General mapping for bosonic and fermionic operators in Fock space

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In this article, we provide an alternative and general way to construct the result of the action of any particle-conserving bosonic or fermionic operator represented in second quantized form on a state vector, without resorting to the matrix representation of operators or even its elements. This approach is based on our proposal to compactly enumerate the configurations (i.e., determinants for fermions, permanents for bosons) that are the elements of the state vector. This extremely simplifies the calculation of the action of an operator on a state vector. The computations of statical properties and the evolution dynamics of a system become much more efficient, and applications to systems made of more particles become feasible. Explicit formulations are given for spin-polarized fermionic systems and spinless bosonic systems, as well as to general (two-component) fermionic systems, two-component bosonic systems, and mixtures thereof.

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I. INTRODUCTION

The well-known time-dependent Schrödinger equation governs the dynamics of many-particle quantum systems in different fields of modern physics [1–7]. To define a quantum system means to specify its Hamiltonian. A quantum system is considered to be made of interacting constituent parts, usually treated as point particles with some known characteristics such as mass and charge. If the interaction potential between these particles is known, then the Hamiltonian of the quantum system is defined. Eigenvectors and eigenvalues of this Hamiltonian provide complete description of all the properties of the considered isolated quantum system.

In general, exact solutions for many-particle Hamiltonians are not known and, therefore, different numerical approaches and techniques are in use [1–8]. The most basic and simplest approach is to represent the *unknown* many-body wave function as a linear combination of some *known* many-body wave functions, that is, to expand the solution in a known basis set. To solve the problem means to find the expansion coefficients or their evolution, depending on whether one performs time-independent or time-dependent studies.

For a quantum system made of indistinguishable particles (e.g., fermions or bosons) along with the Hamiltonian, one has also to specify the quantum statistics of the system. Statistics enters the many-body solution via the basis set used: If each and every basis function fulfills a defined quantum statistics, then any linear combination of the basis functions also possesses the same statistics. From the other end, statistics reduces the required size of the Hilbert subspace; that is, it allows one to operate with a smaller number of many-body basis functions.

In this article, we specifically deal with a system of N identical particles. We utilize the commonly used many-body basis functions for bosons, permanents [5], which are constructed as symmetrized products of N one-particle functions or orbitals, and for fermions, determinants, which are antisymmetrized Hartree products of orbitals [8]. All many-body basis functions (determinants or permanents) are attributed to configurations where N particles reside in M orbitals; for bosons, $M \geqslant 1$, and for fermions, $M \geqslant N$. For orthonormal many-body basis sets, one can associate the number of the many-body basis functions used with the size of the respective Hilbert subspace. Intuitively, it is clear that a larger number of independent many-body basis functions provides a better description of the many-body solution. The expansion spanned by all possible permutations for fixed M and N is referred to as a full configurational expansion or a full Fock subspace. If the many-body wavefunction is represented as a linear combination of permanents for bosons and determinants for fermions, then the Hamiltonian of the system as well as any other operator can also be expressed in second quantized form.

Once the finite many-body basis set is specified, one can construct the respective Hamiltonian matrix. Straightforward implementation of the standard quantum mechanical rules requires construction and operations with this Hamiltonian matrix. For example, typical diagonalization or propagation schemes, such as the short iterative Lanczos (SIL) [9], utilize as a standard building block the product of this matrix to a corresponding state vector, representing the many-body wave function. In this work, we propose an absolutely different "ideology," which allows us to get the required result of the action of the Hamiltonian on a state vector without construction of the Hamiltonian matrix at all. The proposed theory can be effectively and naturally applied to any general particle-conserving operator represented in second quantized form. The construction and operation with the corresponding matrix is not needed. We show the generality and applicability of this theory to systems of fermions, bosons, and mixtures thereof. In the present work, we treat particle-conserving operators only. In the following, we do not indicate explicitly "particle-conserving" when it is unambiguous.

The proposed theory has already been implemented for bosonic systems [10,11] within the multiconfigurational

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time-dependent Hartree for bosons (MCTDHB) [12]. Applications to multiboson long-time dynamics in double-well [10] and triple-well [11] traps have already been performed successfully. These studies demonstrate that the ideas proposed in this work are indeed very beneficial in computing dynamics.

The structure of the article is as follows. For the sake of expositional clarity, we first consider in Sec. II a system of spin-polarized fermions, that is, a system where all spins of all fermions are identical, so each and every fermionic orbital can be occupied only by one particle. In Sec. II B, we enumerate and address the fermionic configurations in a simple, compact, and practical way. The ideas of how to get the action of one- and two-body fermionic operators on a state vector as well as of the general Hamiltonian are explained in Sec. II C. Section II D deals with other quantities such as expectation values of the Hamiltonian and density matrices. In Sec. III, we consider a system of bosons and apply the proposed theory to get the result of the action of a bosonic Hamiltonian on a state vector, without construction of the corresponding Hamiltonian matrix. In Sec. III B, we first describe how to map the fermionic onto the bosonic configurations. This allows us to adopt, after small modification, the fermionic enumeration scheme for bosons. Next, in Sec. III C, we see how bosonic one- and two-body operators act on a state vector and then give explicitly the desired total action of the bosonic Hamiltonian on it as well as related quantities such as expectation values of the Hamiltonian and other one- and two-body operators. In Sec. IV, we generalize our ideas and findings to multicomponent systems. In Sec. IV A, we first deal with general fermions, that is, the system where fermions with up and down spin projections coexist. Then we demonstrate the applicability of the theory to binary mixtures of bosons in Sec. IV B and to systems made of spinless bosons and spin-polarized fermions in Sec. IV C. Extension of the proposed theory to multicomponent systems is given in Sec. IV D. In Sec. V, we discuss the practical implementation of the proposed ideas, and in Sec. VI, we summarize and conclude the discussion.

II. THE CASE OF SPIN-POLARIZED FERMIONS

A. Hamiltonian of interacting systems and the state vector $|\Psi\rangle$

Let us define the system first. We consider a general Hamiltonian in the second quantization form with one-body and two-body interaction terms,

$$\hat{H} = \sum_{k,q} h_{kq} \hat{b}_k^\dagger \hat{b}_q + \frac{1}{2} \sum_{k,s,q,l} W_{ksql} \hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q, \tag{1}$$

where the matrix elements h_{kq} of the one- and W_{ksql} of the two-body operators are assumed to be known. Three-body and higher order interaction terms can also be included in an obvious way. To complete the definition of the system, one has to specify the commutation relations for the creation and annihilation operators $\hat{b}_k^\dagger$ and $\hat{b}_q$. Here, we operate with the systems of indistinguishable fermions, and therefore, the usual anticommutation relations are fulfilled: $\hat{b}_k \hat{b}_q^\dagger + \hat{b}_q^\dagger \hat{b}_k = \delta_{kq}$.

We expand the generic state vector of the many-body system in a linear combination of N_{conf} *known* many-body basis functions $|\vec{n}\rangle$:

$$|\Psi\rangle = \sum_{\vec{n}}^{N_{\mathrm{conf}}} C_{\vec{n}} |\vec{n}\rangle . \tag{2}$$

Traditionally, Slater determinants are taken as $|\vec{n}\rangle$ for fermionic systems. Using fermionic creation operators $\hat{b}_k^\dagger$, each Slater determinant is assembled as

$$|\vec{n}\rangle = (\hat{b}_1^\dagger)^{n_1} (\hat{b}_2^\dagger)^{n_2} \cdots (\hat{b}_M^\dagger)^{n_M} |\mathrm{vac}\rangle, \tag{3}$$

where n_i can be either "0" or "1" for spin-polarized fermions. The symbol $\vec{n} = (n_1, n_2, n_3, \ldots, n_M)$ represents the occupations of the orbitals that preserve the total number of particles $n_1 + n_2 + n_3 + \cdots + n_M = N$, M is a number of the one-particle functions, here $M \geqslant N$, and $|\mathrm{vac}\rangle$ is the vacuum.

In the written expansion, Eq. (2), we did not specify explicitly the size N_{conf} of the problem, that is, the size or length of the $|\Psi\rangle$ vector. Let us now consider the configurational space spanned by *all* possible distributions of N fermions over M fermionic orbitals, that is, a full Fock subspace of the respective configurational space. For spin-polarized fermions, the size of such a full Fock subspace [8,13] is

$$N_{\mathrm{conf}} = \binom{M}{N}, \tag{4}$$

where $\binom{n}{k} = \frac{n!}{k!(n-k)!}$. On the other hand, N_{conf} is the dimension, that is, the number of the elements of any state vector $|\Psi\rangle$ of the system.

B. Enumeration of the Slater determinants

Our goal is to provide a simple and compact scheme for enumeration of the configurations. More strictly, we can reformulate this enumeration as a requirement to map M integers $n_1, n_2, n_3, \ldots, n_M$ characterizing each configuration, that is, the Slater determinant [see Eq. (3)] to *one* integer addressing it as a coordinate (index) of the state vector. Clearly, there are many ways to solve this problem. Here we report on one that utilizes the so-called Combinadic numbers [14].

Every fermionic configuration can be represented as a vector with M components, filled by "1" or "0". The number of orbitals M must be larger than the number of spin-polarized fermions N. Each appearing "1" means that the corresponding orbital is occupied by one fermion, and "0" means that it is not occupied (i.e., it has a hole). Since the total number of "1" and "0" characterizing a configurational vector (i.e., its length) is M, there are N particles ("1") and $M_v = M - N$ holes ("0"). Here, M_v specifies the number of unoccupied (i.e., virtual) orbitals. The general fermionic configuration reads as follows:

$$|\overbrace{\underbrace{11111110}_{i_1}1111110\cdots111110}^{i_2}\underbrace{1111111}_{i_{M_v}}\rangle. \tag{5}$$

For example, for the system of $N = 7$ polarized fermions distributed over $M = 10$ fermionic orbitals, there are $N = 7$ occupied orbitals and $M_v = M - N = 3$ unoccupied ones.

Then, for instance, the fermionic configuration $|1011101011\rangle$ means that the second, sixth, and eighth fermionic orbitals are vacant (i.e., not occupied), while the first, third, fourth, fifth, seventh, ninth, and tenth orbitals are occupied by one fermion. The problem of enumeration of M dimensional vectors filled by "1" and "0" has been successfully solved in the context of Ref. [14]; here we utilize it.

For a given system with N fermions and M fermionic orbitals, the *address* of every fermionic configuration can be uniquely defined either by specifying the positions of all the "1"s (i.e., particles) or alternatively by giving the positions of all holes (i.e., the "0"s). For the sake of definitiveness and without loss of generality, we use the positions of the holes to specify the configurations. The general configuration defined in Eq. (5) is described by $M_v = M - N$ holes placed at positions $i_1, i_2, \ldots, i_{M_v}$. It is convenient to order the holes as $i_1 < i_2 < i_3 < \cdots < i_{M_v}$. The address of this configuration is computed as follows:

$$J(i_1, i_2, \ldots, i_{M_v}) = 1 + \sum_{k=1}^{M_v} \binom{N + M_v - i_k}{M_v + 1 - k}. \qquad (6)$$

So, each and every fermionic configuration in a fermionic state vector $|\Psi\rangle$ has its own unique address (index), defined by the numbers $i_1, i_2, \ldots, i_{M_v}$. For the previously considered fermionic configuration $|1011101011\rangle$ with $N = 7$ particles and $M_v = 3$ holes, the "0"s are located at $i_1 = 2, i_2 = 6, i_3 = 8$ when we count their positions from the left [see Eq. (5)]. By using Eq. (6), we obtain the address of this configuration $J(2, 6, 8) = \binom{10-2}{3} + \binom{10-6}{2} + \binom{10-8}{1} + 1 = 65$. We note that the enumeration scheme provided in Ref. [14] uses positions of the "1"s counted from the right, whereas in our scheme we count the positions of the "0"s (i.e., holes) from the left. The inverse problem, a restoration of the hole positions, $i_1, i_2, \ldots, i_{M_v}$, according to a given address J also can be solved [14] if needed. Our goal is fulfilled: Spin-polarized fermionic configurations are enumerated in an easy and compact way.

Let us summarize: N spin-polarized fermions distributed over M fermionic orbitals span the full subspace of the Fock space of $N_{\text{conf}} = \binom{N+M_v}{N}$ configurations; here $M_v = M - N$ is the number of unoccupied fermionic orbitals. The dimension of any state vector $|\Psi\rangle$ of this system is N_{conf}. Every fermionic configuration, Eq. (5), in the respective Fock subspace is characterized by the positions of M_v holes placed at $i_1, i_2, \ldots, i_{M_v}$. We can attribute a unique address J to each fermionic configuration according to the rule in Eq. (6): $J = J(i_1, i_2, \ldots, i_{M_v})$. This Combinadic-based mapping is a one-to-one and onto mapping. In particular, the index J takes all values between 1 and N_{conf}. The inverse mapping, from the distinct integers $1, 2, \ldots, N_{\text{conf}} - 1, N_{\text{conf}}$ to the N_{conf} distinct configurations is, of course, well defined. We do not construct it here explicitly since the inverse mapping is not needed for the usefulness and practical implementation of the presented formalism.

Now, a general $|\Psi\rangle$, Eq. (2), can be rewritten in a specific form:

$$|\Psi\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J |J(i_1, i_2, \ldots, i_{M_v})\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J \, |J(\mathbf{i})\rangle \,, \qquad (7)$$

where it is explicitly stated that every fermionic configuration (i.e., Slater determinant) $|J(\mathbf{i})\rangle$ is specified by M_v holes placed at $(i_1, i_2, \ldots, i_{M_v}) \equiv \mathbf{i}$. It has a unique address $J = J(i_1, i_2, \ldots, i_{M_v})$, which can be computed according to Eq. (6). The index (address) J runs over all N_{conf} configurations.

C. Applying operators to $|\Psi\rangle$

The Hamiltonian (1) is defined as a sum of terms; each of them is a product of creation and annihilation operators—a pair $\hat{b}_k^\dagger \hat{b}_q$ for the one-body and a quartet $\hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q$ for the two-body terms, scaled by respective prefactors, that is, integrals h_{kq} and W_{ksql}. In principle, any other operator can be represented in a similar way as a sum of contribution of one-, two-, or higher order terms. The idea is quite simple: If one would know the result of action of each of these terms on a state vector $|\Psi\rangle$, the sum of all of them would give the required total result of the action of the Hamiltonian on a state vector. Here we recall that the total number of terms in the Hamiltonian is defined by the number of the orbitals used. In the most general case of M orbitals, the total number of the one-body terms is M^2, and the total number of the two-body terms is M^4. Any symmetry in the problem, including hermicity, reduces these numbers.

1. *Action of one- and two-body operators*

Let us consider the action of a pair $\hat{b}_k^\dagger \hat{b}_q$ of creation and annihilation operators on every fermionic configuration, Eq. (5), of a general state vector $|\Psi\rangle$. As a first step, we consider a specific, say $\hat{b}_2^\dagger \hat{b}_3$, term that kills a particle in the third orbital and creates a particle in the second one. For spin-polarized fermions due to Fermi-Dirac statistics, the term $\hat{b}_2^\dagger \hat{b}_3$ provides a nonzero action only on the subset of configurations $|n_1, 0, 1, \ldots, n_M\rangle$ having $n_2 \equiv 0, n_3 \equiv 1$:

$$\hat{b}_2^\dagger \hat{b}_3 |n_1, 0, 1, \ldots, n_M\rangle = (-1)^0 |n_1, 1, 0, \ldots, n_M\rangle,$$

where the remaining n_i can be 0 or 1. Similarly, for a general $\hat{b}_k^\dagger \hat{b}_q$ case, $n_k \equiv 0, n_q \equiv 1$:

$$\hat{b}_k^\dagger \hat{b}_q |n_1, n_2, n_3, \ldots, n_M\rangle = (-1)^{\sum_{i\in(k,q)} n_i} |n_1, n_2, \ldots, n_q - 1, \ldots, n_k + 1, \ldots, n_M\rangle,$$

where $(-1)^{\sum_{i\in(k,q)} n_i}$ is a prefactor ensuring correct fermionic statistics of the antisymmetrized wave function and the summation $i \in (k, q)$ runs over all occupations n_i between the kth and qth orbitals. We can interpret this well-known result as follows: Operation of any even combination of creation and annihilation operators on a configuration (determinant) results in readdressing this configuration (determinant) to another one. Since the occupation numbers of the incoming $|n_1, n_2, n_3, \ldots, n_M\rangle$ and resulting $|n_1, n_2, \ldots, n_q - 1, \ldots, n_k + 1, \ldots, n_M\rangle$ configurations are explicitly known, the numbers of the orbitals with zero occupations (i.e., the hole positions) are also available; therefore, according to Eq. (6), we can also compute their addresses in a state vector, Eq. (7). By applying the enumeration scheme (mapping) introduced previously, one gets

$$\hat{b}_k^\dagger \hat{b}_q |J(\mathbf{i})\rangle = (-1)^{d_J^{kq}} |J(\mathbf{i}')\rangle, k \in \mathbf{i}, q \notin \mathbf{i}.$$

In other words, the Jth configuration is readdressed to a new configuration with index $J' \equiv J(\mathbf{i}')$ with some sign prefactor. For a given configuration $|J(\mathbf{i})\rangle$ and fixed k, q, the integer d_J^{kq} is equal to the number of fermions, that is, "1"s located between the kth and qth orbitals: $d_J^{kq} = \sum_{i\in(k,q)} n_i$. Note that there is no difference in whether to count the number of fermions between the kth and qth orbitals in the original configuration J or in the resulting J' configuration, namely, $d_J^{kq} = d_{J'}^{kq}$. It is important to stress that the operation with even combinations of creation and annihilation operators results in a single-valued readdressing; that is, an initial configuration having address J is readdressed to a single configuration with address J'.

Having at hand the result of the action of the pair $\hat{b}_k^\dagger \hat{b}_q$ on a general configuration (determinant), we can find out its action on the total state vector [see Eq. (7)]:

$$|\Psi^{kq}\rangle \equiv \hat{b}_k^\dagger \hat{b}_q |\Psi\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J \hat{b}_k^\dagger \hat{b}_q |J\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J^{kq} |J(\mathbf{i})\rangle ,$$
$$C_J^{kq} = \begin{cases} C_{J^{kq}}(-1)^{d_J^{kq}}; & k \notin \mathbf{i}, q \in \mathbf{i} \\ 0; & \text{otherwise} \end{cases} , \tag{8}$$

where at the last step we have changed variables of the summation index from J' to J. Note that this closed-form result of the action of the basic one-body operator on a state vector has been obtained without referring to the matrix representation of the respective operator. How are we to understand this result? Every element C_J^{kq} of the resulting vector having address J is obtained as a product of the $C_{J^{kq}}$ element of the incoming vector having address J^{kq} scaled by the $(-1)^{d_J^{kq}}$ fermionic prefactor. The configuration J^{kq} is related to J by making a hole at kth and filling a hole at qth orbitals. The $\hat{b}_k^\dagger \hat{b}_q$ term acts only if the index k coincides with one of the holes' positions $(i_1, \ldots, k, \ldots, i_{M_v})$ and the index q does not coincide with either of them. If these two conditions are not fulfilled, the respective configuration does not contribute at all to the resulting state vector. The addresses $J^{kq} = J(i_1, \ldots, k, \ldots, i_{M_v})$ and $J = J(i_1, \ldots, q, \ldots, i_{M_v})$ are computed by Eq. (6). In Eq. (8), the summation runs over the index J, implying that for a given J one has to restore the holes' positions $i_1, i_2, \ldots, i_{M_v}$ first. However, this complication can be easily avoided if, instead, one starts M_v nested loops running over the positions of the holes $i_1 < i_2 < \cdots < i_{M_v}$ directly. In the latter case, all $i_1, \ldots, i_{M_v}$ are explicitly available, as well as the resulting address $J = J(i_1, \ldots, q, \ldots, i_{M_v})$ via Eq. (6). Hence, at each step, to get the desired element C_J^{kq} of the resulting vector, one has to compute one integer d_J^{kq} and apply Eq. (6) only once to get the index $J^{kq} = J(i_1, \ldots, k, \ldots, i_{M_v})$ of the respective incoming configuration and its value $C_{J^{kq}}$.

The action of a general $(k \neq s \neq l \neq q)$ two-body $\hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q$ term on the incoming state vector $|\Psi\rangle$ can be obtained using a similar strategy:

$$|\Psi^{kslq}\rangle \equiv \hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q |\Psi\rangle = \hat{b}_s^\dagger \hat{b}_l |\Psi^{kq}\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J^{kslq} |J(\mathbf{i})\rangle,$$
$$C_J^{kslq} = \begin{cases} C_{J^{kslq}} (-1)^{d_{J^{sl}}^{kq}} (-1)^{d_J^{sl}}; & k, s \notin \mathbf{i}, l, q \in \mathbf{i} \\ 0; & \text{otherwise} \end{cases} . \tag{9}$$

To get the Jth element C_J^{kslq} of the resulting state vector one has to take the element $C_{J^{kslq}}$ of the incoming vector having address J^{kslq} and multiply it by $(-1)^{d_{J^{sl}}^{kq} + d_J^{sl}}$ prefactor. Using Eq. (6), we compute the addresses of the resulting $J = J(i_1, \ldots, l, \ldots, q, \ldots, i_{M_v})$ and incoming $J^{kslq} = J(i_1, \ldots, k, \ldots, s, \ldots, i_{M_v})$ configurations. The configuration J^{ksql} is related to J by making holes at kth and sth and filling holes at qth and lth orbitals. For a given quartet k, s, l, q, every component J of the incoming state vector is characterized by the integers $d_{J^{sl}}^{kq} + d_J^{sl}$, computed as a sum of the number d_J^{sl} of fermions located between the sth and lth orbitals of the configuration J, and $d_{J^{sl}}^{kq}$, the number of fermions between the kth and qth ones of the configuration J^{sl}. The $\hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q$ term provides nonzero action only on the smaller subset of the configurations having $n_k \equiv n_s \equiv 0$, $n_l \equiv n_q \equiv 1$. Therefore, in practical computations one needs to address only this subset.

2. *Action of the Hamiltonian*

Considering configurations as coordinates of the state vector $|\Psi\rangle$, we have seen that the action of each term of the Hamiltonian on the state vector readdresses the coordinates of the original state vector, multiplying them by some known prefactors. So, instead of constructing the full Hamiltonian matrix and performing matrix-to-vector multiplications, we obtained the same result by reordering the components of the incoming state vector according to the action of every $\hat{b}_k^\dagger \hat{b}_q$ and $\hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q$ term, multiplying them by the corresponding integrals h_{kq} and W_{ksql}, and summing the results up.

The general Hamiltonian Eq. (1) is a sum of the one-body $\hat{h} = \sum_{k,q} h_{kq} \hat{b}_k^\dagger \hat{b}_q$ and two-body $\hat{W} = \frac{1}{2} \sum_{k,s,q,l} W_{ksql} \hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q$ terms. Using the results of the previous subsection, we find the total action of all one-body terms on the initial state vector $|\Psi\rangle$:

$$\hat{h}\,|\Psi\rangle = \sum_{k,q} h_{kq} [\hat{b}_k^\dagger \hat{b}_q |\Psi\rangle] = \sum_{k,q} h_{kq} |\Psi^{kq}\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J^{\hat{h}} |J(\mathbf{i})\rangle,$$
$$C_J^{\hat{h}} = \sum_{k,q} h_{kq} C_J^{kq}. \tag{10}$$

Here, all the components C_J^{kq} have been computed using Eq. (8). Analogously, we sum up all the contributions from all two-body terms:

$$\hat{W}|\Psi\rangle = \frac{1}{2} \sum_{k,s,q,l} W_{ksql} [\hat{b}_k^\dagger \hat{b}_s^\dagger \hat{b}_l \hat{b}_q |\Psi\rangle]$$
$$= \frac{1}{2} \sum_{k,s,q,l} W_{ksql} |\Psi^{kslq}\rangle = \sum_{J=1}^{N_{\text{conf}}} C_J^{\hat{W}} |J(\mathbf{i})\rangle, \tag{11}$$
$$C_J^{\hat{W}} = \frac{1}{2} \sum_{k,s,q,l} W_{ksql} C_J^{kslq}.$$

Finally, the desired action of the Hamiltonian on the state vector $|\Psi\rangle$ is a sum of the two vectors obtained in Eqs. (10)

and (11):

$$\hat{H}|\Psi\rangle = \hat{h}\,|\Psi\rangle + \hat{W}\,|\Psi\rangle = \sum_{J=1}^{N_{\rm conf}} C_J^{\hat{H}}\,|J(\mathbf{i})\rangle\,,$$
$$C_J^{\hat{H}} = C_J^{\hat{h}} + C_J^{\hat{W}}\,, \tag{12}$$

which fulfills our initial goal. This closed-form result of the action of the Hamiltonian on a state vector is constructed without building the respective Hamiltonian matrix or even referring to its matrix elements.

D. Other quantities of interest

In the preceding subsections, we have successfully derived a simple and straightforward technique to operate with state vectors without representing the respective operators in matrix form. In particular, we have utilized the basic fact that the result of action of any operator represented as a sum of products of creation and annihilation operators on a state vector is equal to the sum of action of each of these terms. So, the action of any operator on a state vector (called incoming state vector) results in a new state vector (called resulting state vector). Let us now show that the expectation value of the respective operator can be immediately computed as a dot product of the incoming and resulting state vectors.

Indeed, according to the standard definition [15–17], for a given state vector $|\Psi\rangle$ the elements of the reduced one-body density matrix read as follows:

$$\rho_{kq} = \langle\Psi|\hat{b}_k^\dagger\hat{b}_q|\Psi\rangle \equiv \langle\Psi|[\hat{b}_k^\dagger\hat{b}_q|\Psi\rangle] = \langle\Psi|\Psi^{kq}\rangle$$
$$= \sum_{J=1}^{N_{\rm conf}} C_J^* C_J^{kq}\,, \tag{13}$$

where we substitute the result for $\hat{b}_k^\dagger\hat{b}_q|\Psi\rangle$ from Eq. (8). Thus, the elements of the reduced one-body density matrix ρ_{kq} are obtained as a dot product of the incoming $|\Psi\rangle$ and resulting $|\Psi^{kq}\rangle$ state vectors.

Similarly, the elements of the reduced two-body density matrix are obtained as a dot product of the incoming $|\Psi\rangle$ and resulting [see Eq. (9)] $|\Psi^{kslq}\rangle$ state vectors:

$$\rho_{kslq} = \langle\Psi|\,\hat{b}_k^\dagger\hat{b}_s^\dagger\hat{b}_l\hat{b}_q\,|\Psi\rangle \equiv \langle\Psi|\,[\hat{b}_k^\dagger\hat{b}_s^\dagger\hat{b}_l\hat{b}_q\,|\Psi\rangle] = \left\langle\Psi|\Psi^{kslq}\right\rangle$$
$$= \sum_{J=1}^{N_{\rm conf}} C_J^* C_J^{kslq}\,. \tag{14}$$

So, in the discussed scheme, the elements of the reduced one- and two-body density matrices appear very naturally. Moreover, the elements of the reduced three- and higher order density matrices can be obtained in a very similar way.

Finally, taking the result of the action of the Hamiltonian on an initial state vector $\hat{H}|\Psi\rangle$ from Eq. (12), we compute the respective expectation value of the Hamiltonian as a dot product as well:

$$\langle\Psi|\,\hat{H}\,|\Psi\rangle \equiv \langle\Psi|\,[\hat{H}\,|\Psi\rangle] = \sum_{J=1}^{N_{\rm conf}} C_J^* C_J^{\hat{H}}\,. \tag{15}$$

We have prescribed here a few expectation values of particular interest in a many-body theory. Other quantities can be represented and computed in a similar way.

III. THE CASE OF STUCTURELESS BOSONS

A. General remarks

Here, we deal with a system of N identical interacting bosons. The terms "structureless" and "spinless" are often used to specify that the bosons do not have an internal structure. Our goal is to show that our ideas of how to operate with state vectors without resorting to the matrix representation of the respective operators proposed previously for fermions can naturally be extended and applied to bosonic systems. The generic Hamiltonian Eq. (1) introduced previously for the system of spin-polarized fermions is also applicable to the system of structureless bosons with the only modification concerning the commutation relations of creation and annihilation operators. Here, we operate with the systems of indistinguishable bosons, and therefore, we use the usual commutation relations: $\hat{b}_k\hat{b}_q^\dagger - \hat{b}_q^\dagger\hat{b}_k = \delta_{kq}$.

The generic bosonic state vector is expanded as a linear combination of $N_{\rm conf}$ known many-body basis functions $|\vec{n}\rangle$:

$$|\Psi\rangle = \sum_{\vec{n}}^{N_{\rm conf}} C_{\vec{n}}\,|\vec{n}\rangle\,, \tag{16}$$

where $|\vec{n}\rangle$ are permanents that are assembled as

$$|\vec{n}\rangle = \frac{1}{\sqrt{n_1!n_2!n_3!\cdots n_M!}}(\hat{b}_1^\dagger)^{n_1}(\hat{b}_2^\dagger)^{n_2}\cdots(\hat{b}_M^\dagger)^{n_M}|\text{vac}\rangle. \tag{17}$$

Here, $\vec{n} = (n_1, n_2, n_3, \ldots, n_M)$ represents the occupations of the orbitals that preserve the total number of particles $n_1 + n_2 + n_3 + \cdots + n_M = N$, $|\text{vac}\rangle$ is the vacuum, and M is the number of the one-particle functions. For bosons, $M \geqslant 1$.

The number of elements $N_{\rm conf}$ in the bosonic state vector $|\Psi\rangle$ is equal to the number of the configurations used. Here we consider the configurational space spanned by *all* possible distributions of N bosons over M orbitals, that is, a *full* subspace of the respective configurational space. We recall that one of the key consequences of this fullness is that an action of any operator on the state vector results in a new state vector defined in the *same* configurational subspace.

The size of this full Fock subspace is [13] as follows:

$$N_{\rm conf} = \binom{N+M-1}{N}. \tag{18}$$

This number is equal to the size of the configurational space spanned by N spin-polarized fermions distributed over $M' = N + M - 1$ fermionic orbitals; see Sec. II A. Therefore, there exists one-to-one mapping between the configurational spaces of the N-boson system distributed over M bosonic orbitals and a fermionic system made of N fermions distributed over $M' = N + M - 1$ fermionic orbitals, and vice versa. In other words, every fermionic configuration having $N + M - 1$ components (occupation numbers) should be attributed to a bosonic configuration characterized by M components. Let us compare these isomorphic bosonic and fermionic systems.

TABLE I. Mapping between fermionic and bosonic configurations made of N particles. The number of the unoccupied fermionic orbitals is equal to the total number of the bosonic orbitals minus one: $M_v \equiv M - 1$. Now, we can adopt the fermionic enumeration scheme for bosons.

Enumeration index J	N fermions, $N + M - 1$ orbitals	N bosons, M orbitals
1	$\lvert \underbrace{1111\cdots111}_{N}\underbrace{000\cdots00}_{M-1}\rangle$	$\lvert N, \underbrace{0,\ldots,0}_{M-1}\rangle$
2	$\lvert \underbrace{1111\cdots11}_{N-1}01\underbrace{000\cdots00}_{M-2}\rangle$	$\lvert N-1, 1, \underbrace{0,\ldots,0}_{M-2}\rangle$
...	...	...
J	$\lvert \underbrace{11111}_{5}0\underbrace{111}_{3}0\underbrace{1111}_{4}0\cdots0\underbrace{111}_{3}00\underbrace{111111}_{6}\rangle$	$\lvert 5, 3, 4, \ldots, 3, 0, 6\rangle$
...	...	...
$N_{\text{conf}} - 1$	$\lvert \underbrace{000\cdots00}_{M-2}10\underbrace{1111\cdots111}_{N-1}\rangle$	$\lvert \underbrace{0,\ldots,0}_{M-2}, 1, N-1\rangle$
N_{conf}	$\lvert \underbrace{000\cdots00}_{M-1}\underbrace{1111\cdots111}_{N}\rangle$	$\lvert \underbrace{0,\ldots,0}_{M-1}, N\rangle$

What is also equal in these two systems, apart from the total number N of particles? The number of the fermionic unoccupied orbitals $M_v = M' - N$, that is, the number of fermionic holes, is equal to the maximal number of the bosonic holes: $M_v = M - 1$. We note that the maximal number of bosonic holes appear in configurations such as $|N, 0, \ldots, 0\rangle$ and $|0, N, 0, \ldots, 0\rangle$. Since we already know how to enumerate fermionic configurations in terms of holes (see Sec. II B), we can adopt the fermionic enumeration scheme to the respective bosonic system.

B. Mapping and enumeration of the permanents

Our goal is to provide a simple and compact scheme for enumeration of the bosonic configurations. To utilize the formal isomorphism between the bosonic and fermionic systems considered previously, we first have to show how to map, or attribute, a fermionic configuration to the bosonic one. The rule is very simple: the number of bosons residing in the first bosonic orbital n_1 is equal to the number of fermions occupying successively the lowest fermionic orbitals from the bottom to the first fermionic hole. In other words, the occupation of the first bosonic orbital is defined as the number of "1"s appearing in the $(N + M - 1)$-component fermionic vector [Eq. (5)] up to the first hole, that is, the first "0", when counting from the left. The occupation number of the second bosonic orbital n_2 is defined as the number of "1"s between the first and second "0" (i.e., between the first and second fermionic holes). The third bosonic occupation number n_3 is defined as the number of "1"s between the second and third "0", and so on. Table I illustrates this mapping.

Consequently, the bosonic occupation numbers and the positions of the fermionic holes are simply connected:

$$\begin{aligned} n_1 &= i_1 - 1, \\ n_2 &= i_2 - i_1 - 1, \\ &\cdots \\ n_k &= i_k - i_{k-1} - 1, \\ &\cdots \\ n_{M-1} &= i_{M-1} - i_{M-2} - 1, \\ n_M &= N + M - i_{M-1} - 1. \end{aligned} \tag{19}$$

So, having a set of the bosonic occupation numbers $|n_1, n_2, n_3, \ldots, n_M\rangle$, by using this scheme we can restore the positions of the $M - 1$ fermionic holes $(i_1, i_2, \ldots, i_{M-1})$ and the respective fermionic configuration, and vice versa. Now we can explicitly use the relations Eq. (19) between bosonic occupation numbers and fermionic holes to uniquely address bosonic configurations utilizing Eq. (6). Finally, omitting all intermediate steps, we get the address of a generic bosonic configuration $|n_1, n_2, n_3, \ldots, n_M\rangle$ in the bosonic state vector:

$$\begin{aligned} &J(n_1, n_2, \ldots, n_{M-1}, n_M) \\ &\quad = 1 + \sum_{k=1}^{M-1} \binom{N + M - 1 - k - \sum_{l=1}^{k} n_l}{M - k}. \end{aligned} \tag{20}$$

Here n_M enters the expression implicitly via the identity $N = n_1 + n_2 + n_3 + \cdots + n_M$.

Let us summarize. The system of N bosons and M bosonic orbitals spans the full subspace of the Fock space of N_{conf} configurations [see Eq. (18)]. The dimension of any state vector $|\Psi\rangle$ of the system is N_{conf}. Every bosonic configuration in the respective Fock subspace is characterized by the set of M occupation numbers $|n_1, n_2, n_3, \ldots, n_M\rangle$. We can attribute a unique address J to each of the configurations according to the rule of Eq. (20): $J = J(n_1, n_2, \ldots, n_{M-1}, n_M)$. The proposed enumeration schemes in Eqs. (6) and (20) are equivalent and connected via Eq. (19) to each other. They can be equally applied to enumerate bosonic and fermionic configurations. In other words, every many-body basis function written in the "fermionic style" (hole positions representation) can be translated via Eq. (19) to the "bosonic style" (occupation numbers representation): $|n_1, n_2, \ldots, n_M\rangle$. However, the explicit use of the bosonic representation for fermions is neither as economic nor appealing as it is for bosons. Therefore, once Eq. (20) has been derived, we preserve for the sake of clarity the hole enumeration scheme for fermions and occupation number enumeration scheme for bosons.

Now, we can represent the bosonic state vector $|\Psi\rangle$ in a form similar to Eq. (7):

$$|\Psi\rangle = \sum_{J=1}^{N_{\rm conf}} C_J\,|J(n_1,n_2,\ldots,n_M)\rangle = \sum_{J=1}^{N_{\rm conf}} C_J\,|J(\mathbf{n})\rangle\,, \quad (21)$$

with the only difference that every bosonic configuration $|n_1,n_2,n_3,\ldots,n_M\rangle$ has a unique address J, which is computed according to Eq. (20), that is, using bosonic occupation number representation. The index J runs over all $N_{\rm conf}$ configurations.

C. Applying operators to $|\Psi\rangle$

Any bosonic operator can be represented as a sum of products of bosonic creation and annihilation operators. If we now show that the action of any even combination of creation and destruction operators on a bosonic state vector [Eq. (21)] leads, as in the case of fermions, only to readdressing (reindexing) of the configurations (coordinates), we can adopt all the ideas developed for fermions to bosonic systems.

Let us first consider a specific (say, the $\hat{b}_3^\dagger\hat{b}_2$) term that kills a boson in the second bosonic orbital and creates a boson in the third one. The result of the action of this pair of creation and annihilation operators on an arbitrary permanent is known and reads as follows:

$$\hat{b}_3^\dagger\hat{b}_2|n_1,n_2,n_3,\ldots,n_M\rangle = \sqrt{n_2}\sqrt{n_3+1}|n_1,n_2-1,n_3+1,\ldots,n_M\rangle.$$

It acts on every many-body configuration having nonzero occupation n_2. We can interpret this result as follows: The operation of any even combination of bosonic creation and annihilation operators on a permanent results in the readdressing of this permanent to another one multiplied with a trivial bosonic prefactor. Clearly, all the ideas proposed for fermions in Sec. II can be easily adopted here for bosons.

1. Action of one- and two-body operators

To derive the results of the actions of bosonic one- and two-body operators on a state vector, one can follow the strategy used for fermions in Sec. II C1. We provide the final results and briefly discuss their meanings. The action of one-body bosonic operator $\hat{b}_k^\dagger\hat{b}_q$ on an incoming $|\Psi\rangle$ results in $|\Psi^{kq}\rangle$:

$$|\Psi^{kq}\rangle \equiv \hat{b}_k^\dagger\hat{b}_q\,|\Psi\rangle = \sum_{J=1}^{N_{\rm conf}} C_J^{kq}\,|J(\mathbf{n})\rangle\,,$$
$$C_J^{kq} = C_{J^{kq}}\sqrt{n_k}\sqrt{n_q+1}. \quad (22)$$

Let us explain this expression. According to Eq. (20), every configuration $|n_1,\ldots,n_k,\ldots,n_q,\ldots,n_M\rangle$ of the resulting vector $|\Psi^{kq}\rangle$ has a unique address (index) $J = J(n_1,\ldots,n_k,\ldots,n_q,\ldots,n_M)$. The respective coefficient C_J^{kq} is obtained as a product of the J^{kq}th component of the incoming vector $C_{J^{kq}}$ scaled by the bosonic $\sqrt{n_k}\sqrt{n_q+1}$ prefactor. On the right-hand side of Eq. (22), we "exchange" the kth and qth indices because of a change of variables of the summation index J applied, similar to how it was done in Eq. (8). The index J^{kq} is computed according to Eq. (20) and corresponds to the configuration $|n_1,\ldots,n_k-1,\ldots,n_q+1,\ldots,n_M\rangle$. This simple and straightforward methodology is ideally suitable for programming.

The action of a general ($k\neq s\neq l\neq q$) two-body $\hat{b}_k^\dagger\hat{b}_s^\dagger\hat{b}_l\hat{b}_q$ term on the incoming state vector $|\Psi\rangle$ is defined as

$$|\Psi^{kslq}\rangle \equiv \hat{b}_k^\dagger\hat{b}_s^\dagger\hat{b}_l\hat{b}_q\,|\Psi\rangle = \sum_{J=1}^{N_{\rm conf}} C_J^{kslq}\,|J(\mathbf{n})\rangle\,,$$
$$C_J^{kslq} = C_{J^{kslq}}\sqrt{n_k}\sqrt{n_s}\sqrt{n_l+1}\sqrt{n_q+1}, \quad (23)$$

where, after the change of variables of the summation index J, the addresses of the incoming $J^{kslq} = J(n_1,\ldots,n_k-1,\ldots,n_s-1,\ldots,n_l+1,\ldots,n_q+1,\ldots,n_M)$ and resulting $J = J(n_1,\ldots,n_k,\ldots,n_s,\ldots,n_l,\ldots,n_q,\ldots,n_M)$ configurations are computed using Eq. (20). For other combinations of the indices k,s,l,q, Eq. (23) is valid as well, of course, with the corresponding bosonic prefactors. For instance, for $k=q, s=l$ the bosonic prefactor [see second line of Eq. (23)] is $n_k n_s$.

2. Action of the Hamiltonian

Using the same strategy as for the fermionic case, we group together the actions of all one-body and all two-body operators to get the total action of the Hamiltonian on an initial bosonic state vector $|\Psi\rangle$ [Eq. (21)].

The one-body contributions read as

$$\hat{h}|\Psi\rangle = \sum_{k,q} h_{kq}[\hat{b}_k^\dagger\hat{b}_q|\Psi\rangle] = \sum_{k,q} h_{kq}|\Psi^{kq}\rangle = \sum_{J=1}^{N_{\rm conf}} C_J^{\hat{h}}\,|J(\mathbf{n})\rangle\,,$$
$$C_J^{\hat{h}} = \sum_{k,q} h_{kq}C_J^{kq}. \quad (24)$$

The two-body terms are

$$\hat{W}\,|\Psi\rangle = \frac{1}{2}\sum_{k,s,q,l} W_{ksql}[\hat{b}_k^\dagger\hat{b}_s^\dagger\hat{b}_l\hat{b}_q\,|\Psi\rangle] = \frac{1}{2}\sum_{k,s,q,l} W_{ksql}|\Psi^{kslq}\rangle$$
$$= \sum_{J=1}^{N_{\rm conf}} C_J^{\hat{W}}\,|J(\mathbf{n})\rangle\,, \quad (25)$$
$$C_J^{\hat{W}} = \frac{1}{2}\sum_{k,s,q,l} W_{ksql}C_J^{kslq}.$$

By combining the contributions from the one- and two-body terms, we get the desired action of the Hamiltonian on a state vector $|\Psi\rangle$:

$$\hat{H}|\Psi\rangle = \hat{h}\,|\Psi\rangle + \hat{W}\,|\Psi\rangle = \sum_{J=1}^{N_{\rm conf}} C_J^{\hat{H}}\,|J(\mathbf{n})\rangle\,,$$
$$C_J^{\hat{H}} = C_J^{\hat{h}} + C_J^{\hat{W}}, \quad (26)$$

which concludes our constructions for bosons.

3. Other quantities of interest

We have seen that the action of any bosonic operator on the state vector results in a new (resulting) state vector. Similar to fermionic systems, the expectation value of the respective operator is immediately available as a dot product of the incoming and resulting state vectors. The matrix elements of

the reduced one- and two-body density matrices as well as the expectation value of the Hamiltonian can be obtained in a very similar way, as have already been done for fermions in Eqs. (13)–(15), respectively. Other expectation values are also amenable to this formulation.

IV. THE CASE OF MULTICOMPONENT SYSTEMS AND BINARY MIXTURES

In this section, we generalize the new ideas for effective and efficient operations in Fock space proposed previously for systems of spinless bosons and spin-polarized fermions to multicomponent systems. More specifically, we show that the mapping and enumeration scheme discussed previously can be naturally extended to more general systems.

Let us considered binary mixtures with $N = N_A + N_B$ particles. The mixture consists of N_A identical particles (bosons or fermions) of type A and N_B identical particles (bosons or fermions) of type B. In what follows, whenever needed we denote the quantities in the mixture by A, B, or AB superscripts.

The many-body Hamiltonian of the mixture has three kinds of terms:

$$\begin{aligned}\hat{H}^{(AB)} &= \hat{H}^{(A)} + \hat{H}^{(B)} + \hat{W}^{(AB)},\\ \hat{W}^{(AB)} &= \sum_{k,k',q,q'} W^{(AB)}_{kk'qq'} \hat{a}^\dagger_k \hat{a}_q \hat{b}^\dagger_{k'} \hat{b}_{q'}.\end{aligned} \tag{27}$$

The first two terms of $\hat{H}^{(AB)}$ are the A and B single-species Hamiltonians and can be read directly from Eq. (1), formally replacing in the first case the $\hat{b}_q$ and $\hat{b}^\dagger_k$ operators with $\hat{a}_q$ and $\hat{a}^\dagger_k$, respectively. The third term of $\hat{H}^{(AB)}$ is the interaction between the two species. We call $\hat{H}^{(A)}$, $\hat{H}^{(B)}$ intraspecies parts and $\hat{W}^{(AB)}$ the interspecies part.

The many-body wavefunction $\Psi^{(AB)}$ is a linear combination of all possible products of permutational-symmetry-adapted configurations:

$$|\Psi^{(AB)}\rangle = \sum_{\vec{n},\vec{m}} C_{\vec{n}\vec{m}}(t)\,|\vec{n}\rangle \times |\vec{m}\rangle \equiv \sum_{\vec{n},\vec{m}} C_{\vec{n}\vec{m}}\,|\vec{n},\vec{m}\rangle\,. \tag{28}$$

The configurations $\{|\vec{n}\rangle\}$, $\{|\vec{m}\rangle\}$ are either Slater determinants (3) or permanents (17), depending on whether we deal with Bose-Bose, Fermi-Fermi, or Bose-Fermi mixtures.

In this work, we make an assumption. The total number of particles of each kind, N_A and N_B, is conserved. In other words, there is no conversion between the particles; that is, the particles of A kind cannot become of B kind and vice versa. The Fock subspace of the A subsystem is spanned by all possible permutations of N_A particles over M_A orbitals ($N^A_{\rm conf}$ configurations), and the configurational subspace of the B subsystem is spanned by permutations of N_B particles over M_B orbitals ($N^B_{\rm conf}$ configurations). Practically, in this case we work in the full configurational subspaces, that is, the summation in Eq. (28) over $\vec{n}$ runs from 1 until $N^A_{\rm conf}$ and over $\vec{m}$ from 1 until $N^B_{\rm conf}$. More strictly, the total configurational space is a tensor product of two full subspaces, and any state vector of such a binary system has $N^A_{\rm conf}N^B_{\rm conf}$ components.

In Secs. II and III, we have seen that enumeration schemes of the full bosonic and fermionic configurational subspaces can be easily done by counting either holes [Eq. (6)] for fermions or particles [Eq. (20)] for bosons. Therefore, if J_A and J_B label configurations in the A and B subspaces, respectively, then the two-component vector index $\vec{J} = (J^A, J^B)$ enumerates all possible configurations in the total product Fock subspace. Now, we can represent the state vector of the mixture, Eq. (28), in a form where enumeration of the configurations in the A and B subspaces are explicitly specified:

$$|\Psi^{(AB)}\rangle = \sum_{J_A=1}^{N^A_{\rm conf}} \sum_{J_B=1}^{N^B_{\rm conf}} C_{J_A J_B}\,|J_A, J_B\rangle = \sum_{J_A=1}^{N^A_{\rm conf}} \sum_{J_B=1}^{N^B_{\rm conf}} C_{J_A J_B}|\vec{J}\rangle. \tag{29}$$

The key goal of this section is to demonstrate that the action of the total Hamiltonian, Eq. (27), on the state vector of the mixture can also be represented and computed without construction of the respective Hamiltonian matrix.

A. General fermionic system

We consider the mixture of fermions of two different kinds, A and B. Despite such an unusual abbreviation, it is a standard system of spin-up and spin-down fermions where the A subsystem is associated with spin-up fermions and B with spin-down fermions. Here, we consider the general, so-called unrestricted case where particles are not constrained to occupy the same spatial orbitals; that is, the one-particle functions of the spin-up fermions can differ from the respective orbitals of the spin-down fermions. Such a treatment is allowed if the Hamiltonian does not have terms leading to spin-flip phenomena, taking place, for example, in external magnetic fields. The Hamiltonian, Eq. (27), does not have such terms.

Let us first show that the action of typical one- and two-body terms contributing to the $\hat{H}^{(A)}$, $\hat{H}^{(B)}$, and $\hat{W}^{(AB)}$ parts on a basic configuration $|\vec{J}\rangle \equiv |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle$ translates or readdresses it to another configuration, multiplied by the respective fermionic prefactors. Indeed, the configuration $|\vec{J}\rangle$ is specified when the $M^A_v = M_A - N_A$ positions of the holes characterizing the A subsystem, that is, the $(i_1, i_2, \ldots, i_{M^A_v})$ set, and the $M^B_v = M_B - N_B$ positions of the holes characterizing the B subsystem, that is, the $(i'_1, i'_2, \ldots, i'_{M^B_v})$ set, are given. Then, the $J_A(\mathbf{i})$ and $J_B(\mathbf{i}')$ numbers available via Eq. (6) provide unique indices of the two-component address of this configuration in the state vector $|\Psi^{(AB)}\rangle$.

If the initial holes of the A subsystem are located at positions $(i_1, \ldots, k, \ldots, i_{M^A_v})$, the action of the $\hat{a}^\dagger_k \hat{a}_q$ operator kills a particle of A kind in the qth orbital and creates the particle of A kind in the kth orbital. We then obtain the holes at $(i_1, \ldots, q, \ldots, i_{M^A_v})$. Hence, according to Eq. (6), we get its new index J^{kq}_A of the two-component address (J^{kq}_A, J_B), where the standard fermionic prefactor has to be added to account for the correct permutation symmetry:

$$\hat{a}^\dagger_k \hat{a}_q |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle = (-1)^{d^{kq}_{J_A}} \left|J^{kq}_A, J_B\right\rangle, \quad k \in \mathbf{i}, \quad q \notin \mathbf{i}. \tag{30}$$

Clearly, the actions of the two-body terms would also lead to readdressings with some other fermionic prefactors:

$$\hat{a}_k^\dagger \hat{a}_s^\dagger \hat{a}_l \hat{a}_q |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle = \hat{a}_s^\dagger \hat{a}_l (-1)^{d_{J_A}^{kq}} \left| J_A^{kq}, J_B \right\rangle$$
$$= (-1)^{d_{J_A}^{kq}} (-1)^{d_{J_A^{kq}}^{sl}} \left| J_A^{ksl q}, J_B \right\rangle, k, s \in \mathbf{i}, l, q \notin \mathbf{i}. \quad (31)$$

The action of creation and annihilation operators from the A subspace changes the address of J_A component only and does not touch the J_B ones. Similarly, the actions of the one- and two-body B terms of the Hamiltonian read as follows:

$$\hat{b}_{k'}^\dagger \hat{b}_{q'} |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle = (-1)^{d_{J_B}^{k'q'}} \left| J_A, J_B^{k'q'} \right\rangle, \quad k' \in \mathbf{i}', \quad q' \notin \mathbf{i}', \quad (32)$$

$$\hat{b}_{k'}^\dagger \hat{b}_{s'}^\dagger \hat{b}_{l'} \hat{b}_{q'} |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle = \hat{b}_{s'}^\dagger \hat{b}_{l'} (-1)^{d_{J_B}^{k'q'}} \left| J_A, J_B^{k'q'} \right\rangle$$
$$= (-1)^{d_{J_B}^{k'q'}} (-1)^{d_{J_B^{k'q'}}^{s'l'}} \left| J_A, J_B^{k's'l'q'} \right\rangle,$$
$$k', s' \in \mathbf{i}', \quad l', q' \notin \mathbf{i}'. \quad (33)$$

Now, we show that the action of the interspecies terms from the $\hat{W}^{(AB)}$ part also results in a readdressing of the initial configuration to another one with a different fermionic prefactor:

$$\hat{a}_k^\dagger \hat{a}_q \hat{b}_{k'}^\dagger \hat{b}_{q'} |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle = (-1)^{d_{J_A}^{kq}} (-1)^{d_{J_B}^{k'q'}} \left| J_A^{kq}, J_B^{k'q'} \right\rangle, \quad (34)$$
$$k \in \mathbf{i}, \quad q \notin \mathbf{i}, \quad k' \in \mathbf{i}', \quad q' \notin \mathbf{i}'.$$

We have shown that the action of each term of the Hamiltonian, Eq. (27), on a general configuration readdresses it to another one within the same Fock subspace. This allows us to conclude that the action of the total Hamiltonian, Eq. (27), on a state vector, Eq. (29), can be obtained directly without construction of the respective Hamiltonian matrix:

$$\hat{H}^{(AB)} |\Psi^{(AB)}\rangle = \sum_{J_A=1}^{N_{\text{conf}}^A} \sum_{J_B=1}^{N_{\text{conf}}^B} C_{J_A J_B}^{\hat{H}^{(AB)}} |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle,$$
$$C_{J_A J_B}^{\hat{H}^{(AB)}} = C_{J_A J_B}^{\hat{H}^{(A)}} + C_{J_A J_B}^{\hat{H}^{(B)}} + C_{J_A J_B}^{\hat{W}^{(AB)}}, \quad (35)$$

where $C^{\hat{H}^{(A)}}$ and $C^{\hat{H}^{(A)}}$ can be read from Eqs. (8)–(12) and the $C_{J_A J_B}^{\hat{W}^{(AB)}}$ can be easily derived using Eq. (34):

$$\hat{W}^{(AB)} |\Psi^{(AB)}\rangle = \sum_{k,k',q,q'} W_{kk'qq'}^{(AB)} \hat{a}_k^\dagger \hat{a}_q \hat{b}_{k'}^\dagger \hat{b}_{q'} |\Psi^{(AB)}\rangle = \sum_{J_A=1}^{N_{\text{conf}}^A} \sum_{J_B=1}^{N_{\text{conf}}^B} C_{J_A J_B}^{\hat{W}^{(AB)}} |J_A(\mathbf{i}), J_B(\mathbf{i}')\rangle,$$
$$C_{J_A J_B}^{\hat{W}^{(AB)}} = \sum_{k,k',q,q'} W_{kk'qq'}^{(AB)} C_{J_A J_B}^{kk'qq'}, \quad (36)$$
$$C_{J_A J_B}^{kk'qq'} = \begin{cases} C_{J_A^{kq} J_B^{k'q'}} (-1)^{d_{J_A}^{kq}} (-1)^{d_{J_B}^{k'q'}}; & k \notin \mathbf{i}, q \in \mathbf{i}, k' \notin \mathbf{i}', q' \in \mathbf{i}' \\ 0; & \text{otherwise} \end{cases}.$$

Each element of the resulting vector has a unique address $(J_A(\mathbf{i}), J_B(\mathbf{i}'))$ characterized by the two sets of holes $(i_1, \ldots, q, \ldots, i_{M_v^A})$ and $(i'_1, \ldots, q', \ldots, i'_{M_v^B})$, that is, J_A and J_B are obtained by using Eq. (6). The value of the element $C_{J_A J_B}^{\hat{W}^{(AB)}}$ is computed as a sum of the $C_{J_A^{kq} J_B^{k'q'}}$ components of the incoming state vector scaled by the respective integrals $W_{kk'qq'}^{(AB)}$ and fermionic prefactors. The address $(J_A^{kq}, J_B^{k'q'})$ of each of these components is obtained for every given set k, k', q, q' by applying Eq. (6) to $(i_1, \ldots, k, \ldots, i_{M_v^A})$ and $(i'_1, \ldots, k', \ldots, i'_{M_v^B})$. Finally, the expectation value of the Hamiltonian as well as that of any other operator are available as a dot product of the incoming and respective resulting vectors in a manner very similar to what has been done in the single-component case, Eq. (15).

B. Mixture of bosons

Here, we consider the mixture of bosons of two different kinds, A and B. In Sec. III, we have seen that operations with single-component bosonic systems can be done without representing the respective operators in the matrix form. Now, we demonstrate the usefulness of this theory and ideas to bosonic mixtures.

The general configuration $|\vec{J}\rangle \equiv |J_A(\mathbf{n}), J_B(\mathbf{n}')\rangle$ is specified by the bosonic occupation numbers corresponding to the first $(n_1, n_2, \ldots, n_{M_A})$ and second $(n'_1, n'_2, \ldots, n'_{M_B})$ bosonic subsystems. Let us first show that the actions of typical intraspecies terms from the A subsystem lead to readdressings:

$$\hat{a}_k^\dagger \hat{a}_q |J_A(\mathbf{n}), J_B(\mathbf{n}')\rangle = \sqrt{n_k + 1}\sqrt{n_q} \left| J_A^{kq}, J_B \right\rangle, \quad (37)$$

$$\hat{a}_k^\dagger \hat{a}_s^\dagger \hat{a}_l \hat{a}_q |J_A(\mathbf{n}), J_B(\mathbf{n}')\rangle = \hat{a}_s^\dagger \hat{a}_l \sqrt{n_k + 1}\sqrt{n_q} \left| J_A^{kq}, J_B \right\rangle$$
$$= \sqrt{n_k+1}\sqrt{n_q}\sqrt{n_s+1}\sqrt{n_l} \left| J_A^{ksl q}, J_B \right\rangle. \quad (38)$$

Similar expressions can be obtained for the action of the intraspecies terms associated with the B subsystem. Clearly, the interbosonic term, acting on a general configuration, translates it to another one, weighted by the respective bosonic prefactor:

$$\hat{a}_k^\dagger \hat{a}_q \hat{b}_{k'}^\dagger \hat{b}_{q'} |J_A(\mathbf{n}), J_B(\mathbf{n}')\rangle$$
$$= \sqrt{n_k + 1}\sqrt{n_q}\sqrt{n_{k'} + 1}\sqrt{n_{q'}} \left| J_A^{kq}, J_B^{k'q'} \right\rangle. \quad (39)$$

Having verified that the actions of intra- and interspecies terms of the bosonic operators on a general configuration result in its readdressing with some scaling prefactors, we can explicitly express the result of the action of the Hamiltonian on a state vector, Eq. (29); that is, to sum up the contributions from all the terms of Eq. (27),

$$\hat{H}^{(AB)}|\Psi^{(AB)}\rangle = \sum_{J_A=1}^{N_{\mathrm{conf}}^A}\sum_{J_B=1}^{N_{\mathrm{conf}}^B} C_{J_AJ_B}^{\hat{H}^{(AB)}}|J_A(\mathbf{n}), J_B(\mathbf{n}')\rangle$$
$$C_{J_AJ_B}^{\hat{H}^{(AB)}} = C_{J_AJ_B}^{\hat{H}^{(A)}} + C_{J_AJ_B}^{\hat{H}^{(B)}} + C_{J_AJ_B}^{\hat{W}^{(AB)}}, \tag{40}$$

where $C^{\hat{H}^{(A)}}$ and $C^{\hat{H}^{(A)}}$ can be deduced from Eqs. (22)–(26) and the $C_{J_AJ_B}^{\hat{W}^{(AB)}}$ can be derived using Eq. (39) in a way very similar to that done in Eq. (36).

We conclude that the operation of the Hamiltonian representing a binary mixture of bosons on a state vector can be performed directly without constructing the respective Hamiltonian matrix.

C. Mixture of bosons and fermions

In the two preceding subsections, we have seen that effective and efficient operations and manipulations with state vectors of a binary mixture of bosons or a binary mixture of fermions are possible without resorting to the matrix representation of the respective operators. Actually, the final Eqs. (35) and (40) for $\hat{H}^{(AB)}|\Psi^{(AB)}\rangle$ are almost identical, with the only exception of the enumeration scheme used to address fermionic and bosonic configurations. In the Fermi-Fermi case, we use the positions of the holes $\mathbf{i}, \mathbf{i}'$ of the A and B subsystems to specify the fermionic configurations and Eq. (6) to compute the indices of the two-component address of the mixture, whereas in the Bose-Bose case, we utilize bosonic occupation numbers $\mathbf{n}, \mathbf{n}'$ to specify the bosonic configurations and Eq. (20) to compute the components of the respective address. The goal of this subsection is to demonstrate, for completeness, the validity and applicability of the theory to a mixed system of bosons and fermions.

Let A be the fermionic subsystem and B be the bosonic one. Now, to specify the general configuration $|\vec{J}\rangle \equiv |J_A(\mathbf{i}), J_B(\mathbf{n})\rangle$, one has to provide a set of the fermionic holes $(i_1, i_2, \ldots, i_{M_v^A})$ and a set of the bosonic occupation numbers $(n_1, n_2, \ldots, n_{M_B})$. The two-component address of this configuration is defined by the two numbers $J_A(\mathbf{i})$ and $J_B(\mathbf{n})$ computed using Eqs. (6) and (20), respectively.

Clearly, the operation of the one- and two-body fermionic terms on the general configuration changes the positions of the fermionic holes and does not affect the bosonic occupation numbers. In other words, only the first (fermionic) index of the two-component address $|\vec{J}\rangle$ is changed, like in Eqs. (30) and (31). Similarly, the action of the pure bosonic terms on a general configuration readdresses only the bosonic index, analogously to Eqs. (37) and (38). The Bose-Fermi interaction terms lead to the change of both fermionic and bosonic parts of the two-component address:

$$\hat{a}_k^\dagger \hat{a}_q \hat{b}_{k'}^\dagger \hat{b}_{q'}\,|J_A(\mathbf{i}), J_B(\mathbf{n})\rangle$$
$$= (-1)^{d_{J_A}^{kq}}\sqrt{n_{k'}+1}\sqrt{n_{q'}}\,\big|J_A^{kq}, J_B^{k'q'}\big\rangle, \quad k \in \mathbf{i}, \quad q \notin \mathbf{i}. \tag{41}$$

Every configuration characterized by $\mathbf{i} = (i_1, i_2, \ldots, i_{M_v^A})$ and $\mathbf{n} = (n_1, n_2, \ldots, n_{M_B})$ and therefore having the address $\mathbf{(}J_A(\mathbf{i}), J_B(\mathbf{n})\mathbf{)}$ is translated to a configuration $(J_A^{kq}, J_B^{k'q'})$ where the kth fermionic hole was filled and a new hole at q was created, that is, $(i_1, \ldots, q, \ldots, i_{M_v^A})$, and simultaneously one boson from bosonic orbital q' was transfered to orbital k', that is, $(n_1, \ldots, n_{k'}+1, \ldots, n_{q'}-1, \ldots, n_{M_B})$.

The action of any term of the Bose-Fermi Hamiltonian on a general configuration leads to its translation, that is, readdressing with some known prefactor. This allows us to apply the developed theory and write down the result of the action of the Hamiltonian on a state vector of the system as follows:

$$\hat{H}^{(AB)}|\Psi^{(AB)}\rangle = \sum_{J_A=1}^{N_{\mathrm{conf}}^A}\sum_{J_B=1}^{N_{\mathrm{conf}}^B} C_{J_AJ_B}^{\hat{H}^{(AB)}}\,|J_A(\mathbf{i}), J_B(\mathbf{n})\rangle,$$
$$C_{J_AJ_B}^{\hat{H}^{(AB)}} = C_{J_AJ_B}^{\hat{H}^{(A)}} + C_{J_AJ_B}^{\hat{H}^{(B)}} + C_{J_AJ_B}^{\hat{W}^{(AB)}}, \tag{42}$$

where the contributions $C^{\hat{H}^{(A)}}$ and $C^{\hat{H}^{(B)}}$ from the actions of the intraspecies Hamiltonians can be deduced from Eqs. (8)–(12) and Eqs. (22)–(26), respectively. The results of the action of the Bose-Fermi interactions $C_{J_AJ_B}^{\hat{W}^{(AB)}}$ can be derived using Eq. (41) in a way very similar to that done in Eq. (36).

D. More components

In the previous subsections, we have shown that the total configurational spaces of quantum systems made of two kinds of particles, that is, Fermi-Fermi, Bose-Bose, and Bose-Fermi mixtures, can be labeled by two-component vector index $\vec{J} = (J_A, J_B)$. A system with a larger number of components can be addressed by a multicomponent vector index $\vec{J} = (J_A, J_B, J_C, \ldots)$. Then, all the experience collected here can be expanded to these systems as well. The only constrain is that the total number of particles of each kind is conserved, that is, there are no terms in the Hamiltonian leading to particle conversion. We recall that, depending on the quantum statistics of the subsystem (i.e., whether we are dealing with fermions or bosons), we apply different schemes to enumerate the respective configurations. Both derived enumeration schemes, that is, Eq. (6) for fermions and Eq. (20) for bosons, are applicable only if $N_A = \mathrm{const}$, $N_B = \mathrm{const}$, $N_C = \mathrm{const}$, ... We just mention here that a generalization of the presented enumeration schemes can be adopted also to systems with particle conversion. This issue is out of the scope of the present study.

The most relevant conclusion is that for multicomponent Hamiltonians the action of each term on a state vector leads to readdressing the configurations with some quantum-statistics-dependent but simple and known prefactors. We can find the results of actions of each of these terms on the state vector independently. The total action of the Hamiltonian is obtained by summing over all the resulting vectors. Having at hand the initial and resulting state vectors, we can readily compute the expectation value of the Hamiltonian as a simple dot product of these two vectors.

V. REMARKS ON IMPLEMENTATION

Here, to discuss a strategy for a practical implementation of the ideas presented in all previous sections, we refer to the single-component bosonic or fermionic system. To define the system means to specify the number of particles N, their quantum statistics, and the number of the orbitals M. The integrals h_{kq} and W_{ksql} specify the Hamiltonian or any other operator of interest. Depending on the type of the quantum statistics, the N and M define the length of the state vector N_{conf} according to Eqs. (4) or (18), respectively. It is equal to the number of the elements in the one-dimensional vector-array of complex numbers $\{C_J\}_{J=1}^{N_{\mathrm{conf}}}$ representing the state vector $|\Psi\rangle$ of the system.

Now we explain basic computational steps needed to get the result of the action of the Hamiltonian on a state vector. As a first step, for a given incoming state vector $|\Psi\rangle$, that is, a vector-array of expansion coefficients $\{C_J\}_{J=1}^{N_{\mathrm{conf}}}$, the action of every pair or quartet of creation and annihilation operators is evaluated using Eqs. (8) and (9) for fermionic or Eqs. (22) and (23) for bosonic systems. The result of the action of each such operator on a state vector is another state vector; that is, as an outcome we get again a one-dimensional vector-array of some other complex numbers $\{C'_J\}_{J=1}^{N_{\mathrm{conf}}}$ of the same length N_{conf}. It is very important to stress that the action of each of these operators can be computed independently, implying an effective parallelization. For example, each available computational node is designated to a specific pair or quartet of creation and annihilation operators. Next, the incoming array $\{C_J\}_{J=1}^{N_{\mathrm{conf}}}$ is broadcasted to every node, and the respective actions take place, producing the resulting arrays. We apply Eqs. (13) and (14) on each node to compute the corresponding element of the reduced one- or two-body density matrices as dot products of the incoming and respective resulting vector-arrays. Then, by multiplying each and every element of the resulting vector-array by the corresponding integral h_{kq} or W_{ksql}, we get on each node the desired action of the respective Hamiltonian term. Now, to sum up the resulting vectors from all the nodes, we can use an appropriate collective operation and get the desired total action of the Hamiltonian on the incoming state vector. Finally, using Eq. (15), we easily compute the expectation value of the Hamiltonian $\langle\Psi|\hat{H}|\Psi\rangle$ as a dot product of the total resulting and incoming state vectors.

This technique has several advantages. First of all, it does not require the evaluation of the Hamiltonian matrix elements in the given many-body basis set. Consequently, there is no need to construct, store, and address these elements of the Hamiltonian matrix at all. Second, the elements of the reduced one- and two-body matrices are immediately and naturally available. Third, this technique can be easily extended to three- and higher body interaction potentials. Last but not the least, such a strategy implies very effective parallelization schemes, which are of high demand in modern computational physics. Finally, in the formulation of this method we did not specify explicitly the h_{kq} and W_{ksql} numbers; therefore, it is valid for general many-body Hamiltonians or for any other operators represented in the second quantization form. Consequently, this scheme can be successfully applied to standard real-space Hamiltonians as well as to discrete ones (e.g., of the Bose-Hubbard type). The derivations of the readdressing scheme have been done for the full Fock subspace spanned by permutation of N particles over M orbitals, but in principle, any selected subspace can be used. For example, an implementation of additional constraints on possible excitation patterns for fermions or restrictions on occupancies of the higher bosonic orbitals leads to considerable reduction of the respective configurational subspaces. In these cases, the enumeration schemes derived previously have to be modified accordingly. Moreover, one has to pay additional attention to the readdressing cases leading beyond the selected configurational subspace. This opens, on the other hand, a new vision on size-consistency issues [8,13]; it can be now explicitly considered and analyzed.

The present mapping, as mentioned before, assumes the integrals h_{kq} and W_{ksql} to be known. In relevant computations, these integrals are evaluated from self-consistent or even from time-dependent one-body functions (orbitals) that have to be computed "on the fly". It is relevant to discuss the usefulness of the present formalism in this situation as well. We have already implemented the present mapping for interacting bosons (see Refs. [10,11]), where we treated their rich many-body dynamics utilizing a few million time-dependent configurations assembled from up to $M = 12$ orbitals. There was no difficulty in this case at all to compute for each and every time point the time-dependent orbitals underlying the integrals h_{kq} and W_{ksql}. These computations were practically impossible without the present mapping.

VI. SUMMARY AND CONCLUSIONS

In this article, we provide a novel, effective, and general technique to construct the result of the action of any particle-conserving operator represented in the second quantized form on a many-body state vector. Within a standard framework, one represents the corresponding operator in a matrix form and obtains the desired action of the operator by applying a matrix-to-vector multiplication. We have shown that the same result can be reached without even referring to the respective matrix elements. Considering configurations as coordinates of the many-body state vector, we first demonstrated that the action of any even combination of creation and annihilation operators on a configuration translates or readdresses it to another configuration. In other words, we have seen that such an action is equivalent to permutation of coordinates of the initial state vector, weighted by some trivial prefactors. The total action of any operator, represented in the second quantized form on a state vector, is a sum of the actions of all its terms.

Next, for a full subspace of the configurational space spanned by permutation of N fermions over M orbitals, we present a simple and compact scheme to enumerate the fermionic configurations according to the given set of the holes' positions. Then, using the formal isomorphism between the configurational spaces formed by this fermionic system and the system of N bosons distributed over the corresponding number of bosonic orbitals, we invent a simple and compact scheme to enumerate bosonic configurations according to the given set of the bosonic occupation numbers. Using these enumeration algorithms, we directly construct the result of the action of any pair or quartet of the annihilation and creation

operators on a state vector. Moreover, the respective matrix elements of the reduced one- and two-body density matrices are naturally available as simple dot products of the initial and resulting state vectors. This allows us to combine the total action of the Hamiltonian as a sum of all its terms into simple and compact formulas, which can be directly implemented and permit straightforward parallelization. The proposed ideas to operate with fermionic and bosonic Hamiltonians have been directly extended to binary mixtures of fermions and of bosons as well as to Bose-Fermi mixtures. We have also shown that the same ideas can be naturally applied to systems made of a larger number of components as well.

Finally, since the $\hat{H}|\Psi\rangle$ is the basic building block appearing in the computations of statical properties as well as of the evolution dynamics of many-body systems, we expect that the implementation of the theory into the respective computational approaches will increase their efficiency and enable applications to systems made of larger number of particles than currently possible. Indeed, the proposed ideas have recently been implemented for bosonic systems [10,11] within the MCTDHB [12], and applications to multiboson long-time dynamics in double-well [10] and triple-well [11] traps have already been performed successfully.

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