\Phi\rangle \tag{42}
$$

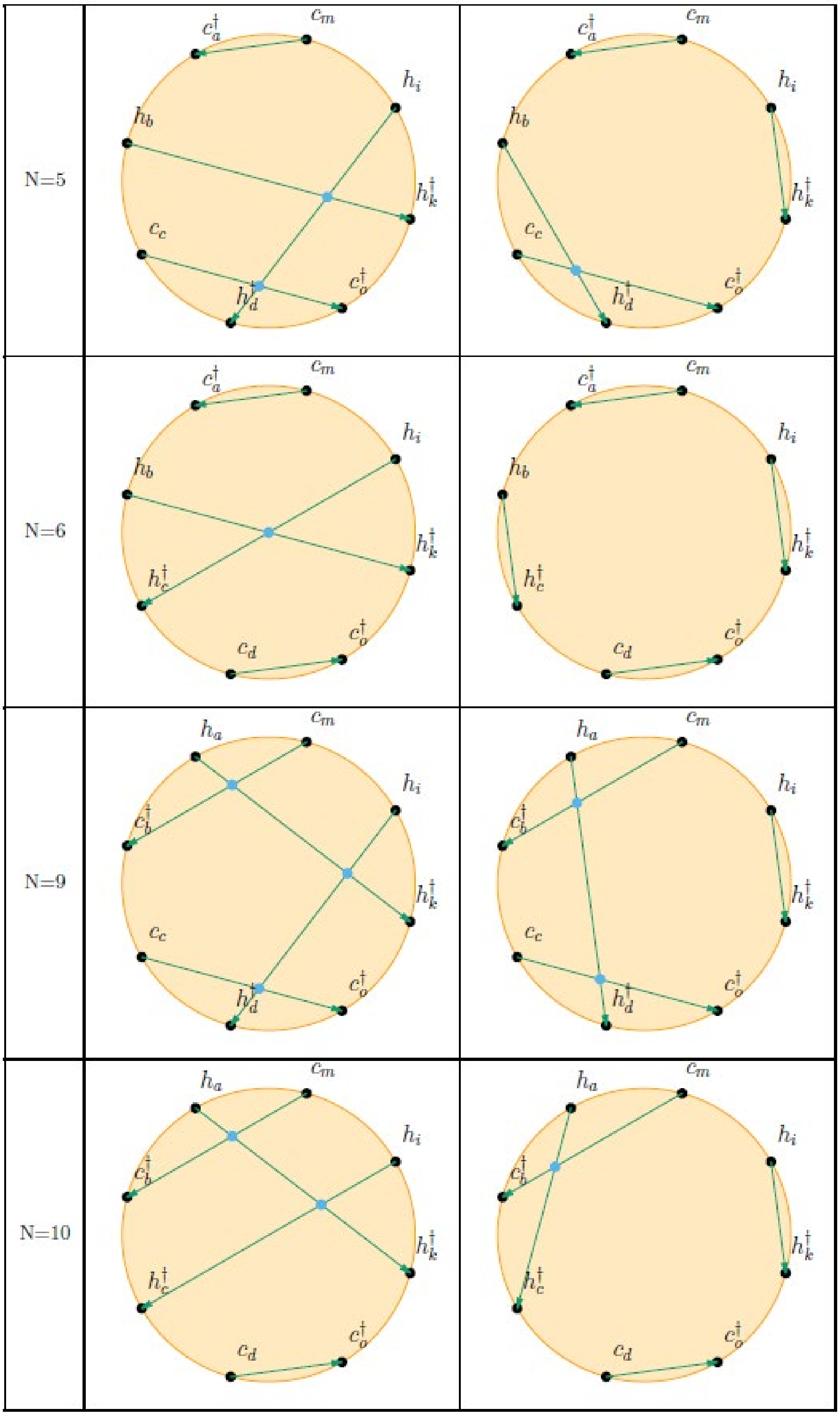


Fig. 6. Geometrical interpretation of the full Wick's contractions (set W) related with calculation of the expectation value of the operators of the particle-hole contribution to the RPA A matrix, in particular sets from S_1 to S_4 from Example 1.

It describes the process in which the response of the system to the external field is first manifested in the creation of the particle-hole pair $n4$, with the realization amplitude C_{n4}. The mentioned pair is then propagated until the moment when, due to the interaction with the rest of the system, i.e. the particles within the Fermi sea, the particle scatters from the n state to the 2 state, which is the annihilation process of the mentioned pair, and the (simultaneous) creation of the $m2$ pair which is propagated until some later moment in which the annihilation occurs due to the relaxation of the system. The amplitude of the annihilation realization of the particle-hole pair is shown by C^*_{mi}. This process is shown in the first row and the second column of the Fig.8. First term in eq. (41) also contains the Fock contribution:

$$C^*_{m2}C_{n4}v_{m4n2}\langle\Phi|h_2c_mc^\dagger_m h_4h^\dagger_2c_nc^\dagger_n h^\dagger_4|\Phi\rangle \tag{43}$$

which represents the case when we first have the formation of the particle-hole pair $n4$, where due to mutual interaction, the hole scatters from state 4 to state 2, and the particle from state n to state m, that would later lead to the annihilation of the pair $m2$. As before, we relate the coefficients C_{n4} and C^*_{m2} to the creation and annihilation of the particle-hole pairs. This process is shown in the first row and the third column of the Fig.7. Variation with respect to the density matrix, i.e., corresponding expansion coefficients C^*_{mi} and C_{nj} from Thouless theorem, leads to the RPA A matrix.

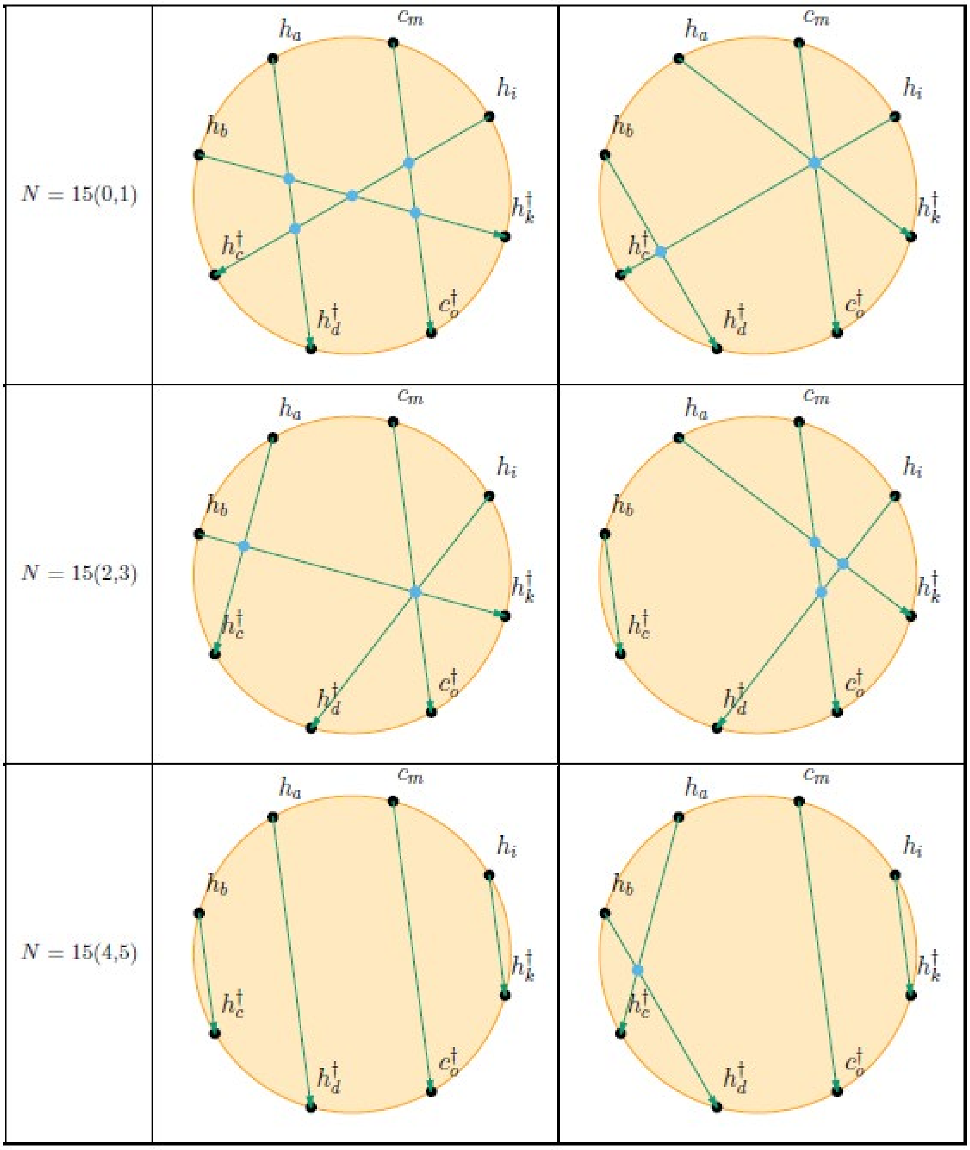


Fig. 7. Geometrical interpretation of the full Wick's contractions (set W) related with calculation of value of the operators of the particle-hole contribution to the RPA A matrix, in particular set from Example 1.

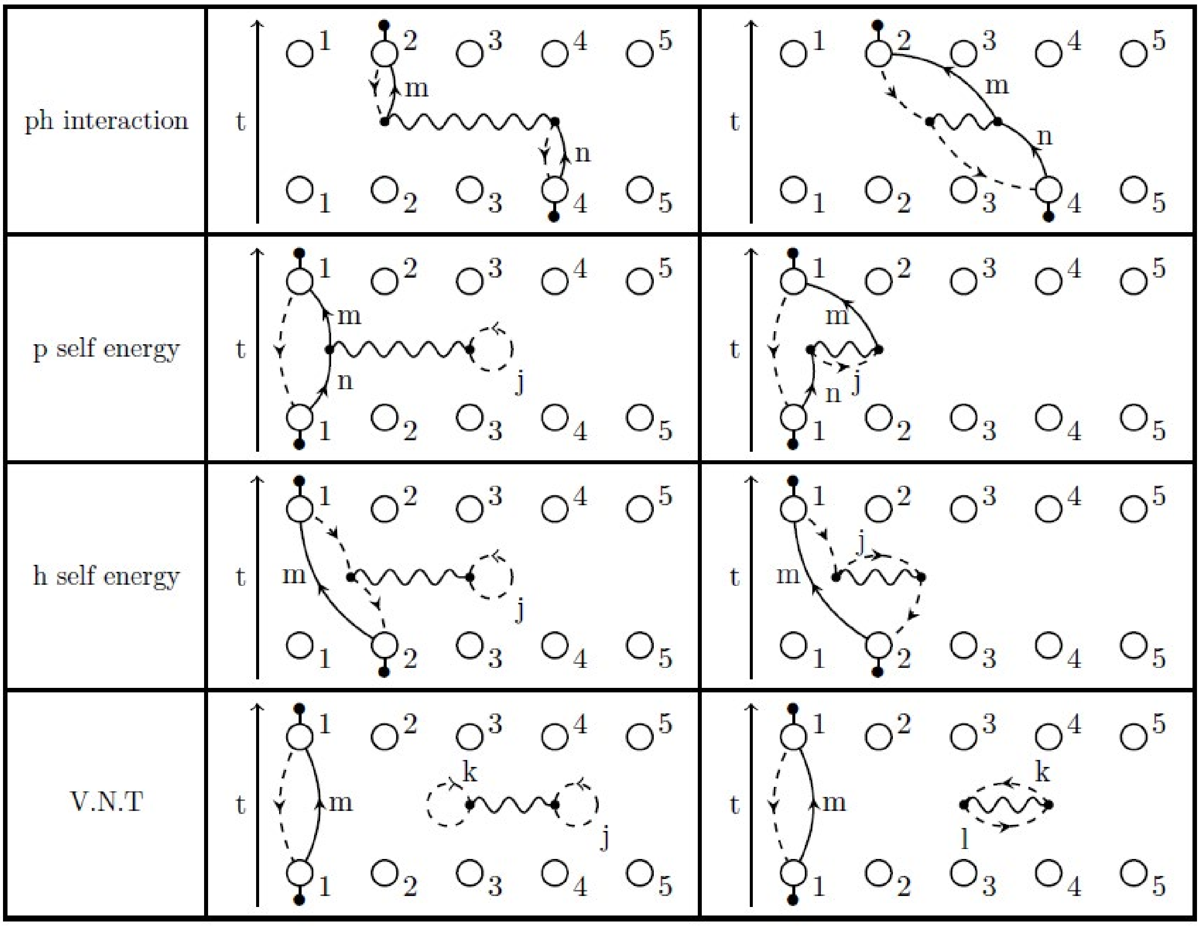


Fig. 8. Goldstone-Da Providencia diagrams for physical processes related to RPA A matrix. Vertical arrow represents time flow. Empty large circles represent states below Fermi level, smaller filled circles amplitudes of creation or annihilation of phonons, arrows propagation of particle and dashed arrows of hole state (Da Providência, 1963; Mattuck 1967). The abbreviation V. N. T. stands for "vacuum normalization terms", i.e., terms which are cancelled after variation with respect to density matrix.

Summary

In conclusion, Wick's contractions are an essential tool in the study of quantum many body systems. We have formulated two theorems related to the observed isomorphism between graph-like objects which are in fact contained in the full Wick's contractions and some geometrical objects, such as circle or regular rectangle with internal structure, and an isomorphism between two induced groups, i.e., permutations of one end of Wick's lines and rotations of directed lines inside geometrical object.

In this paper we have presented fast and efficient algorithm for the calculation of Wick's contractions based on the observed isomorphisms. We have tested the execution time of the computer program for different numbers of creation and annihilation operators of the same kind and found that time of the execution increases almost exponentially with the total number of operators, and the case which involves general operators, which results in few times larger execution time with respect to the case of operators of one kind due to additional canonical transformation procedure. We have presented the tex and geometrical output (figures) of the computer program for few representative cases. Also, we have given the connection between results of the Wick's contractions and related physical process in Hartree-Fock theory and Random phase approximation.

Wick's contractions allow physicists to gain a deeper understanding of many body systems, and they continue to play a crucial role in our understanding of the behavior and interactions of particles on a microscopic scale.

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Sažetak

Wickove kontrakcije, također povezane s Wickovim teoremom, predstavljaju važnu matematičku tehniku koja se koristi u kvantnoj mnogočestičnoj teoriji za pojednostavljenje izračuna koji uključuje operatore stvaranja i poništenja. U ovom radu proučavali smo svojstva potpunih Wickovih kontrakcija i detaljno raspravili kontrakcije s aspekta teorije grafova i teorije grupa. Promatrali smo izomorfizam između objekata nalik grafovima koji su zapravo sadržani u punoj Wickovoj kontrakciji i nekoliko geometrijskih objekata, poput kružnice i pravilnog poligona koji imaju unutarnju strukturu. Također smo pronašli izomorfizam između dvije inducirane grupe, jedne koja je povezana s permutacijama jednog kraja Wickovih linija i druge koja odgovara rotacijama usmjerenih linija unutar geometrijskog objekta. Predstavili smo brz i učinkovit algoritam za izračun očekivane vrijednosti velikog broja operatora stvaranja i poništenja čestica i šupljina kako bismo izračunali različite čestično-čestične ili čestično-šupljinske članove u mnogočestičnim teorijama, od nuklearne fizike do fizike čvrstog stanja ili kvantne kemije. Naš algoritam temelji se na opaženim izomorfizmima. Potpune Wick-ove kontrakcije svodi na jednostavne relacije susjedstva i geometrijske odnose, koje smo također iskoristili za određivanje njihova predznaka. Također, prezentirali smo nekoliko ilustrativnih primjera računanja, poput dvočestičnih čestica-šupljina članova koji se pojavljuju u Hartree-Fockovoj teoriji i aproksimaciji slučajnih faza.

Ključne riječi: *Wickov teorem, Wick-ove kontrakcije, teorija grupa, teorija grafova, kvantna mehanika, kvantna mnogočestična teorija, Hartree-Fock, aproksimacija slučajnih faza*