Back and forth from Fock space to Hilbert space: a guide for commuters

Andrea Beggi[1], **Ilaria Siloi**[2], **Claudia Benedetti**[3], **Enrico Piccinini**[4], **Luca Razzoli**[5], **Paolo Bordone**[5], **Matteo G. A. Paris**[3,6]

[1]I.I.S. *Primo Levi*, I-41058 Vignola, Italy.
[2]Department of Physics, University of North Texas, 76201 Denton, Texas, USA.
[3]Quantum Technology Lab, Dipartimento di Fisica *Aldo Pontremoli*, Università degli Studi di Milano, I-20133 Milano, Italy.
[4]Dipartimento di Ingegneria dell'Energia Elettrica e dell'Informazione *Guglielmo Marconi*, Università di Bologna, I-40136 Bologna, Italy.
[5]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, I-41125 Modena, Italy.
[6]The Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai, 600113, India.

Abstract. Quantum states of systems made of many identical particles, e.g. those described by Fermi-Hubbard and Bose-Hubbard models, are conveniently depicted in the Fock space. However, in order to evaluate some specific observables or to study the system dynamics, it is often more effective to employ the Hilbert space description. Moving effectively from one description to the other is thus a desirable feature, especially when a numerical approach is needed. Here we recall the construction of the Fock space for systems of indistinguishable particles, and then present a set of recipes and advices for those students and researchers in the need to commute back and forth from one description to the other. The two-particle case is discussed in some details and few guidelines for numerical implementations are given.

1. Introduction

The wave function describing the quantum state of a collection of identical bosons is symmetric under the exchange of any two particles, and is thus naturally described in the Hilbert space of symmetric functions, which is a subspace of the tensor product of single-particle states. On the contrary, the wave function for a collection of identical fermions is antisymmetric, which means that it must change sign when we exchange any two particles. These wave functions are elements of a Hilbert space of antisymmetric functions, which is another subspace of the tensor product of single-particle states. Indistinguishability thus introduces correlations in the wave function, and this is true even for non-interacting particles, a feature that prompted attempts to do quantum information processing exploiting only the statistical properties of quantum systems [1, 2].

The above facts are usually summarised by saying that for quantum particles with a definite statistics not all available states are permitted, also in those situations where one addresses free particles. In graduate physics courses, second quantization and the Fock space [3, 4, 5, 6, 7], are presented as the natural framework where this constraint may be naturally taken into account. Indeed, the Fock space is a crucial tool in the description of systems made of a variable, or unknown, number of identical particles. In particular, the Fock space allows one to build the space of states starting from the single-particle Hilbert space. As a side effect, the usual introduction of the Fock space may somehow give the impression that the Hilbert space description may be left behind. On the other hand, the representation of operators in the Fock space is not straightforward since the indexing of the basis set states, as well as the interpretation of the number states in terms of particle states, are usually not trivial. A known example is that of fermionic operators on a lattice system [8]: anti-commutation rules have to be taken into account and additional phases appear in the components of hopping operators from a site to another through periodic boundary conditions. Additionally, one often encounters operators that are symmetrized or anti-symmetrized versions of a distinguishable particle operator, e.g. the kinetic term in Hubbard models [8, 9, 10], and in this case one may assume that those operators contain both bosonic and fermionic features, which should be then discriminated (separated) using a suitable transformation [11].

For all the above reasons, it is often more transparent to employ the Hilbert space description and to study *there* the dynamics of a physical system [12], as done in some recent works concerning the study of quantum walks of identical particles [13, 14, 15, 16]. On the other hand, Fock number states appear quite naturally in the description of systems of identical particles and thus a question arises on how and whether we may go from Fock space to Hilbert space and vice versa with minimum effort.

The main goal of this paper is to provide a gentle introduction to details of the transformation rules between the different description of states and operators in the two spaces. We start smoothly, by recalling the construction of the Fock space for systems of indistinguishable particles, and then offer a set of recipes, guidelines, and advices for those people interested in going back and forth from one description to the other. We devote some attention to the two-particle case, which already contains most of the interesting features related to indistinguishability, and briefly discuss how to take care of the two different representations in numerical implementations. The material presented in this paper is intended to be a concise reference about the different representations employed in many-body physics, and it aims at being useful to students and researchers working with systems of identical particles, ranging from photons in a black-body cavity to interacting electrons in a lattice, and from neutrons in a neutron star to helium atoms in a superfluid.

The paper is structured as follows. In Section 2.1 we recall few basic notions about indistinguishable particles and the construction of the Fock space. In Section 3 we illustrate in details how to change description from Hilbert space to Fock space and vice versa in the operator representation and the system evolution. Section 4 presents some specific applications, whereas Section 5 contains guidelines to numerical implementations. Finally, Section 6 closes the paper with some concluding remarks.

2. Identical particles and the Fock space

2.1. From distinguishable to indistinguishable particles

Let us start by considering a collection of N identical but distinguishable particles, each of which can be put in one of the K *modes* of a quantum system, e.g. the K eigenstates of its Hamiltonian. The collective state describing the system is given by

$$|\Psi\rangle = |k_1\rangle \otimes |k_2\rangle \otimes ... \otimes |k_N\rangle = |k_1, k_2, ..., k_N\rangle \,, \tag{1}$$

or by any linear combination of states of this kind, which all belong to the K^N-dimensional N-particles Hilbert space $\mathscr{H}_N = \mathscr{H}_1^{\otimes N}$ given by the tensor product of N single-particle spaces $\mathscr{H}_1$, each one with dimension K and basis $\{|k_i\rangle\}_i$.

Let us now introduce the notion of indistinguishability [17]. We start by the definition of the permutation operator $\hat{P}_{ij}$, whose effect is to exchange the states of the particles i and j inside any state $|\{k_i\}_i\rangle$:

$$\hat{P}_{ij}\,|k_1, k_2, ..., k_i, ..., k_j, ..., k_N\rangle = |k_1, k_2, ..., k_j, ..., k_i, ..., k_N\rangle \,. \tag{2}$$

If the particles are indistinguishable, the overall state of the system $|\Psi\rangle_{id}$ will be given by linear combination of states (of distinguishable particles) which is invariant under action of $\hat{P}_{ij}$, e.g. states like $|\{k_i\}_i\rangle$. It means that $\hat{P}_{ij}\,|\Psi\rangle_{id}$ is a state physically indistinguishable from the previous one, i.e. they can differ only for a phase:

$$\hat{P}_{ij}\,|\Psi\rangle_{id} = e^{\mathrm{i}\phi}\,|\Psi\rangle_{id} \,. \tag{3}$$

Of course, two identical permutations must reproduce the initial state, i.e.:

$$\hat{P}_{ij}^2\,|\Psi\rangle_{id} = e^{2\mathrm{i}\phi}\,|\Psi\rangle_{id} = |\Psi\rangle_{id} \,, \tag{4}$$

and thus the eigenvalues for $\hat{P}_{ij}$ are given by $e^{\mathrm{i}\phi} = \pm 1$.

According to the spin-statistics theorem we have two categories of identical particles: *fermions*, which are characterized by half-integer spins and anti-symmetric wavefunctions, and *bosons*, which are characterized by integer spins and symmetric wavefunctions. High precision experiments have confirmed the spin-statistics and established strict probability bounds for a violation to occur [18, 19, 20, 21]. Alternative para-statistics have been suggested earlier in the history of quantum mechanics [22], however we are not discussing here the properties of those kind of particles, e.g. anyons [23].

A state is symmetric or anti-symmetric under the action of $\hat{P}_{ij}$ if, respectively, it maintains or it changes its sign, i.e.:

$$\hat{P}_{ij} \left|\Psi\right\rangle_F = - \left|\Psi\right\rangle_F , \tag{5}$$

$$\hat{P}_{ij} \left|\Psi\right\rangle_B = + \left|\Psi\right\rangle_B . \tag{6}$$

A symmetric or anti-symmetric state can be built with the proper symmetrization operator $\hat{S}$ or $\hat{A}$, acting on the distinguishable particle state $\left|\Psi\right\rangle$:

$$\hat{S} \left|\Psi\right\rangle = \left|\Psi\right\rangle_B , \tag{7}$$

$$\hat{A} \left|\Psi\right\rangle = \left|\Psi\right\rangle_F . \tag{8}$$

In general, the symmetrization operators can be built as

$$\begin{bmatrix} \hat{S} \\ \hat{A} \end{bmatrix} \left|\Psi\right\rangle = \begin{bmatrix} \left|\Psi\right\rangle_B \\ \left|\Psi\right\rangle_F \end{bmatrix} = \sqrt{\frac{n_1! n_2! ... n_K!}{N!}} \sum_{\hat{P}} (\pm 1)^{\sigma(P)} \hat{P} \left|\Psi\right\rangle , \tag{9}$$

where we are applying on $\left|\Psi\right\rangle$ all the possible distinct permutations $\hat{P}$ of the N single-particle states $\left|k_i\right\rangle$ included in $\left|\Psi\right\rangle$, each one multiplied by the sign of the permutation $(-1)^{\sigma(P)}$, where $\sigma(P)$ is the number of particle exchanges occurred in the permutation $\hat{P}$, when we are dealing with fermions. Notice that any N-particle permutation $\hat{P}$ can be built by composing a proper sequence of two-particle permutations $\hat{P}_{ij}$, and the same is true for the operators $\hat{A}$ and $\hat{S}$. The states should be then properly normalized with the prefactor under square root, where n_k indicates the number of particles occupying the state k, i.e., the number of times that k occurs in $\left|\Psi\right\rangle$.

¿From the anti-symmetrization procedure for fermions, we derive the *Pauli exclusion principle*, that forbids two fermions to occupy the same state: indeed, if this was the case, e.g. for the particles i and j, we would have contemporarily

$$\hat{P}_{ij} \left|\Psi\right\rangle_F = - \left|\Psi\right\rangle_F , \tag{10}$$

$$\hat{P}_{ij} \left|\Psi\right\rangle_F = \left|\Psi\right\rangle_F , \tag{11}$$

where the first equality comes from Eq. (5), while the second one comes from the fact that the two particles occupy the same state. The only possible conclusion is that our state is the null vector.

In order to properly describe states and operators taking into account the indistinguishability of particles we should move to the formalism of second quantization [24], where states belong to the bosonic or fermionic Fock space $\mathscr{F}$, that is a space containing states with a number of particles that in principle is not fixed. The *number states* (basis states) of the Fock space can be represented as

$$\left|n_1, n_2, ..., n_K\right\rangle_{B(F)} , \tag{12}$$

with the fundamental constraint $n_i \in \{0, 1\}$ holding only for fermions, because of Pauli's principle. If we deal with a fixed number N of particles, there is the additional constraint $\sum_{i=1}^{K} n_i = N$. In this last case, we are operating in the subspace of $\mathscr{F}$ called $\mathscr{F}_N$. Indeed the Fock space is given by:

$$\mathscr{F} = \bigoplus_{N=0}^{\infty} \mathscr{F}_N . \tag{13}$$

These number states coincide with the states of Eq. (1) except for the relabeling (and the symmetrization). Indeed, while in the *first quantization* formalism we specify for each particle i ($i = 1, ..., N$) the state/mode k_i that it occupies, in the second quantization formalism we treat particles as excitation of the modes of a field, therefore for each mode i ($i = 1, ..., K$) we specify how many excitation/particles n_i it contains, since we cannot distinguish among them (see Fig. 1).

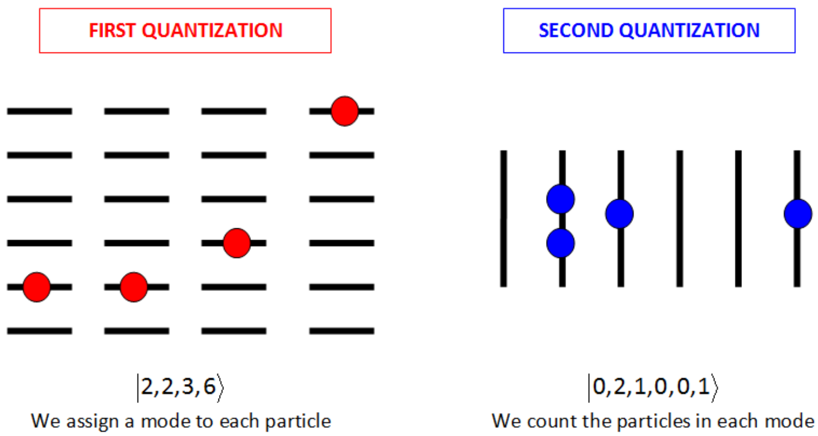

Figure 1: First and Second Quantization compared for $N = 4$ particles and $K = 6$ modes available to each particle.

The total number of particles N can be changed through the application of *creation* and *annihilation* (or *destruction*) operators, respectively denoted as $\hat{a}_i^\dagger$ and $\hat{a}_i$. These operators create or destroy a particle in the mode/state i, so they connect the Fock subspaces with a different number of particles:

$$\hat{a}_i^\dagger : \mathscr{F}_N \to \mathscr{F}_{N+1}, \tag{14}$$
$$\hat{a}_i : \mathscr{F}_N \to \mathscr{F}_{N-1}. \tag{15}$$

In more detail, these operators are defined by the following commutation rules:

$$[\hat{a}_i, \hat{a}_j]_\mp = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right]_\mp = 0, \tag{16}$$
$$\left[\hat{a}_i, \hat{a}_j^\dagger\right]_\mp = \delta_{i,j}, \tag{17}$$

where the upper sign, denoting the commutator, holds for bosons, while the lower sign, denoting the anti-commutator, holds for fermions. It is quite important to stress, therefore, that fermionic creation (annihilation) operators do anticommute: therefore, when we exchange their order, we have to add a minus sign for each permutation we perform.

Upon denoting by $|0\rangle$ the *vacuum state*, corresponding to a state with no particle, i.e. $|0, 0, ..., 0\rangle$ (not to be confused with the null vector), we can build any number state as

$$|n_1, n_2, ..., n_K\rangle_{B(F)} = \prod_{i=1}^{K} \frac{1}{\sqrt{n_i!}} \left(\hat{a}_i^\dagger\right)^{n_i} |0\rangle \, . \tag{18}$$

From the commutation rules, we also deduce the action of the creation and annihilation operators on the number states:

$$\hat{a}_i^\dagger \left|n_1, n_2, ..., n_i, ..., n_K\right\rangle_{B(F)} = \begin{cases} \sqrt{n_i+1}\left|n_1, n_2, ..., n_i+1, ..., n_K\right\rangle_B \\ (1-n_i)(-1)^{\sigma_i}\left|n_1, n_2, ..., 1-n_i, ..., n_K\right\rangle_F \,, \end{cases} \tag{19}$$

$$\hat{a}_i \left|n_1, n_2, ..., n_i, ..., n_K\right\rangle_{B(F)} = \begin{cases} \sqrt{n_i}\left|n_1, n_2, ..., n_i-1, ..., n_K\right\rangle_B \\ n_i(-1)^{\sigma_i}\left|n_1, n_2, ..., 1-n_i, ..., n_K\right\rangle_F \,, \end{cases} \tag{20}$$

where the σ_i exponent is due to the anti-commuting rules and is given by

$$\sigma_i = \sum_{k=1}^{i-1} n_k. \tag{21}$$

From Eqs. (19)-(20) we straightforwardly deduce that

$$\hat{a}_i \left|n_1, n_2, ..., n_i, ..., n_K\right\rangle = 0 \quad \text{if } n_i = 0, \tag{22}$$

$$\hat{a}_i^\dagger \hat{a}_i \left|n_1, n_2, ..., n_i, ..., n_K\right\rangle = n_i \left|n_1, n_2, ..., n_i, ..., n_K\right\rangle. \tag{23}$$

The last equation gives the definition of the *number operator*

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i, \tag{24}$$

that counts the number of particles in the mode i.

Let us now consider a single-particle operator $\hat{O}_j$ acting on the particle j. It is apparent that we must have

$$\hat{P}_{ij}\hat{O}_j\hat{P}_{ij} = \hat{O}_i. \tag{25}$$

Then, for a many-particle operator $\hat{O}$, we will say that this operator is invariant under particle exchange (*permutation symmetry*) if, for any couple of particles i and j, the following relation holds:

$$\hat{P}_{ij}\hat{O}\hat{P}_{ij} = \hat{O}. \tag{26}$$

However, the previous property does not mean that the operator $\hat{O}$ must be invariant also under the action of $\hat{A}$ and $\hat{S}$, but it implies that these symmetry operators must commute with $\hat{O}$. It means, therefore, that for $\hat{O} = \hat{H}$ the evolution preserves the symmetry of bosonic and fermionic states, i.e. their subspaces

$$\mathscr{F}_N^B = \hat{S}\mathscr{H}_N \tag{27}$$

and

$$\mathscr{F}_N^F = \hat{A}\mathscr{H}_N \tag{28}$$

are not mixed, since the Hamiltonian $\hat{H}$ and $\hat{S}\,(\hat{A})$ have a common set of orthogonal eigenstates. Therefore, this kind of operators can be used in the second quantization formalism with identical particle states in the same way they were used in first quantization, because they preserve the permutation symmetry. We remind here that second quantization representation is strictly connected with the choice of the basis $\{|a_i\rangle\}_i$ in which the operators $\hat{a}_i^\dagger\,(\hat{a}_i)$ are creating (destroying) particles: indeed, if

$\hat{a}_i^\dagger$ ($\hat{a}_i$) creates (destroys) a particle in the i-th eigenstate of the Hamiltonian, we can define a change of basis and build a new set of operators $\hat{b}_i^\dagger$ ($\hat{b}_i$) that create (destroy) particles in the i-th eigenstate of any other operator $\hat{O}$ (e.g. in the i-th site of a lattice for the position operator):

$$|b_i\rangle = \left[\hat{b}_i^\dagger\right]|0\rangle = \sum_j \langle a_j|b_i\rangle\,|a_j\rangle = \left[\sum_j \langle a_j|b_i\rangle\,\hat{a}_j^\dagger\right]|0\rangle\,. \tag{29}$$

2.2. Two-particle case

Here and in the rest of the article we apply the tools introduced in the previous section to the specific case of $N = 2$ identical particles. Despite the small number of particles, this example shows most of the peculiarities related to indistinguishability, and illustrates how to deal with both Fock and Hilbert descriptions to conveniently describe the physics of the system.

In the Hilbert space $\mathscr{H}_2$ (for distinguishable particles), the basis set is given by $\{|i,j\rangle\}_{i,j}$. According to the symmetrization procedures described above for a 2-boson state we have

$$|i,j\rangle_s = \begin{cases} \frac{1}{\sqrt{2}}\left(|i,j\rangle + |j,i\rangle\right) & \text{for}\, i<j \\ |i,i\rangle & \text{for}\, i=j\,, \end{cases} \tag{30}$$

while for a 2-fermion state the allowed basis set is given by:

$$|i,j\rangle_a = \frac{1}{\sqrt{2}}\left(|i,j\rangle - |j,i\rangle\right) \quad \text{for}\, i<j, \tag{31}$$

where the constraint $j > i$ avoids overcounting in the basis set, since

$$|j,i\rangle_s = |i,j\rangle_s\,, \tag{32}$$

$$|j,i\rangle_a = -\,|i,j\rangle_a\,. \tag{33}$$

It is easy to check that these two new basis sets are orthogonal and related to the previous one by

$$\{|i,j\rangle\}_{i,j} = \{|i,j\rangle_s\}_{i,j} \cup \{|i,j\rangle_a\}_{i,j}. \tag{34}$$

Indeed, the dimension d_B of the basis set for bosonic particles is given by

$$d_B = K + \frac{K(K-1)}{2} = \frac{K(K+1)}{2}, \tag{35}$$

while the dimension d_F of the fermionic basis set is given by

$$d_F = \frac{K(K-1)}{2}, \tag{36}$$

and

$$d_B + d_F = K^2 = \dim(\mathscr{H}_2). \tag{37}$$

Overall, the Hilbert space $\mathscr{H}_2$ is decomposed into two subspaces [25]: one contains only symmetric states, while the other one only anti-symmetric states, see Fig. 2. These subspaces are, in turn, the 2-particle restrictions of the Fock spaces for bosons and fermions, namely $\mathscr{F}_2^B$ and $\mathscr{F}_2^F$:

$$\mathscr{H}_2 = \mathscr{F}_2^B \oplus \mathscr{F}_2^F. \tag{38}$$

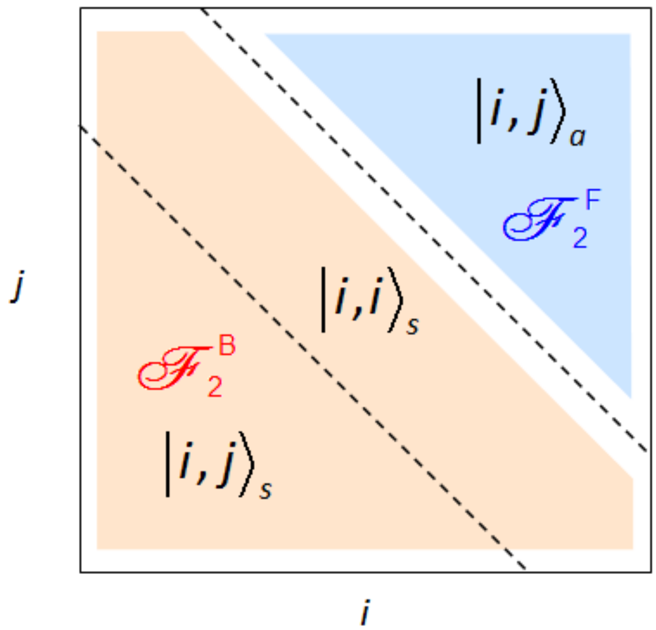

Figure 2: Hilbert space decomposition into symmetry-defined Fock subspaces for $N = 2$ particles.

Each subspace is obtained, in general, by applying the proper symmetry operators over $\mathscr{H}_2$:

$$\mathscr{F}_2^B = \hat{S}\mathscr{H}_2, \tag{39}$$

$$\mathscr{F}_2^F = \hat{A}\mathscr{H}_2, \tag{40}$$

which are given by the following projectors:

$$\hat{S} = \sum_i |i,i\rangle\langle i,i| + \sum_{i,j>i} \frac{1}{2}\left(|i,j\rangle + |j,i\rangle\right)\left(\langle i,j| + \langle j,i|\right), \tag{41}$$

$$\hat{A} = \sum_{i,j>i} \frac{1}{2}\left(|i,j\rangle - |j,i\rangle\right)\left(\langle i,j| - \langle j,i|\right). \tag{42}$$

However, the action of $\hat{S}$ and $\hat{A}$ is not enough to write operators (or states) in the Fock space. Indeed, if we consider the bosonic operator $\hat{O}_B = \hat{S}\hat{O}\hat{S}$, in order to properly represent it in the Fock space we still have to perform a change of basis. Therefore, sometimes it could be useful to perform both operations in a single step, by writing the symmetry operators in a mixed-basis representation (where the bras are states of $\mathscr{H}_2$, while kets are states of $\mathscr{F}_2$):

$$\hat{S} = \sum_i |i,i\rangle_s \langle i,i| + \sum_{i,j>i} |i,j\rangle_s \frac{1}{\sqrt{2}} \left(\langle i,j| + \langle j,i|\right), \tag{43}$$

$$\hat{A} = \sum_{i,j>i} |i,j\rangle_a \frac{1}{\sqrt{2}} \left(\langle i,j| - \langle j,i|\right). \tag{44}$$

so that we can write the operator $\hat{O}_B$ in $\mathscr{F}_2$ directly as $\hat{S}\hat{O}\hat{S}^\dagger$ (a similar discussion also holds for fermionic operators).

Even if in general this is not true, we observe that for the case $N = 2$ we have

$$\hat{S} + \hat{A} = \hat{I}, \tag{45}$$

in agreement with Eq. (34). In conclusion, a distinguishable-particle operator $\hat{O}$ in $\mathscr{H}_2$ is invariant under particle-exchange symmetry if and only if the following decomposition holds:

$$\hat{O} = \hat{S}\hat{O}\hat{S} + \hat{A}\hat{O}\hat{A} = \hat{O}_s + \hat{O}_a, \tag{46}$$

i.e. the operator is the sum of its projections over the bosonic and fermionic subspaces of $\mathscr{H}_2$. This means that $\hat{O}$ does not mix states belonging to subspaces with different symmetries (i.e., fermionic and bosonic), and it commutes with $\hat{A}$ and $\hat{S}$. If this property holds also for the Hamiltonian $\hat{H}$, it is possible to perform a symmetrization only over the state vectors without modifying the operators. Indeed, $\hat{S}$ and $\hat{A}$ are projectors, $\hat{S} = \hat{S}^\dagger$ and $\hat{S}^n = \hat{S}$, and are orthogonal, i.e. $\hat{S}\hat{A} = \hat{A}\hat{S} = 0$. The dynamics thus conserves symmetries, and this is sufficient to get the right expectation values:

$$\hat{H}_s = \hat{S}\hat{H}\hat{S} = \hat{H}\hat{S}^2 = \hat{H}\hat{S}, \tag{47}$$

$$\hat{H}_s |\Psi\rangle_s = \hat{H}\hat{S}^2 |\Psi\rangle = \hat{H} |\Psi\rangle_s, \tag{48}$$

$$O_s = {}_s\langle\Psi|\hat{O}_s|\Psi\rangle_s = \langle\Psi| \hat{S}^2\hat{O}\hat{S}^2 |\Psi\rangle = \langle\Psi| \hat{S}\hat{O}\hat{S} |\Psi\rangle = {}_s\langle\Psi|\hat{O}|\Psi\rangle_s. \tag{49}$$

Clearly for the 2-particle case, the evaluation of expectation values and dynamics of the system can be conveniently obtained in the Hilbert space, starting with a properly (anti-)symmetrized state[26], namely $|\Psi\rangle_{(a)s}$. Then, with a proper *reshaping operation*, observables may be recast in the Fock space, see Fig. 3. This procedure presents advantages compared to a direct calculation in the Fock space where each particle loses its identity. For instance, the operation of partial trace over the degrees of freedom of one particle is straightforward in the Hilbert space, while it is more delicate in the Fock space, where the natural basis set is the occupation number. Moreover, the indexing of the basis in the Fock space is not trivial to handle [27], and a convenient way to rank the basis vectors should be considered in the numerical implementation (see Section 5). Therefore, it is often the case that the dynamics and all the required observables are evaluated in the Hilbert space, after a proper symmetrization of the initial state.

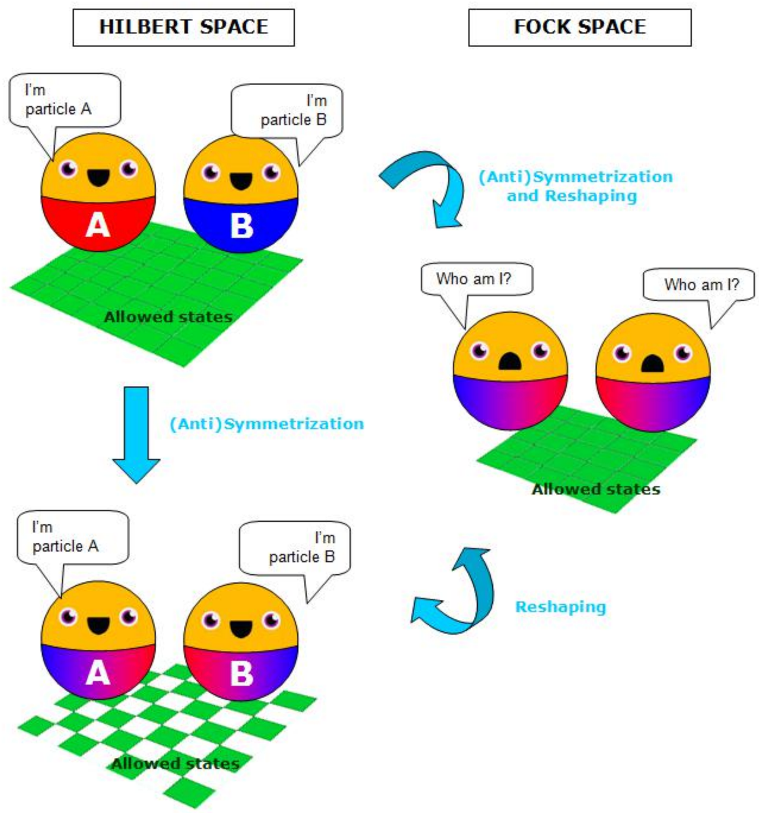

Figure 3: Pictorial representation of *symmetrization* and *reshaping* processes, which transform states and operators, respectively, from Hilbert to Fock space and vice versa. Notice that in the Hilbert space all particles have a clear identity (A or B in the example) and may even possess well defined states (the colors in the example) if they are distinguishable, whereas in the Fock space no particle has a clear identity or a well defined state. Switching from Hilbert to Fock space requires to properly (anti-)symmetrize states and to remove states with the wrong symmetry (reshaping), while going back to Hilbert space requires to reshape both operators and states, but the number of allowed states remains the same.

3. From Hilbert space to Fock space and vice versa

3.1. Operator representation: from Fock to Hilbert

Given the basis sets for the symmetric and antisymmetric subspaces, $\{|i,j\rangle_s\}_{i,j\geq i}$ and $\{|i,j\rangle_a\}_{i,j>i}$, their union $\mathcal{B}^* = \{|i,j\rangle_s\}_{i,j\geq i} \cup \{|i,j\rangle_a\}_{i,j>i}$ is a basis set for the whole Hilbert space $\mathscr{H}_2$. As discussed in the previous section, we typically use the distinguishable-particle basis set, hereafter labeled $\mathcal{B} = \{|i,j\rangle\}_{i,j}$.

The bosonic operator $\hat{O}_B$ may be represented with a $d_B \times d_B$ matrix defined on $\mathscr{F}_2^B$, but also with a $K^2 \times K^2$ matrix acting on $\mathscr{H}_2$. Adding d_F rows and d_F columns full of zeros, we may extend the Fock matrix $\hat{O}_B^{\mathscr{F}}$: the first d_B rows and columns involve only bosonic states, while the additional lines only the fermionic states (none, since it is a bosonic operator):

$$\hat{O}_B^{\mathscr{H}}|_{\mathcal{B}^*} = \left(\begin{array}{c|c} \hat{O}_B^{\mathscr{F}} & 0 \\ \hline 0 & 0 \end{array}\right). \tag{50}$$

When the basis set is given by $\mathcal{B}^*$, whose symmetric part coincides with the basis of $\mathscr{F}_2^B$, the representation $\hat{O}_B^{\mathscr{H}}|_{\mathcal{B}^*}$ is valid in $\mathscr{H}_2$. In order to represent operators in the basis $\mathcal{B}$ of distinguishable particles, we need to reverse this transformation, that is:

$$\hat{O}_B^{\mathscr{H}}|_{\mathcal{B}} = \hat{S}^\dagger \hat{O}_B^{\mathscr{H}}|_{\mathcal{B}^*} \hat{S}. \tag{51}$$

The relation between the elements of a bosonic operator in the Fock (basis $\mathcal{B}_s^* = \{|i,j\rangle_s\}_{i,j\geq i}$) and in the Hilbert space (basis $\mathcal{B} = \{|i,j\rangle\}_{i,j}$) is the following:

$$\left(O_B^{\mathscr{H}}\right)_{i,j;k,l} = \langle i,j|\, \hat{O}_B^{\mathscr{H}}|_{\mathcal{B}}\, |k,l\rangle = \frac{1}{2}\left(O_B^{\mathscr{F}}\right)_{i,j;k,l}(1+\epsilon\delta_{i,j})(1+\epsilon\delta_{k,l}), \tag{52}$$

where $\epsilon = \sqrt{2}-1$.

Analogous arguments apply to the fermionic case, thus

$$\hat{O}_F^{\mathscr{H}}|_{\mathcal{B}} = \hat{A}^\dagger \hat{O}_F^{\mathscr{H}}|_{\mathcal{B}^*} \hat{A}, \tag{53}$$

where

$$\hat{O}_F^{\mathscr{H}}|_{\mathcal{B}^*} = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \hat{O}_F^{\mathscr{F}} \end{array}\right). \tag{54}$$

Again, the transformation of a fermionic operator in the Fock space (basis $\mathcal{B}_a^* = \{|i,j\rangle_a\}_{i,j>i}$) to the Hilbert space (basis $\mathcal{B} = \{|i,j\rangle\}_{i,j}$) is given by

$$\left(O_F^{\mathscr{H}}\right)_{i,j;k,l} = \frac{1}{2}\left(O_F^{\mathscr{F}}\right)_{i,j;k,l}(1-\delta_{i,j})(1-\delta_{k,l})\,\varsigma_{i,j}\varsigma_{k,l}, \tag{55}$$

where $\varsigma_{i,j} = \mathrm{sgn}(j-i)$.

In the case of a 2-particle bosonic (fermionic) operator, the transformation laws from Fock to Hilbert space of distinguishable particles are thus given by equations (52) and (55), respectively. However, one should remind that the Fock space elements exist only for $i \leq j$ ($i < j$ for fermions), so indices in $\left(O_F^{\mathscr{F}}\right)_{i,j;k,l}$ must be exchanged if $i > j$ and/or $k > l$. Moreover, if $i = j$ or $k = l$, the corresponding elements are zero.

Notice that if the dynamics is evaluated in the Hilbert space, the reshaping operation needed to recast observables in the Fock space is given by the inverse equations of (52) and (55).

3.2. Symmetrized and antisymmetrized operators of distinguishable particles

Let us consider a *native* Hilbert operator $\hat{T}^{\mathscr{H}}$, i.e. an operator which arises naturally in the distinguishable particles Hilbert space $\mathscr{H}_2$ where the basis set is given by $\mathcal{B}$. Such an operator conserves parity, being invariant under particle exchange, thus it does not mix states with different symmetries; therefore it is equivalent to the sum of its projections with defined symmetries: $\hat{T}^{\mathscr{H}} = \hat{S}\hat{T}^{\mathscr{H}}\hat{S}^{\dagger} + \hat{A}\hat{T}^{\mathscr{H}}\hat{A}^{\dagger}$, see Fig. 4. Overall, we have that $\mathscr{H}_2^s$ and $\mathscr{H}_2^a$ are invariant subspaces for $\hat{T}^{\mathscr{H}}$.

Since the operator acts on states of distinguishable particles, it contains both bosonic and fermionic components, which can be isolated with a suitable transformation. An interesting example is the kinetic term $\hat{T}$ in the Hubbard model, which can be derived from the discretization of the laplacian terms in the Schrödinger equation, and describes the hopping of the two particles along a chain with K sites. In the distinguishable particles framework we have

$$\hat{T}^{\mathscr{H}} = \left[-J\sum_{i=1}^{K}(|i\rangle\langle i+1| + |i+1\rangle\langle i|)\right]\otimes I_1 + I_1\otimes\left[-J\sum_{i=1}^{K}(|i\rangle\langle i+1| + |i+1\rangle\langle i|)\right], \tag{56}$$

where $I_1 = \sum_{i=1}^{K}|i\rangle\langle i|$ is the single-particle identity operator, and J is a scale factor that represents the tunneling amplitude between adjacent sites and depends on physical parameters of the system, such as the particle mass and the distance between the discrete sites. The form of $\hat{T}$ for identical particles in the Fock space is

$$\hat{T}^{\mathscr{F}} = -J\sum_{i=1}^{K}(\hat{c}_i^{\dagger}\hat{c}_{i+1} + \hat{c}_{i+1}^{\dagger}\hat{c}_i), \tag{57}$$

where $\hat{c}_i$ is an annihilation operator (for bosons or fermions) and $\hat{c}_i^{\dagger}$ the corresponding creation operator for the mode i. Given the results of the previous section, we conclude that the representation of the bosonic/fermionic operator in the Fock space can be obtained from $\hat{T}^{\mathscr{H}}$ by a simple change of basis, followed by a projection over the subspace with the required symmetry. Considering $\hat{T}$ a bosonic operator, we have

$$\hat{T}_B^{\mathscr{F}} = \hat{S}\hat{T}^{\mathscr{H}}\hat{S}^{\dagger}. \tag{58}$$

Let us check the previous results in some significant cases:

$$ {}_s\langle k,k+1|\hat{T}_B^{\mathscr{F}}|k,k\rangle_s = -J\,{}_s\langle k,k+1|\hat{c}_{k+1}^{\dagger}\hat{c}_k|k,k\rangle_s = -\sqrt{2}J, \tag{59}$$

$$ {}_s\langle k,k+1|\hat{S}\hat{T}^{\mathscr{H}}\hat{S}^{\dagger}|k,k\rangle_s = \frac{1}{\sqrt{2}}\left(\langle k,k+1| + \langle k+1,k|\right)\hat{T}^{\mathscr{H}}|k,k\rangle = -\sqrt{2}J, \tag{60}$$

$$ {}_s\langle k,l+1|\hat{T}_B^{\mathscr{F}}|k,l\rangle_s \underset{l\neq k,k-1}{=} -J\,{}_s\langle k,l+1|\hat{c}_{l+1}^{\dagger}\hat{c}_l|k,l\rangle_s = -J, \tag{61}$$

$$ \begin{aligned} {}_s\langle k,l+1|\hat{S}\hat{T}^{\mathscr{H}}\hat{S}^{\dagger}|k,l\rangle_s &\underset{l\neq k,k-1}{=} \frac{1}{\sqrt{2}}\left(\langle k,l+1| + \langle l+1,k|\right)\hat{T}^{\mathscr{H}}\frac{1}{\sqrt{2}}\left(|k,l\rangle + |l,k\rangle\right) \\ &= -J. \end{aligned} \tag{62}$$

Analogous results may be obtained for fermions, where additional attention to the anticommutation relation is required to handle periodic boundary conditions (PBC).

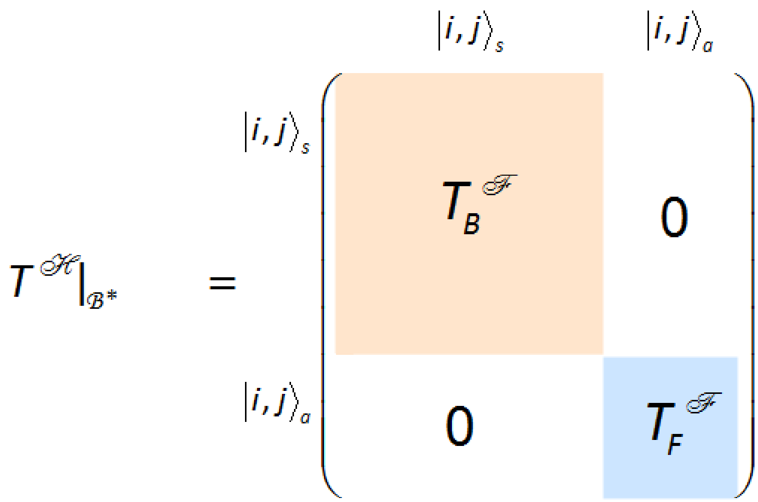

Figure 4: Representation of a parity-conserving operator: symmetry-defined subspaces are invariant.

If a state like $|k, K\rangle_a$ is connected to a state like $|1, k\rangle_a$, e.g. K jumps over the border, we should account for an additional minus sign due to the reordering of the anti-commuting fermionic operators. Indeed (we denote the state with no particle with $|0\rangle$):

$$|1, k\rangle_a = \hat{c}_1^\dagger \hat{c}_k^\dagger |0\rangle , \tag{63}$$

$$\hat{c}_{K+1}^\dagger \hat{c}_K |k, K\rangle_a \underset{PBC}{=} \hat{c}_1^\dagger \hat{c}_K |k, K\rangle_a = \hat{c}_1^\dagger \hat{c}_K \hat{c}_k^\dagger \hat{c}_K^\dagger |0\rangle$$
$$= -\hat{c}_1^\dagger \hat{c}_k^\dagger \hat{c}_K \hat{c}_K^\dagger |0\rangle = -\hat{c}_1^\dagger \hat{c}_k^\dagger |0\rangle = -|1, k\rangle_a . \tag{64}$$

The same results may be obtained without any change of basis, that is by simply applying the operator $\hat{T}^{\mathscr{H}}$ only over the proper (anti-)symmetrized states (this is equivalent to applying the transformation described by $\hat{S}$ or $\hat{A}$). However, the spectrum of the operator $\hat{S}\hat{T}^{\mathscr{H}}\hat{S}^\dagger$ is substantially the spectrum of the bosonic operator, while the spectrum of $\hat{T}^{\mathscr{H}}$ contains also the fermionic eigenvalues of $\hat{A}\hat{T}^{\mathscr{H}}\hat{A}^\dagger$.

Further, we observe that the representation of $\hat{T}_B^{\mathscr{F}}$ in the basis $\mathcal{B}$ of $\mathscr{H}_2$ is quite interesting. Indeed, it contains terms like $-J|i+1, j\rangle_{ss}\langle i, j|$, which can be rewritten as:

$$-J|i+1, j\rangle_{ss}\langle i, j| = \tag{65}$$
$$= -\frac{J}{2}\left(|i+1, j\rangle \langle i, j| + |j, i+1\rangle \langle j, i| + |j, i+1\rangle \langle i, j| + |i+1, j\rangle \langle j, i|\right).$$

This suggests that the Fock operator not only produces transitions where one particle hops from a site to a nearest-neighbour one, but can also allows the two particles to exchange their position: the third term in brackets in the RHS of the previous equation sees the second particle in position i jumping on the site $i+1$, and then exchanging its position with the first particle, previously located on site j. These *exchange terms* are a consequence of the fact that when we rewrite the operator in the Hilbert space of distinguishable particles, it must bear signs of the exchange symmetry, due to the fact that it is actually acting on identical particles (in this case, bosons). The original operator $\hat{T}^{\mathscr{H}}$ does not contain these terms, but they appear when we apply the transformation $\hat{S}\hat{T}^{\mathscr{H}}\hat{S}^{\dagger}$.

3.3. Evolution of the system and symmetrization

Let us now consider our quantum system of $N = 2$ identical particles, whose evolution is ruled by the Hamiltonian $\hat{H}^{\mathscr{F}}$. Their dynamics can be directly calculated in the Hilbert space of distinguishable particles $\mathscr{H}_2$: we can properly (anti-)symmetrize the initial state and get the final state of the evolution with the required symmetry, exactly as we had carried over the evolution in the Fock space. This can be done either using the Fock Hamiltonian $\hat{H}^{\mathscr{F}}$ rewritten in the Hilbert space (see Eqs. (52) and (55)), or using directly the equivalent Hamiltonian $\hat{H}^{\mathscr{H}}$ for distinguishable particles, provided that it conserves parity (i.e., it is invariant under particle exchange). Indeed, projecting $\hat{H}^{\mathscr{H}}$ over the subspaces with the proper symmetry (i.e., using $\hat{S}$ or $\hat{A}$) - and/or applying it only over properly symmetrized states - is equivalent to using $\hat{H}^{\mathscr{F}}$, as we have just seen in the previous section.

4. Expectation values and projections

4.1. Density operator

In order to simplify the notation, let us define a factor g to distinguish between bosons ($g = +1$) and fermions ($g = -1$). If needed, we will use the subscript $|...\rangle_g$ to denote symmetrized or anti-symmetrized states.

The density operator is the fundamental quantity for evaluating the expectation values of all the observables characterizing the system. The density operator can be calculated in the Hilbert space as usual:

$$\rho^{\mathscr{H}}(t) = |\Psi(t)\rangle \langle\Psi(t)|\,, \tag{66}$$

and then recast in the Fock space using Eq. (52) for bosons ($j \geq i$, $l \geq k$):

$$\rho^{\mathscr{F}}_{i,j;k,l} = \frac{2}{(1+\epsilon\delta_{i,j})\,(1+\epsilon\delta_{k,l})}\rho^{\mathscr{H}}_{i,j;k,l}, \tag{67}$$

and Eq. (55) for fermions ($j > i$, $l > k$):

$$\rho^{\mathscr{F}}_{i,j;k,l} = 2\rho^{\mathscr{H}}_{i,j;k,l}, \tag{68}$$

where, within the index constraint, we have $\varsigma_{i,j} = \varsigma_{k,l} = 1$. Notice that if $|\Psi(t)\rangle = \sum_{i,j}\beta_{i,j}(t)\,|i,j\rangle$, we should remember that for exchange symmetry

$$\beta_{i,j}(t) = g \cdot \beta_{j,i}(t), \tag{69}$$

and then we have

$$\rho^{\mathscr{H}}(t) = \sum_{i,j}\sum_{k,l}\beta_{i,j}(t)\beta^*_{k,l}(t)\,|i,j\rangle\langle k,l|\,. \tag{70}$$

If in the Fock space we have

$$\rho^{\mathscr{F}}(t) = \sum_{i,j\geq i} \sum_{k,l\geq k} \alpha_{i,j}(t)\alpha^*_{k,l}(t)|i,j\rangle_{g\,g}\langle k,l|, \tag{71}$$

it is easy to show that the proper (anti-)symmetrization of the Hilbert matrix elements

$$\alpha_{i,j}(t) = \begin{cases} \dfrac{\beta_{i,j}(t) + g\cdot\beta_{j,i}(t)}{\sqrt{2}} = \sqrt{2}\beta_{i,j}(t) & \forall\, i<j \\ \beta_{i,i}(t)\dfrac{(1+g)}{2} & \forall\, i=j \end{cases} \tag{72}$$

gives exactly the expected results in the Fock space (see Eqs. (67) and (68)).

4.2. Occupation numbers

The expectation value of the number operator $\hat{n}_k$, corresponding to the average number of particles in the mode k, can be calculated as follows:

$$\begin{aligned} \langle n_k\rangle &= \mathrm{Tr}[\rho^{\mathscr{F}}(t)\hat{n}_k] = \mathrm{Tr}[\rho^{\mathscr{F}}(t)\hat{c}_k^\dagger\hat{c}_k] \\ &= \sum_i {}_g\langle i,i|\rho^{\mathscr{F}}(t)\hat{c}_k^\dagger\hat{c}_k|i,i\rangle_g + \sum_{i,j>i} {}_g\langle i,j|\rho^{\mathscr{F}}(t)\hat{c}_k^\dagger\hat{c}_k|i,j\rangle_g \\ &= \sqrt{2}\sqrt{2}\rho^{\mathscr{F}}_{k,k;k,k}(t) + \sum_{i<k} {}_g\langle i,k|\rho^{\mathscr{F}}(t)\hat{c}_k^\dagger\hat{c}_k|i,k\rangle_g + \sum_{j>k} {}_g\langle k,j|\rho^{\mathscr{F}}(t)\hat{c}_k^\dagger\hat{c}_k|k,j\rangle_g \\ &= 2\rho^{\mathscr{F}}_{k,k;k,k}(t) + \sum_{i<k}\rho^{\mathscr{F}}_{i,k;i,k}(t) + \sum_{j>k}\rho^{\mathscr{F}}_{k,j;k,j}(t). \end{aligned} \tag{73}$$

Upon recalling that in the Hilbert space the symmetry exchange requires

$$\rho^{\mathscr{H}}_{i,j;k,l}(t) = g\cdot\rho^{\mathscr{H}}_{j,i;k,l}(t) = g\cdot\rho^{\mathscr{H}}_{i,j;l,k}(t), \tag{74}$$

we may rewrite $\langle n_k\rangle$ in the Hilbert space, also using Eq. (68), as follows:

$$\begin{aligned} \langle n_k\rangle &= 2\rho^{\mathscr{H}}_{k,k;k,k}(t) + \sum_{i<k} 2\rho^{\mathscr{H}}_{i,k;i,k}(t) + \sum_{j>k} 2\rho^{\mathscr{H}}_{k,j;k,j}(t) \\ &= 2\left(\rho^{\mathscr{H}}_{k,k;k,k}(t) + \sum_{i\neq k}\rho^{\mathscr{H}}_{i,k;i,k}(t)\right) = 2\sum_i \rho^{\mathscr{H}}_{i,k;i,k}(t), \end{aligned} \tag{75}$$

since $\rho^{\mathscr{H}}_{k,j;k,j} = g^2\rho^{\mathscr{H}}_{j,k;j,k} = \rho^{\mathscr{H}}_{j,k;j,k}$.

4.3. Entropies

Given a quantum system, it is natural to ask how to measure the amount of quantum correlations in it. Besides representing an intriguing trait of quantum mechanics, quantum entanglement has turned into a fundamental resource for quantum information theory and quantum computing, since it can be used to implement protocols and tasks that could not be accomplished within the classical framework [28]. The term entanglement refers to an intrinsic relation between subsystems of a composite quantum system: in an entangled state, each subsystem

cannot be described independently of the state of the other one, or, in other words, what we know (ignore) about A, is what we know (ignore) about B, and vice-versa. For a system composed of two subsystems A and B (bipartite) described by the density matrix ρ_{AB}, the entanglement among A and B can be quantified in different ways [29], depending on the reduced state of the subsystem $\rho_{A(B)}$ and the size $d_{A(B)}$ of the subsystem $A(B)$. In the case of pure states, the entanglement can always be measured with the von Neumann entropy $\mathcal{S}(\rho_A) = -\rho_A \log_2 \rho_A$, with $\mathcal{S}(\rho_A) = \mathcal{S}(\rho_B)$, [30].
Here we consider a compound system described the total density matrix ρ_{SE}, where a quantum system S is coupled to an external bath E, acting as a noise source. In this case the entanglement between system and environment gives a measure of the decoherence, which quantifies the loss of coherence in the quantum correlations of the system [31]. In this picture, decoherence can be evaluated via the von Neumann entropy of the quantum system $\mathcal{S}(\rho_S)$, with $\rho_S = \mathrm{Tr}_E\, \rho$. Whenever the quantum system S contains indistinguishable particles, this quantity should be evaluated in the Fock space, which is the natural space for the system since it accounts for the exchange symmetry. Indeed, we have

$$\mathcal{S}(\rho_S^{\mathscr{F}}) = -\frac{1}{\ln(d_g)}\mathrm{Tr}[\rho_S^{\mathscr{F}} \ln \rho_S^{\mathscr{F}}] > -\frac{1}{\ln(K^2)}\mathrm{Tr}[\rho_S^{\mathscr{H}} \ln \rho_S^{\mathscr{H}}] = \mathcal{S}(\rho_S^{\mathscr{H}}), \tag{76}$$

since $\rho_S^{\mathscr{H}}$ and $\rho_S^{\mathscr{F}}$ have the same eigenvalues: they only differ for a unitary transformation, and the additional eigenvalues of $\rho_S^{\mathscr{H}}$ are zeros that do not contribute to the entropy. We therefore conclude that $\mathrm{Tr}[\rho_S^{\mathscr{H}} \ln \rho_S^{\mathscr{H}}] = \mathrm{Tr}[\rho_S^{\mathscr{F}} \ln \rho_S^{\mathscr{F}}]$, and the only difference between $\mathcal{S}(\rho_S^{\mathscr{F}})$ and $\mathcal{S}(\rho_S^{\mathscr{H}})$ is given by different normalization ($d_g = \frac{K(K+g)}{2} < K^2$): so we conclude that $\mathcal{S}(\rho_S^{\mathscr{H}})$ underestimates the loss of quantum correlations with respect to $\mathcal{S}(\rho_S^{\mathscr{F}})$. The reason is intuitively obvious: since the system always possesses a residual amount of correlations due to exchange symmetry, these correlations are seen as quantum correlations by the entropy of the Hilbert space, which is devised for distinguishable particles. On the other hand, they are correctly not counted by the von Neumann entropy evaluated in the Fock space. Indeed, they are not genuine quantum correlations - like entanglement or quantum discord [32]- which may be exploited to perform quantum information tasks.

5. Guidelines for Numerical implementation

5.1. Base ordering and indexing

One of the main problems in implementing numerically the calculations of operators is the different indexing in Hilbert and Fock spaces. This situation is made more involved by the differences between allowed states for fermions and bosons. Let us see this with an example. Let us consider a system with $N = 2$ identical particles, which can occupy $K = 4$ sites, or modes. The allowed states in the Hilbert and Fock spaces are given in Table 1.

Since any vector or matrix must be indexed with a progressive index m, we have to define a global index m that depends on the single-particle states i and j and follows the correct ordering when basis set states $|m\rangle$ are $|i,j\rangle$, $|i,j\rangle_s$ or $|i,j\rangle_a$. It turns out that we have

$$\mathscr{H}_2 : \quad m = K(i-1) + j, \tag{77}$$

$$\mathscr{F}_2^{B/F} : \quad m = K(i-1) + j - s(g,i)\,, \tag{78}$$

Space	**Basis set**				**Dimension**
	$\vert 1,1\rangle$	$\vert 1,2\rangle$	$\vert 1,3\rangle$	$\vert 1,4\rangle$	
$\mathscr{H}_2$	$\vert 2,1\rangle$	$\vert 2,2\rangle$	$\vert 2,3\rangle$	$\vert 2,4\rangle$	16
(distinguishable)	$\vert 3,1\rangle$	$\vert 3,2\rangle$	$\vert 3,3\rangle$	$\vert 3,4\rangle$	
	$\vert 4,1\rangle$	$\vert 4,2\rangle$	$\vert 4,3\rangle$	$\vert 4,4\rangle$	
	$\vert 1,1\rangle_s$	$\vert 1,2\rangle_s$	$\vert 1,3\rangle_s$	$\vert 1,4\rangle_s$	
$\mathscr{F}_2^B$		$\vert 2,2\rangle_s$	$\vert 2,3\rangle_s$	$\vert 2,4\rangle_s$	10
(bosons)			$\vert 3,3\rangle_s$	$\vert 3,4\rangle_s$	
				$\vert 4,4\rangle_s$	
$\mathscr{F}_2^F$		$\vert 1,2\rangle_a$	$\vert 1,3\rangle_a$	$\vert 1,4\rangle_a$	
			$\vert 2,3\rangle_a$	$\vert 2,4\rangle_a$	6
(fermions)				$\vert 3,4\rangle_a$	

Table 1: Basis sets for Hilbert and Fock spaces of $N = 2$ identical particles, which can occupy $K = 4$ sites.

where $s(g, i)$ is a correction term that takes into account the fact that states with indices exchanged must not be counted again in Fock space, and also that states with identical indices are forbidden for fermions ($g = -1$). From an intuitive point of view, we can think that i and j in $|i, j\rangle$ are two numbers living on a ring $\mathbb{Z}_K = \{1, 2, ..., K\}$: i plays the role of the tens, while j plays the role of units and, overall, we have $m = K(i-1) + j$. By a simple combinatorial reasoning we find:

$$s(g, i) = \frac{i(i-g)}{2}. \tag{79}$$

Indeed, for a fixed value of i, denoted as i^*, the number of forbidden states which must be subtracted from m is

$$B: \quad \mathrm{card}\{|i, j\rangle \mid i \leq i^* \wedge j < i\} = \sum_{i=1}^{i^*} (i-1) = \sum_{i=0}^{i^*-1} i\,, \tag{80}$$

$$F: \quad \mathrm{card}\{|i, j\rangle \mid i \leq i^* \wedge j \leq i\} = \sum_{i=1}^{i^*} i = \sum_{i=0}^{i^*} i\,. \tag{81}$$

In both cases, we calculate the result with the Gauss formula $\sum_{i=0}^{n} i = \frac{1}{2}n(n+1)$. One can easily verify that $\{|i, j\rangle_{s(a)} \mid i \leq i^* \wedge j \underset{(-)}{<} i\}$ are exactly the states not appearing in Table 1 since forbidden.

So, according to Eqs. (78) and (79), the state $|3, 4\rangle$, e.g., is the basis state $|m\rangle = |12\rangle$ in $\mathscr{H}_2$, the basis state $|m\rangle = |9\rangle$ in $\mathscr{F}_2^B$, and the basis state $|m\rangle = |6\rangle$ in $\mathscr{F}_2^F$. This allows us to scan all the elements of vector states and operators in terms of the single-particle states i and j, and it also lets us to switch easily from their Hilbert representation to the Fock one and vice versa.

5.2. Reshaping cycle

Now, it is worth noting that, in order to fill-in properly the elements of an operator O in the space $\mathscr{F}_2^{B/F}$, starting from the corresponding operator in the Hilbert space (the so-called *reshaping* operation), we must use cycles like

```
for i=1,N
    for j=i+Δ,N
        for k=1,N
            for l=k+Δ,N
              O^𝓕(i,j;k,l) = O^𝓗(i,j;k,l) · ...
            end
        end
    end
end
```

where the correction

$$\Delta = \frac{1-g}{2} \tag{82}$$

is 0 for bosons (i.e., states with $i = j$ are allowed) and 1 for fermions (i.e., states with $i = j$ are forbidden).

5.3. Computational and storage considerations

Working in the Hilbert space offers an obvious advantage from the physical point of view, since one has a clear identification of the degrees of freedom associated to each particle, and a better indexing of states. On the other hand, a couple of issues arises from the point of view of numerical implementation. The first is linked to the larger dimension of the space and may be properly addressed by opportunely inverting Eqs. (78) and using reshaping cycles as those presented in Section 5.2, so that the number of operations is not significantly larger in the Hilbert space [33]. Let us define the function

$$\begin{aligned} f^{\mathrm{g}}_{\mathrm{K}}(r) &:= \begin{cases} m-1-\displaystyle\sum_{n=K-\Delta-r+1}^{K-\Delta} n & \text{for } r\in\mathbb{N}^+ \\ m-1 & \text{for } r=0 \end{cases} \\ &= m-1-\frac{r}{2}\,(2K+g-r) \qquad \text{for } r\in\mathbb{N}\,, \end{aligned} \tag{83}$$

where Δ is defined in Eq. (82), $g = {}_{(-)}^{+} 1$ for bosons (fermions), and K is the number of modes of the quantum system. The expression in Eq. (83), which is in principle the result for $r \in \mathbb{N}^+$, returns $m-1$ for $r = 0$, thus it already summarizes the two distinct cases. Let $\bar{r}^{\mathrm{g}}_{\mathrm{K}}$ be the greater value of $r \in \{0, 1, ..., K-1\}$ such that $f^{\mathrm{g}}_{\mathrm{K}}(r) \geq 0$, i.e.

$$\bar{r}^{\mathrm{g}}_{\mathrm{K}} = \max\{r \mid r \in \{0, 1, ..., K-1\} \wedge f^{\mathrm{g}}_{\mathrm{K}}(r) \geq 0\}. \tag{84}$$

Hence, the inverse formulae of Eqs. (78) are given by

$$\begin{cases} i^{\mathrm{g}}_{\mathrm{K}}(m) &= 1+\bar{r}^{\mathrm{g}}_{\mathrm{K}} \\ j^{\mathrm{g}}_{\mathrm{K}}(m) &= \Delta + i^{\mathrm{g}}_{\mathrm{K}}(m) + f^{g}_{\mathrm{K}}(\bar{r}^{\mathrm{g}}_{\mathrm{K}})\,. \end{cases} \tag{85}$$

The other and major issue is instead related to the storage of the matrix elements of states and operators, since in both cases using the Hilbert space description amounts to storing several empty cells, i.e. those corresponding to states with the wrong symmetry. This problem may be addressed by exploiting the above mapping, and also noticing that the involved matrices are often sparse, e.g. when systems with only nearest-neighbour interactions are considered [34], so that sparse matrix declarations and algorithms may be exploited to reduce the storage space.

6. Concluding remarks

In graduate physics courses, second quantization and the Fock space are presented as the natural framework to deal with quantum systems made of many indistinguishable particles, leaving the impression that the Hilbert space description may be left behind. While this is certainly true for the description of quantum states of those systems, the evaluation of some specific observable or the study of the system dynamics may be often more conveniently pursued using the Hilbert space description.

A research-oriented teaching of these topics should therefore reflect the importance of both descriptions, and provide tools to connect them in the most straightforward way. To this aim, we have provided here a gentle and self-contained introduction to details of the transformation rules between the different description of states and operators in the two spaces. In particular, we have devoted some attention to the two-particle case, since this already contains most of the interesting features related to indistinguishability. The paper aims at being a concise reference about the different representations for students and researchers working with systems made of many identical particles, especially those interested in numerical approaches to the system dynamics.

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