

Indistinguishable particles

- Indistinguishability implies invariance under permutations of particles. The observables must be invariant under permutations and the states must be totally symmetric (Bose statistics) or totally antisymmetric (Fermi statistics).
- Any possible permutation is implemented by an operator $\mathbf{P}_m$. Given N indices, the permutations operators are $N!$ (including the identity) and they form a possible representation of a discrete group P_N , with $\mathbf{P}_m \in P_N$. There are $N - 1$ generators σ_j consisting of the exchange of two “neighbor” elements

$$\sigma_j \in P_N : j \leftrightarrow j + 1 \quad j = 1, \dots, N - 1,$$

which satisfy the involutory property

$$\sigma_j^2 = \mathbf{I}.$$

Any $\mathbf{P}_m$ can be obtained as a product of some generators

$$\mathbf{P}_m = \prod_{\{j_m\}} \sigma_{j_m},$$

where we denote with $\{j_m\}$ a possible sequence of n_m values of j meaning the number of transpositions needed to obtain the permutation.

- Consider N particles and a complete set of p *single-particle* states $\{|\alpha\rangle\}$. Suppose that n_j particles are in the state $|\alpha_j\rangle$ (with $\sum_{j=1}^p n_j = N$), to construct the correctly symmetrized $|\{\alpha\}_N^S\rangle$ state one can start from a possible configuration $|\{\alpha\}_N\rangle = |\alpha_1\rangle^{\otimes n_1} |\alpha_2\rangle^{\otimes n_2} \dots |\alpha_p\rangle^{\otimes n_p}$ and apply to it the (anti)symmetrization operator

$$|\{\alpha\}_N^S\rangle = \frac{1}{\sqrt{N! \prod_{j=1}^p n_j!}} \sum_{m=1}^{N!} \zeta^{n_m} \mathbf{P}_m |\{\alpha\}_N\rangle = \sqrt{\frac{N!}{\prod_{j=1}^p n_j!}} \mathbf{S}_\zeta |\{\alpha\}_N\rangle, \quad (1)$$

where $\mathbf{P}_m$ is a possible permutation. The symbol

$$\zeta = \begin{cases} 1 & \text{bosons} \\ -1 & \text{fermions} \end{cases}$$

refers to the bosonic/fermionic statistics, and

$$\mathbf{S}_\zeta = \frac{1}{N!} \sum_{m=1}^{N!} \zeta^{n_m} \mathbf{P}_m, \quad (2)$$

is the (anti)symmetrization operator¹.

¹Notice that from the property

$$\mathbf{P}_s \mathbf{P}_m = \mathbf{P}_k \Rightarrow \mathbf{P}_s^2 \mathbf{P}_m = \mathbf{P}_m = \mathbf{P}_s \mathbf{P}_k,$$

follows that

$$\zeta^{n_s} \mathbf{P}_s \mathbf{S}_\zeta = \frac{1}{N!} \sum_m \zeta^{n_m + n_s} \mathbf{P}_s \mathbf{P}_m = \frac{1}{N!} \sum_k \zeta^{n_k} \mathbf{P}_k = \mathbf{S}_\zeta,$$

and

$$\mathbf{S}_\zeta^2 = \mathbf{S}_\zeta.$$

Moreover, $\mathbf{S}_\zeta^\dagger = \mathbf{S}_\zeta$ since $\mathbf{P}_m$ are hermitian. This means that $\mathbf{S}_\zeta$ is a projector. In particular, $\mathbf{S}_+$ and $\mathbf{S}_-$ are orthogonal projectors

$$\mathbf{S}_+ \mathbf{S}_- = 0.$$

- If the vectors $\{|\alpha\rangle\}$ form a discrete complete orthonormal basis for the single-particle space, then the resolution of identity for the N -particle space is

$$\sum_{\alpha_1, \dots, \alpha_N} |\{\alpha\}_N^S\rangle \langle \{\alpha\}_N^S| = \mathbf{I}_N, \quad (3)$$

and, if the basis is continuous

$$\int d\alpha_1 \dots d\alpha_N |\{\alpha\}_N^S\rangle \langle \{\alpha\}_N^S| = \mathbf{I}_N. \quad (4)$$

Exercise 1. Consider 3 particles each of them described by a 4-dimension single-particle state in a space spanned by the complete basis

$$|a\rangle, |b\rangle, |c\rangle, |d\rangle.$$

1. How many 3-particle states would the basis be composed of if the particles were distinguishable?
2. How many 3-particle states would the basis be composed of if the particles were classically indistinguishable? Construct them.
3. How many 3-particle states would the basis be composed of if the particles were indistinguishable bosons? Construct them.
4. How many 3-particle states would the basis be composed of if the particles were indistinguishable fermions? Construct them.

Second quantization

The second quantization is formalism which is more suitable to describe a many-body system because:

- It is more compact than “first quantization”,
- It avoids to write explicitly the (anti-)symmetrization of the state, because in second quantization the correct symmetry is already contained in the algebra of the operators,
- It is easier to work with an arbitrary (not necessary fixed) number of particles,
- Gives a more intuitive picture of the interaction in terms of processes of creation and annihilation of particles.
- It is the formal tool to define a quantum field.

One-particle states

Consider a complete basis of single-particle states $\{|\phi_k\rangle\} \in \mathcal{H}^1$ with k a discrete dimensionless index. We can introduce for each of them a **creation operator** as

$$\boxed{\mathbf{a}_k^\dagger |0\rangle = |\phi_k\rangle}, \quad (5)$$

where $|0\rangle$ is called **vacuum state**: it does not belong to $\mathcal{H}^1$ and it is the only normalized state of a one-dimensional Hilbert space $\mathcal{H}^0$. The interpretation is that, starting from the vacuum, a particle is created in that specific state. Then, for each creation operator there is its adjoint $\mathbf{a}_k$ which is called

annihilation operator. In the following we will denote with $\mathbf{a}_k$, $\mathbf{a}_k^\dagger$ the generic operators, with $\mathbf{c}_k$, $\mathbf{c}_k^\dagger$ the fermionic operators and with $\mathbf{b}_k$, $\mathbf{b}_k^\dagger$ the bosonic operators.

The particle statistics is taken into account imposing suitable (anti-)commutation rules. The properties of the bosonic operators are given by the commutation rules

$$\begin{aligned} [\mathbf{b}_k, \mathbf{b}_{k'}] &= 0, \\ [\mathbf{b}_k, \mathbf{b}_{k'}^\dagger] &= \delta_{k,k'}, \end{aligned} \quad (6)$$

while the properties of the fermionic operators are given by the anti-commutation rules

$$\begin{aligned} \{\mathbf{c}_k, \mathbf{c}_{k'}\} &= 0, \\ \{\mathbf{c}_k, \mathbf{c}_{k'}^\dagger\} &= \delta_{k,k'}. \end{aligned} \quad (7)$$

We can use the compact notation

$$[,] = [,]_-, \{ , \} = [,]_+$$

and write

$$\boxed{[\mathbf{a}_k, \mathbf{a}_{k'}]_{-\zeta} = 0; \quad [\mathbf{a}_k, \mathbf{a}_{k'}^\dagger]_{-\zeta} = \delta_{k,k'}}. \quad (8)$$

Occupation-number operator

The **occupation-number operator** for the state k is

$$\mathbf{n}_k = \mathbf{a}_k^\dagger \mathbf{a}_k,$$

which satisfies the following commutation relations (both for fermions and bosons)

$$\boxed{[\mathbf{a}_k, \mathbf{n}_{k'}] = \mathbf{a}_k \delta_{k,k'}, \quad [\mathbf{a}_k^\dagger, \mathbf{n}_{k'}] = -\mathbf{a}_k^\dagger \delta_{k,k'}}. \quad (9)$$

Exercise 2. Remembering that, given three operators $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, the following relations hold

$$\boxed{[\mathbf{AB}, \mathbf{C}] = \mathbf{A} [\mathbf{B}, \mathbf{C}] + [\mathbf{A}, \mathbf{C}] \mathbf{B} = \mathbf{A} \{\mathbf{B}, \mathbf{C}\} - \{\mathbf{A}, \mathbf{C}\} \mathbf{B} = \mathbf{A} [\mathbf{B}, \mathbf{C}]_{-\zeta} + \zeta [\mathbf{A}, \mathbf{C}]_{-\zeta} \mathbf{B}} \quad (10)$$

$$\boxed{[\mathbf{AB}, \mathbf{C}]_{-\zeta} = \mathbf{A} [\mathbf{B}, \mathbf{C}]_{-\zeta} + \zeta [\mathbf{A}, \mathbf{C}] \mathbf{B}} \quad (11)$$

prove Eq. (9).

For a single particle the occupation-number operator gives the probability distribution for the particle to be in the state k

$$p_k = \langle \mathbf{n}_k \rangle \implies \sum_k \langle \mathbf{n}_k \rangle = 1,$$

as a consequence, the identity in $\mathcal{H}^1$ is

$$\mathbf{I} = \sum_k \mathbf{n}_k.$$

Change of basis

Given two different single-particle basis $\{|\phi_k\rangle\}$ e $\{|\nu_k\rangle\}$, corresponding to the operators $\mathbf{a}_k^\dagger$ $\mathbf{d}_k^\dagger$, one can express one basis in terms of the other as

$$|\phi_k\rangle = \sum_l \langle \nu_l | \phi_k \rangle |\nu_l\rangle, \quad (12)$$

so, from (16), the same change of basis can done in term of operators

$$\mathbf{a}_k^\dagger = \sum_l \langle \nu_l | \phi_k \rangle \mathbf{d}_l^\dagger. \quad (13)$$

Field operators

The **field creation operators** are defined analogously from a continuous basis $|x\rangle$ (where x is a generic continuous variable) as

$$\boxed{\Psi^\dagger(x) |0\rangle = |x\rangle}. \quad (14)$$

Since

$$|x\rangle = \sum_k \langle \phi_k | x \rangle |\phi_k\rangle = \sum_k \phi_k^*(x) \mathbf{a}_k^\dagger |0\rangle, \quad (15)$$

the field operator can be expressed as the linear combination

$$\Psi^\dagger(x) = \sum_k \phi_k^*(x) \mathbf{a}_k^\dagger, \quad (16)$$

and vice versa

$$\hat{\mathbf{a}}_k^\dagger = \int dx \phi_k(x) \hat{\Psi}^\dagger(x). \quad (17)$$

The (anti-)commutation relations for the field operators are

$$\boxed{[\Psi(x), \Psi(x')]_{-\zeta} = 0; \quad [\Psi(x), \Psi^\dagger(x')]_{-\zeta} = \delta(x - x')}. \quad (18)$$

Local-density operator

Form the field operators one can define the **local-density operator**

$$\mathbf{n}(x) = \Psi^\dagger(x) \Psi(x),$$

which satisfy the commutation rules

$$\boxed{[\Psi(x), \mathbf{n}(x')] = \Psi(x) \delta(x - x'), \quad [\Psi^\dagger(x), \mathbf{n}(x')] = -\Psi^\dagger(x) \delta(x - x')}. \quad (19)$$

Exercise 3. Prove formula (19).

Exercise 4. It is possible to define also field operators in the momentum representation

$$\tilde{\Psi}(k), \tilde{\Psi}^\dagger(k),$$

write these operators in term of field operators $\Psi^\dagger(x), \Psi(x)$.

As in the discrete case, in $\mathcal{H}^1$ $\mathbf{n}(x)$ represents the probability density function in the continuous variable x

$$p(x) = \langle \mathbf{n}(x) \rangle \implies \int dx \langle \mathbf{n}(x) \rangle = 1.$$

As in the discrete case, in $\mathcal{H}^1$ the identity can be expressed as

$$\mathbf{I} = \int dx \mathbf{n}(x).$$

Many-particle states

To describe a many-particle state, one can introduce the so-called **Fock space** $\mathcal{F}$ which is a Hilbert space given by the direct sum of fixed-particle states

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \mathcal{F}_3 \oplus \dots$$

Starting from $\mathcal{F}_0 = \mathcal{H}^0$ and $\mathcal{F}_1 = \mathcal{H}^1$ (zero and one-particle Hilbert spaces), and from a complete set of single-particle states $\mathbf{a}_k^\dagger |0\rangle$, the so-called **occupation-number representation** for the elements of $\mathcal{F}$ is defined giving how many particles are on each single-particle state

$$|n_1, n_2, \dots\rangle,$$

with the total number of particle given by $\sum_j n_j = N$. Of course

$$n_k = 0, 1$$

for fermions and

$$n_k = 0, 1, 2, \dots, \infty$$

for bosons. Applying a creation/annihilation operator to a N -particle state, one jumps to a $N \pm 1$ particle sector of the Fock space

$$\begin{aligned} \mathbf{a}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle &= \begin{cases} \sqrt{n_k + 1} |n_1, n_2, \dots, (n_k + 1)_k, \dots\rangle & \text{bosons} \\ (-1)^{k+1} \delta_{n_k, 0} |n_1, n_2, \dots, (n_k + 1)_k, \dots\rangle & \text{fermions} \end{cases}, \\ \mathbf{a}_k |n_1, n_2, \dots, n_k, \dots\rangle &= \begin{cases} \sqrt{n_k} |n_1, n_2, \dots, (n_k - 1)_k, \dots\rangle & \text{bosons} \\ (-1)^{k+1} \delta_{n_k, 1} |n_1, n_2, \dots, (n_k - 1)_k, \dots\rangle & \text{fermions} \end{cases}. \end{aligned}$$

In this representation a vector basis for N identical particles can be written as the (normalized) vectors

$$|n_1, n_2, \dots\rangle = \frac{1}{\sqrt{\prod_k n_k!}} \prod_k \left(\mathbf{a}_k^\dagger \right)^{n_k} |0\rangle, \quad (20)$$

(remembering that because of the anti-commutation rules, for the fermions one has $\mathbf{a}_k^{\dagger n_k} = 0$ for $n_k > 1$) with

$$\sum_k n_k = N.$$

For any subspace $\mathcal{F}_N$ a **resolution of identity** is

$$\mathbf{I}_N = \sum_{\{n_k\} | \sum_k n_k = N} \frac{1}{\prod_k n_k!} \left[\prod_k \left(\mathbf{a}_k^\dagger \right)^{n_k} |0\rangle \langle 0| \prod_k \mathbf{a}_k^{n_k} \right] = \frac{1}{N!} \sum_{k_1, k_2, \dots, k_N} \left[\prod_j \mathbf{a}_{k_j}^\dagger |0\rangle \langle 0| \prod_j \mathbf{a}_{k_j} \right],$$

and in particular

$$\mathbf{I}_0 = |0\rangle \langle 0|,$$

$$\mathbf{I}_1 = \sum_k \mathbf{a}_k^\dagger |0\rangle \langle 0| \mathbf{a}_k,$$

$$\mathbf{I}_2 = \frac{1}{2} \sum_{k, k'} \mathbf{a}_k^\dagger \mathbf{a}_{k'}^\dagger |0\rangle \langle 0| \mathbf{a}_{k'} \mathbf{a}_k,$$

and so on.

Continuous basis

Starting from a continuous basis, one can proceed in a similar way, paying attention to the normalization. Applying a field operator to a 1-particle state, one obtains a 2-particle state

$$\Psi^\dagger(x_2) |x_1\rangle = \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle.$$

The possible states constructed in this way are orthogonal

$$\begin{aligned} \langle 0 | \Psi(x_3) \Psi(x_4) \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle &= \langle 0 | \Psi(x_3) (\delta(x_2 - x_4) + \zeta \Psi^\dagger(x_2) \Psi(x_4)) \Psi^\dagger(x_1) | 0 \rangle = \\ &= \delta(x_2 - x_4) \delta(x_1 - x_3) + \zeta \langle 0 | \Psi(x_3) \Psi^\dagger(x_2) \Psi(x_4) \Psi^\dagger(x_1) | 0 \rangle = \\ &= \delta(x_2 - x_4) \delta(x_1 - x_3) + \zeta \delta(x_2 - x_3) \delta(x_1 - x_4), \end{aligned}$$

moreover

$$\begin{aligned} &\left(\int dx_3 dx_4 \Psi^\dagger(x_4) \Psi^\dagger(x_3) | 0 \rangle \langle 0 | \Psi(x_3) \Psi(x_4) \right) \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle = \\ &= \int dx_3 dx_4 (\delta(x_2 - x_4) \delta(x_1 - x_3) + \zeta \delta(x_2 - x_3) \delta(x_1 - x_4)) \Psi^\dagger(x_4) \Psi^\dagger(x_3) | 0 \rangle = \\ &= (\Psi^\dagger(x_2) \Psi^\dagger(x_1) + \zeta \Psi^\dagger(x_1) \Psi^\dagger(x_2)) | 0 \rangle = 2 \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle, \end{aligned}$$

it follows that in the 2-particle space, the **resolution of the identity** is

$$\frac{1}{2} \int dx_3 dx_4 \Psi^\dagger(x_4) \Psi^\dagger(x_3) | 0 \rangle \langle 0 | \Psi(x_3) \Psi(x_4) = \mathbf{I}.$$

This result can be generalized to N particles

$$\frac{1}{N!} \int dx_1 \dots dx_N \Psi^\dagger(x_N) \dots \Psi^\dagger(x_1) | 0 \rangle \langle 0 | \Psi(x_1) \dots \Psi(x_N) = \mathbf{I},$$

giving the correct normalization for the continuous basis for fixed number of particles

$$\boxed{|x_1, x_2, \dots, x_N\rangle = \frac{1}{\sqrt{N!}} \prod_{k=1}^N \Psi^\dagger(x_k) | 0 \rangle}.$$

Important! Notice that in the Fock representation the state has automatically the correct symmetrization of (1) so to say

$$|n_1, n_2, \dots\rangle = |\{k\}_N^S\rangle,$$

as can be verified in the following example.

Example 0.0.1. Two-particle case: consider two particles in the Fock state with $k \neq k'$

$$|\psi\rangle = \mathbf{a}_k^\dagger \mathbf{a}_{k'}^\dagger | 0 \rangle, \tag{21}$$

its wave function is given by

$$\begin{aligned} \psi(x_1, x_2) &= \frac{1}{\sqrt{2}} \langle 0 | \Psi(x_1) \Psi(x_2) \mathbf{a}_k^\dagger \mathbf{a}_{k'}^\dagger | 0 \rangle = \\ &= \frac{1}{\sqrt{2}} \sum_{l,m} \phi_l(x_1) \phi_m(x_2) \langle 0 | \mathbf{a}_l \mathbf{a}_m \mathbf{a}_k^\dagger \mathbf{a}_{k'}^\dagger | 0 \rangle = \\ &= \frac{1}{\sqrt{2}} (\phi_k(x_1) \phi_{k'}(x_2) + \zeta \phi_k(x_2) \phi_{k'}(x_1)), \end{aligned} \tag{22}$$

and it has the correct symmetrization. If the particles are two bosons in the same quantum number

$$|\psi\rangle = \frac{1}{\sqrt{2}} \mathbf{a}_k^{\dagger 2} |0\rangle,$$

the wave function is

$$\begin{aligned} \psi(x_1, x_2) &= \frac{1}{2} \langle 0 | \Psi(x_1) \Psi(x_2) \mathbf{a}_k^{\dagger 2} | 0 \rangle = \\ &= \frac{1}{2} \sum_{l,m} \phi_l(x_1) \phi_m(x_2) \langle 0 | \mathbf{a}_l \mathbf{a}_m \mathbf{a}_k^{\dagger 2} | 0 \rangle = \\ &= \phi_k(x_1) \phi_k(x_2). \end{aligned} \tag{23}$$

Particle-number operator

For a N -particle system, the average of the local-density operator over the N -particle state gives the density of particles for each position x , while the average of the occupation-number operator is the average occupation of the state k .

The **particle-number operator** is

$$\mathbf{N} = \int dx \Psi^\dagger(x) \Psi(x) = \sum_k \mathbf{a}_k^\dagger \mathbf{a}_k.$$

Example 0.0.2. Consider the two-particle state

$$|\phi_{N=2}\rangle = \frac{1}{\sqrt{2}} \int dx_1 dx_2 f(x_1, x_2) \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle.$$

Let us analyze the coefficient $f(x_1, x_2)$.

- They must be (anti-)symmetric $f(x_1, x_2) = \zeta f(x_2, x_1)$:

$$\begin{aligned} |\phi_{N=2}\rangle &= \frac{1}{\sqrt{2}} \int dx_1 dx_2 f(x_1, x_2) \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle = \\ &= \frac{\zeta}{\sqrt{2}} \int dx_1 dx_2 f(x_1, x_2) \Psi^\dagger(x_1) \Psi^\dagger(x_2) |0\rangle = \\ &= \frac{\zeta}{\sqrt{2}} \int dx_1 dx_2 f(x_2, x_1) \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle, \end{aligned}$$

- From the normalization condition derives that $\int dx_1 dx_2 |f(x_1, x_2)|^2 = 1$:

$$\begin{aligned} \langle \phi_{N=2} | \phi_{N=2} \rangle &= \frac{1}{2} \int dx_1 dx_2 dx_3 dx_4 f^*(x_3, x_4) f(x_1, x_2) \times \\ &\quad \times \langle 0 | \Psi(x_3) \Psi(x_4) \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle = \\ &= \frac{1}{2} \int dx_1 dx_2 dx_3 dx_4 f^*(x_3, x_4) f(x_1, x_2) \times \\ &\quad \times [\delta(x_2 - x_4) \delta(x_1 - x_3) + \zeta \delta(x_2 - x_3) \delta(x_1 - x_4)] = \\ &= \frac{1}{2} \int dx_1 dx_2 [|f(x_1, x_2)|^2 + \zeta f^*(x_2, x_1) f(x_1, x_2)] = \\ &= \int dx_1 dx_2 |f(x_1, x_2)|^2. \end{aligned}$$

- The quantity $|f(x_1, x_2)|^2$ represents the probability density function $p(x_1, x_2)$ for two particles to be localized in the positions x_1 and x_2 . The marginal distribution for a single particle is

$$p(x) = \int dx_2 |f(x, x_2)|^2.$$

- The average of the (single particle) local-density operator over the state $|\phi_{N=2}\rangle$ is

$$\langle \mathbf{n}(x) \rangle = 2p(x),$$

as can be found explicitly

$$\begin{aligned} \langle \phi_{N=2} | \mathbf{n}(x) | \phi_{N=2} \rangle &= \int dx_1 dx_2 dx_3 dx_4 \frac{f(x_1, x_2) f^*(x_3, x_4)}{2} \langle 0 | \Psi(x_3) \Psi(x_4) \mathbf{n}(x) \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle = \\ &= \frac{1}{2} \int dx_1 dx_2 dx_3 dx_4 f(x_1, x_2) f^*(x_3, x_4) \times \\ &\quad \times \langle 0 | \Psi(x_3) \Psi(x_4) [\Psi^\dagger(x_2) \delta(x_2 - x) + \Psi^\dagger(x_2) \mathbf{n}(x)] \Psi^\dagger(x_1) | 0 \rangle = \\ &= \frac{1}{2} \int dx_1 dx_2 dx_3 dx_4 f(x_1, x_2) f^*(x_3, x_4) \times \\ &\quad \times [\delta(x_2 - x) \langle 0 | \Psi(x_3) \Psi(x_4) \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle + \\ &\quad + \langle 0 | \Psi(x_3) \Psi(x_4) [\Psi^\dagger(x_2) \Psi^\dagger(x_1) \delta(x_1 - x) + \Psi^\dagger(x_2) \Psi^\dagger(x_1) \mathbf{n}(x)] | 0 \rangle] = \\ &= \frac{1}{2} \int dx_1 dx_2 dx_3 dx_4 f(x_1, x_2) f^*(x_3, x_4) \times (\delta(x_2 - x) + \delta(x_1 - x)) \\ &\quad \times (\delta(x_2 - x_4) \delta(x_1 - x_3) + \zeta \delta(x_2 - x_3) \delta(x_1 - x_4)) = \\ &= \int dx_2 |f(x, x_2)|^2 + \int dx_1 |f(x_1, x)|^2 = 2 \int dx_2 |f(x, x_2)|^2. \end{aligned}$$

Exercise 5. Verify the following relations:

$$[\mathbf{a}_k, \mathbf{N}] = \mathbf{a}_k, \quad [\mathbf{a}_k^\dagger, \mathbf{N}] = -\mathbf{a}_k^\dagger \quad (24)$$

$$[\Psi(x), \mathbf{N}] = \Psi(x), \quad [\Psi^\dagger(x), \mathbf{N}] = -\Psi^\dagger(x) \quad (25)$$

Exercise 6. Show that

$$e^{-a\mathbf{N}} \Psi(x) e^{a\mathbf{N}} = \Psi(x) e^a$$

Observables

A many-body observable $\mathbf{A}$ must be invariant under any particle permutation so it must satisfy

$$[\mathbf{A}, \mathbf{P}_m] = 0.$$

We want to express the operators in terms of creation and annihilation operators. Before to start, we notice that, for one particle

$$(\mathbf{a}_n^\dagger | 0) \langle 0 | \mathbf{a}_l | \psi \rangle = \mathbf{a}_n^\dagger | 0) \langle 0 | \mathbf{a}_l \sum_k \psi_k \mathbf{a}_k^\dagger | 0 \rangle = \psi_l \mathbf{a}_n^\dagger | 0),$$

$$(\mathbf{a}_n^\dagger \mathbf{a}_l | \psi \rangle = \mathbf{a}_n^\dagger \mathbf{a}_l \sum_k \psi_k \mathbf{a}_k^\dagger | 0 \rangle = \psi_l \mathbf{a}_n^\dagger | 0),$$

so one obtains the formal relation

$$\mathbf{a}_n^\dagger | 0) \langle 0 | \mathbf{a}_l = \mathbf{a}_n^\dagger \mathbf{a}_l,$$

that will result useful in the following.

One-particle operators

Let $\mathbf{A}_1$ be an operator acting on the Hilbert space of a single particle. The one-particle many-body operator corresponding to it is

$$\mathbf{A} = \mathbf{A}_1 \otimes \mathbf{I}_{N-1} + \mathbf{I}_1 \otimes \mathbf{A}_1 \otimes \mathbf{I}_{N-2} + \dots + \mathbf{I}_{N-1} \otimes \mathbf{A}_1.$$

This means that, even if the operator acts on the N -particle space, it engages a single particle at a time. In first quantization a one-particle observable $\mathbf{A}_1$ has the following representation in terms of its eigenstates $\mathbf{A}_1 |\phi_k\rangle = F_k |\phi_k\rangle$

$$\mathbf{A}_1 = \sum_k F_k |\phi_k\rangle \langle \phi_k|. \quad (26)$$

In second quantization one has an equivalent representation, given $|\phi_k\rangle = \mathbf{a}_k^\dagger |0\rangle$, the operator can be represented as

$$\mathbf{A}_1 = \sum_k F_k \mathbf{n}_k. \quad (27)$$

As expected, for the single particle case the two pictures are completely equivalent as expected. Taking another basis $\{|\nu_k\rangle = \mathbf{d}_k^\dagger |0\rangle\}$, the observable can be written as

$$\mathbf{A}_1 = \sum_k F_k |\phi_k\rangle \langle \phi_k| = \sum_{k,l,m} F_k |\nu_l\rangle \langle \nu_l|\phi_k\rangle \langle \phi_k|\nu_m\rangle \langle \nu_m| = \sum_{l,m} A_{l,m} |\nu_l\rangle \langle \nu_m| \quad (28)$$

with $A_{l,m} = \sum_k F_k \langle \nu_l|\phi_k\rangle \langle \phi_k|\nu_m\rangle = \langle 0|\mathbf{d}_l \mathbf{A}_1 \mathbf{d}_m^\dagger |0\rangle$, using (13) in (27), one gets

$$\mathbf{A}_1 = \sum_{l,m} A_{l,m} \mathbf{d}_l^\dagger \mathbf{d}_m.$$

The second-quantization representation results more convenient for more than one particle, since *this representation of the operators remains the same also in the N -particle space*, so one gets

$$\boxed{\mathbf{A} = \sum_{l,m} A_{l,m} \mathbf{d}_l^\dagger \mathbf{d}_m} \text{ with } A_{l,m} = \langle 0|\mathbf{d}_l \mathbf{A}_1 \mathbf{d}_m^\dagger |0\rangle, \quad (29)$$

and, in a continuous basis

$$\boxed{\mathbf{A} = \int dx_1 dx_2 A(x_1, x_2) \Psi^\dagger(x_1) \Psi(x_2)} \text{ with } A(x_1, x_2) = \langle 0|\Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_2) |0\rangle. \quad (30)$$

The rigorous proof of this fact is a little long and tedious, so we rather prefer to show it, in the next example, only in the simple case of two particles and let the interested reader to generalize it.

Example 0.0.3. Let us study the case of $N = 2$. The action of a single-particle operator

$$\mathbf{A} = \mathbf{A}_1 \otimes \mathbf{I}_1 + \mathbf{I}_1 \otimes \mathbf{A}_1,$$

on the symmetrized two-particle state *in first quantization* is

$$\begin{aligned}
\sqrt{2}\mathbf{A}\mathbf{S}_\zeta |x_2\rangle |x_1\rangle &= \sqrt{2}\mathbf{S}_\zeta \mathbf{A} |x_2\rangle |x_1\rangle = \\
&= \sqrt{2}\mathbf{S}_\zeta [(\mathbf{A}_1 |x_2\rangle) |x_1\rangle + |x_2\rangle (\mathbf{A}_1 |x_1\rangle)] = \\
&= \frac{1}{\sqrt{2}} [(\mathbf{A}_1 |x_2\rangle) |x_1\rangle + \zeta |x_1\rangle (\mathbf{A}_1 |x_2\rangle)] + \\
&\quad + \frac{1}{\sqrt{2}} [|x_2\rangle (\mathbf{A}_1 |x_1\rangle) + \zeta (\mathbf{A}_1 |x_1\rangle) |x_2\rangle] = \\
&= \int dx_3 A(x_3, x_2) \frac{|x_3\rangle |x_1\rangle + \zeta |x_1\rangle |x_3\rangle}{\sqrt{2}} + \\
&\quad + \int dx_3 A(x_3, x_1) \frac{|x_2\rangle |x_3\rangle + \zeta |x_3\rangle |x_2\rangle}{\sqrt{2}} = \\
&= \frac{1}{\sqrt{2}} \int dx_3 A(x_3, x_2) \Psi^\dagger(x_3) \Psi^\dagger(x_1) |0\rangle + \\
&\quad + \frac{1}{\sqrt{2}} \int dx_3 A(x_3, x_1) \Psi^\dagger(x_2) \Psi^\dagger(x_3) |0\rangle = \\
&= \frac{1}{\sqrt{2}} \Psi^\dagger(x_2) \int dx_3 A(x_3, x_1) \Psi^\dagger(x_3) |0\rangle + \\
&\quad + \frac{1}{\sqrt{2}} \zeta \Psi^\dagger(x_1) \frac{1}{\sqrt{2}} \int dx_3 A(x_3, x_2) \Psi^\dagger(x_3) |0\rangle.
\end{aligned}$$

Using the single-particle property (30) we get

$$\begin{aligned}
\mathbf{A} |x_j\rangle &= \mathbf{A} \Psi^\dagger(x_j) |0\rangle = \int dx_3 dx_4 A(x_3, x_4) \Psi^\dagger(x_3) \Psi(x_4) \Psi^\dagger(x_j) |0\rangle = \\
&= \int dx_3 dx_4 A(x_3, x_4) \Psi^\dagger(x_3) [\delta(x_4 - x_j) + \zeta \Psi^\dagger(x_j) \Psi(x_4)] |0\rangle = \\
&= \int dx_3 A(x_3, x_j) \Psi^\dagger(x_3) |0\rangle,
\end{aligned}$$

so the previous equation becomes

$$\begin{aligned}
\sqrt{2}\mathbf{A}\mathbf{S}_\zeta |x_2\rangle |x_1\rangle &= \frac{1}{\sqrt{2}} \mathbf{A} \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle = \\
&= \frac{1}{\sqrt{2}} (\Psi^\dagger(x_2) \mathbf{A}_1 \Psi^\dagger(x_1) + \zeta \Psi^\dagger(x_1) \mathbf{A}_1 \Psi^\dagger(x_2)) |0\rangle
\end{aligned}$$

obtaining the following identity

$$\mathbf{A} \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle = (\Psi^\dagger(x_2) \mathbf{A}_1 \Psi^\dagger(x_1) + \zeta \Psi^\dagger(x_1) \mathbf{A}_1 \Psi^\dagger(x_2)) |0\rangle.$$

We now introduce two resolutions of the identity

$$\mathbf{A} = \mathbf{I}\mathbf{A}\mathbf{I} = \frac{1}{4} \int dx_1 dx_2 dx_3 dx_4 \Psi^\dagger(x_2) \Psi^\dagger(x_1) |0\rangle \langle 0| \Psi(x_1) \Psi(x_2) \mathbf{A} \Psi^\dagger(x_4) \Psi^\dagger(x_3) |0\rangle \langle 0| \Psi(x_3) \Psi(x_4), \quad (31)$$

let us analyze the central term

$$\langle 0| \Psi(x_1) \Psi(x_2) \mathbf{A} \Psi^\dagger(x_4) \Psi^\dagger(x_3) |0\rangle = \langle 0| \Psi(x_1) \Psi(x_2) (\Psi^\dagger(x_4) \mathbf{A}_1 \Psi^\dagger(x_3) + \zeta \Psi^\dagger(x_3) \mathbf{A}_1 \Psi^\dagger(x_4)) |0\rangle,$$

it splits in two parts

$$\begin{aligned}
\langle 0| \Psi(x_1) \Psi(x_2) \Psi^\dagger(x_4) \mathbf{A}_1 \Psi^\dagger(x_3) |0\rangle &= \delta(x_2 - x_4) \langle 0| \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_3) |0\rangle + \\
&\quad + \zeta \langle 0| \Psi(x_1) \Psi^\dagger(x_4) \Psi(x_2) \mathbf{A}_1 \Psi^\dagger(x_3) |0\rangle = \\
&= \delta(x_2 - x_4) \langle 0| \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_3) |0\rangle + \\
&\quad + \delta(x_1 - x_4) \zeta \langle 0| \Psi(x_2) \mathbf{A}_1 \Psi^\dagger(x_3) |0\rangle
\end{aligned}$$

and, equivalently,

$$\begin{aligned} \zeta \langle 0 | \Psi(x_1) \Psi(x_2) \Psi^\dagger(x_3) \mathbf{A}_1 \Psi^\dagger(x_4) | 0 \rangle &= \zeta \delta(x_2 - x_3) \langle 0 | \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_4) | 0 \rangle + \\ &+ \delta(x_1 - x_3) \langle 0 | \Psi(x_2) \mathbf{A}_1 \Psi^\dagger(x_4) | 0 \rangle. \end{aligned}$$

The two resulting integrals are equivalent, in fact for the second term one can make a change of variables $x_3 \rightleftharpoons x_4$ remembering that $\Psi(x_3) \Psi(x_4) = \zeta \Psi(x_4) \Psi(x_3)$, so eq. (31) becomes

$$\begin{aligned} \mathbf{A} &= \frac{1}{2} \int dx_1 dx_2 dx_3 \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle \langle 0 | \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_3) | 0 \rangle \langle 0 | \Psi(x_3) \Psi(x_2) + \\ &+ \frac{\zeta}{2} \int dx_1 dx_2 dx_3 \Psi^\dagger(x_2) \Psi^\dagger(x_1) | 0 \rangle \langle 0 | \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_3) | 0 \rangle \langle 0 | \Psi(x_3) \Psi(x_1), \end{aligned}$$

also in this case the two terms are equivalent since one can change $x_1 \rightleftharpoons x_2$, so the result is

$$\mathbf{A} = \int dx_1 dx_3 \langle 0 | \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_3) | 0 \rangle \Psi^\dagger(x_1) \left[\int dx_2 \Psi^\dagger(x_2) | 0 \rangle \langle 0 | \Psi(x_2) \right] \Psi(x_3),$$

the part inside the parenthesis is a resolution of the identity in the one-particle state, so we obtain the desired result

$$\mathbf{A} = \int dx_1 dx_3 \langle 0 | \Psi(x_1) \mathbf{A}_1 \Psi^\dagger(x_3) | 0 \rangle \Psi^\dagger(x_1) \Psi(x_3).$$

Example 0.0.4. Single particle Hamiltonian: Take a single-particle Hamiltonian

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \mathbf{V}(\mathbf{x}) \quad (32)$$

in the basis $\{|\phi_k\rangle\}$ one has

$$\boxed{\mathbf{H} = \sum_{i,j} H_{i,j} |\phi_i\rangle \langle \phi_j| = \sum_{i,j} H_{i,j} \mathbf{a}_i^\dagger \mathbf{a}_j}. \quad (33)$$

In the position representation

$$\mathbf{H} = \int dx_1 dx_2 \hat{\Psi}^\dagger(x_1) \hat{\Psi}(x_2) \langle x_1 | \mathbf{H} | x_2 \rangle,$$

since $\mathbf{V}(\mathbf{x})$ is local

$$\langle x_1 | \mathbf{V}(\mathbf{x}) | x_2 \rangle = V(x_1) \delta(x_1 - x_2),$$

and

$$\langle x_1 | \mathbf{p} | x_2 \rangle = -i \delta(x_1 - x_2) \frac{\partial}{\partial x_2},$$

one gets

$$\boxed{\mathbf{H} = \int dx \hat{\Psi}^\dagger(x) H \left(x, \frac{\partial^2}{\partial x^2} \right) \hat{\Psi}(x)}. \quad (34)$$

Exercise 7. Write the spin- $\frac{1}{2}$ operator $\vec{\mathbf{S}}$ in terms creation and annihilation operators of fermions with spin $\frac{1}{2}$ and $-\frac{1}{2}$

$$\mathbf{c}_\sigma, \mathbf{c}_\sigma^\dagger \quad \sigma = \pm \frac{1}{2}.$$

Try to express this result in a compact quadratic form of this kind

$$\vec{\mathbf{S}} = \underline{\mathbf{v}}^\dagger \vec{\mathbf{M}} \underline{\mathbf{v}},$$

where

$$\underline{\mathbf{v}} = \begin{pmatrix} \mathbf{c}_{\frac{1}{2}} \\ \mathbf{c}_{-\frac{1}{2}} \end{pmatrix},$$

and $\vec{\mathbf{M}}$ is a vector whose three components are 2×2 matrices.

Example 0.0.5. Current density operator: In quantum mechanics, the current density of a single particle wavefunction $\psi(x)$

$$J(x) = \frac{1}{m} \Im \left[\psi^* \frac{\partial \psi}{\partial x} \right],$$

is the average value of the so-called **current-density operator**, defined as

$$\mathbf{J}(x) = \frac{1}{2m} \{ \mathbf{p}, \delta(x - \mathbf{x}) \},$$

on the state $|\psi\rangle$

$$\begin{aligned} J(x) &= \langle \psi | \mathbf{J}(x) | \psi \rangle = \\ &= \frac{1}{2m} (\langle \psi | \mathbf{p} \delta(x - \mathbf{x}) | \psi \rangle + \langle \psi | \delta(x - \mathbf{x}) \mathbf{p} | \psi \rangle) = \\ &= \frac{1}{2m} \int dx' (\langle \psi | \mathbf{p} | x' \rangle \langle x' | \delta(x - \mathbf{x}) | \psi \rangle + \langle \psi | \delta(x - \mathbf{x}) | x' \rangle \langle x' | \mathbf{p} | \psi \rangle) = \\ &= \frac{1}{2m} \int dx' \delta(x - x') (\langle \psi | \mathbf{p} | x' \rangle \langle x' | \psi \rangle + \langle \psi | x' \rangle \langle x' | \mathbf{p} | \psi \rangle) = \\ &= \frac{i}{2m} \left(\frac{\partial \psi^*(x)}{\partial x} \psi(x) - \psi^*(x) \frac{\partial \psi(x)}{\partial x} \right) = \frac{1}{m} \Im \left[\psi^* \frac{\partial \psi}{\partial x} \right]. \end{aligned}$$

The current density operator can be expressed in second quantization as

$$\begin{aligned} \mathbf{J}(x) &= \frac{1}{2m} \int dx' dx'' \hat{\Psi}^\dagger(x') \hat{\Psi}(x'') \langle x' | \{ \mathbf{p}, \delta(x - \mathbf{x}) \} | x'' \rangle = \\ &= \frac{-i}{2m} \int dx' dx'' \hat{\Psi}^\dagger(x') \hat{\Psi}(x'') (\delta(x - x'') + \delta(x - x')) \delta'(x' - x'') = \\ &= \frac{i}{2m} \left(\int dx'' \frac{\partial \hat{\Psi}^\dagger(x'')}{\partial x''} \hat{\Psi}(x'') \delta(x - x'') - \int dx' \hat{\Psi}^\dagger(x') \frac{\partial \hat{\Psi}(x')}{\partial x'} \delta(x - x') \right), \end{aligned}$$

$$\boxed{\mathbf{J}(x) = \frac{i}{2m} \left(\frac{\partial \hat{\Psi}^\dagger(x)}{\partial x} \hat{\Psi}(x) - \hat{\Psi}^\dagger(x) \frac{\partial \hat{\Psi}(x)}{\partial x} \right)}.$$

One can expand the operator in a discrete basis

$$\begin{aligned} \Psi^\dagger(x) &= \sum_k \phi_k^*(x) \mathbf{a}_k^\dagger, \\ \mathbf{J}(x) &= \frac{i}{2m} \sum_{k,m} \left(\frac{\partial \phi_k^*(x)}{\partial x} \phi_m(x) \mathbf{a}_k^\dagger \mathbf{a}_m - h.c. \right). \end{aligned}$$

The global current is obtained integrating over all the space

$$\begin{aligned} \mathbf{J} &= i \sum_{k,m} \left(g_{k,m} \mathbf{a}_k^\dagger \mathbf{a}_m - h.c. \right), \\ g_{k,m} &= \frac{1}{2m} \int dx \frac{\partial \phi_k^*(x)}{\partial x} \phi_m(x). \end{aligned}$$

Two-particle operators

Let $\mathbf{A}_2$ be an operator acting on the Hilbert space of two particles. The two-particle many-body operator corresponding to it is

$$\mathbf{A} = \mathbf{A}_2 \otimes \mathbf{I}_{N-2} + \mathbf{I}_1 \otimes \mathbf{A}_2 \otimes \mathbf{I}_{N-3} + \dots + \mathbf{I}_{N-2} \otimes \mathbf{A}_2 = \frac{1}{2} \sum_{i,j} \mathbf{A}_2^{(i,j)} \otimes \mathbf{I}_{N-2}.$$

Given a single-particle basis

$$\mathbf{d}_n^\dagger |0\rangle = |\phi_n\rangle,$$

the two-particle operators have the form

$$\boxed{\mathbf{A} = \frac{1}{2} \sum_{j,n,j',n'} \langle \phi_j, \phi_n | \mathbf{A}_2 | \phi_{n'}, \phi_{j'} \rangle \mathbf{d}_j^\dagger \mathbf{d}_n^\dagger \mathbf{d}_{j'} \mathbf{d}_{n'}}. \quad (35)$$

Notice that the state $|\phi_{n'}, \phi_{j'}\rangle$ is not symmetrized.

Example 0.0.6. Let us check it in the case in which we have only two particles. The matrix element of $\mathbf{A}$ is

$$\langle 0 | \mathbf{d}_{m'} \mathbf{d}_{k'} \mathbf{A} \mathbf{d}_k^\dagger \mathbf{d}_m^\dagger | 0 \rangle = \langle \phi_{k'} \phi_{m'} | \mathbf{A}_2 | \phi_k \phi_m \rangle + \zeta \langle \phi_{k'} \phi_{m'} | \mathbf{A}_2 | \phi_m \phi_k \rangle,$$

where we used the symmetry of the operator

$$\langle \phi_{k'} \phi_{m'} | \mathbf{A}_2 | \phi_k \phi_m \rangle = \langle \phi_{m'} \phi_{k'} | \mathbf{A}_2 | \phi_m \phi_k \rangle.$$

Let us compare it with (35)

$$\langle 0 | \mathbf{d}_{m'} \mathbf{d}_{k'} \mathbf{A} \mathbf{d}_k^\dagger \mathbf{d}_m^\dagger | 0 \rangle = \frac{1}{2} \sum_{j,n,j',n'} \langle \phi_j, \phi_n | \mathbf{A}_2 | \phi_{n'}, \phi_{j'} \rangle \langle 0 | \mathbf{d}_{m'} \mathbf{d}_{k'} \mathbf{d}_j^\dagger \mathbf{d}_n^\dagger \mathbf{d}_{j'} \mathbf{d}_{n'} \mathbf{d}_k^\dagger \mathbf{d}_m^\dagger | 0 \rangle,$$

the right-side term can be expanded

$$\begin{aligned} \langle 0 | \mathbf{d}_{m'} \mathbf{d}_{k'} \mathbf{d}_j^\dagger \mathbf{d}_n^\dagger \mathbf{d}_{j'} \mathbf{d}_{n'} \mathbf{d}_k^\dagger \mathbf{d}_m^\dagger | 0 \rangle &= \langle 0 | \mathbf{d}_{m'} \left(\delta_{k',j} + \zeta \mathbf{d}_j^\dagger \mathbf{d}_{k'} \right) \mathbf{d}_n^\dagger \mathbf{d}_{j'} \left(\delta_{n',k} + \zeta \mathbf{d}_k^\dagger \mathbf{d}_{n'} \right) \mathbf{d}_m^\dagger | 0 \rangle = \\ &= \delta_{k',j} \delta_{n',k} \delta_{m',n} \delta_{j',m} + \zeta \delta_{k',j} \delta_{m',n} \langle 0 | \left(\delta_{j',k} + \zeta \mathbf{d}_k^\dagger \mathbf{d}_{j'} \right) \left(\delta_{n',k} + \zeta \mathbf{d}_m^\dagger \mathbf{d}_{n'} \right) | 0 \rangle + \\ &+ \zeta \delta_{n',k} \delta_{j',m} \langle 0 | \left(\delta_{m',j} + \zeta \mathbf{d}_j^\dagger \mathbf{d}_{m'} \right) \left(\delta_{k',n} + \zeta \mathbf{d}_n^\dagger \mathbf{d}_{k'} \right) | 0 \rangle + \\ &+ \langle 0 | \mathbf{d}_{m'} \mathbf{d}_j^\dagger \mathbf{d}_{k'} \mathbf{d}_n^\dagger \mathbf{d}_{j'} \mathbf{d}_k^\dagger \mathbf{d}_{n'} \mathbf{d}_m^\dagger | 0 \rangle = \\ &= \delta_{k',j} \delta_{n',k} \delta_{m',n} \delta_{j',m} + \zeta \delta_{k',j} \delta_{m',n} \delta_{j',k} \delta_{n',m} + \\ &+ \zeta \delta_{n',k} \delta_{j',m} \delta_{m',j} \delta_{k',n} + \delta_{m',j} \delta_{k',n} \delta_{j',k} \delta_{n',m}, \end{aligned}$$

so to obtain

$$\langle 0 | \mathbf{d}_{m'} \mathbf{d}_{k'} \mathbf{A} \mathbf{d}_k^\dagger \mathbf{d}_m^\dagger | 0 \rangle = \frac{1}{2} (2 \langle \phi_{k'}, \phi_{m'} | \mathbf{A}_2 | \phi_k, \phi_m \rangle + 2\zeta \langle \phi_{k'}, \phi_{m'} | \mathbf{A}_2 | \phi_m, \phi_k \rangle).$$

In a continuous basis

$$\boxed{\mathbf{A} = \frac{1}{2} \int dx_1 dx_2 dx_3 dx_4 \langle x_1, x_2 | \mathbf{A}_2 | x_3, x_4 \rangle \hat{\Psi}^\dagger(x_1) \hat{\Psi}^\dagger(x_2) \hat{\Psi}(x_4) \hat{\Psi}(x_3)}.$$

Global gauge transformations

We know that, in quantum mechanics, one-particle states are defined up to a global phase factor

$$|\psi\rangle \rightarrow e^{i\phi} |\psi\rangle.$$

Equivalently, the observables are unchanged under the transformation

$$e^{-i\phi} \mathbf{A} e^{i\phi} = \mathbf{A}.$$

This phase factor represents for the quantum system a global $U(1)$ symmetry, under which it is invariant. In second quantization and within a one-particle space, this gauge transformation is equivalent to

$$\mathbf{a}_j \rightarrow \mathbf{a}_j e^{i\phi}.$$

In the Fock space, a global gauge transformation is obtained applying the symmetry generated by the operator $\mathbf{N}$

$$\mathbf{U} = e^{i\phi \mathbf{N}}, \quad (36)$$

indeed

$$\mathbf{U}^\dagger \mathbf{a}_j \mathbf{U} = e^{i\phi} \mathbf{a}_j.$$

The system is invariant under this global gauge transformation if and only if the Hamiltonian commutes with its infinitesimal generator, i.e. $\mathbf{N}$, meaning that the total number of particles is a conserved quantity. All the n -body Hamiltonians that we described are obviously invariant under (36), indeed their structure consists of terms with products of n creation and n annihilation operators which transform as

$$\mathbf{U}^\dagger \mathbf{a}_1^\dagger \dots \mathbf{a}_n^\dagger \mathbf{a}_n \dots \mathbf{a}_1 \mathbf{U} = e^{-ni\phi} \mathbf{a}_1^\dagger \dots \mathbf{a}_n^\dagger \mathbf{a}_n \dots \mathbf{a}_1 e^{ni\phi} = \mathbf{a}_1^\dagger \dots \mathbf{a}_n^\dagger \mathbf{a}_n \dots \mathbf{a}_1.$$

The requirement of being particle-preserving is a quite reasonable physical requirement but also non particle-preserving Hamiltonians can be constructed introducing for example terms proportional to

$$\mathbf{a}_i^\dagger \mathbf{a}_j^\dagger + \mathbf{a}_j \mathbf{a}_i.$$

Such terms are commonly allowed when assuming the existence of a reservoir with which the system can exchange particles. A typical example is the BCS mean field Hamiltonian describing a superconductor in the mean field approximation, where these terms appear as the effect of the spontaneous symmetry breaking of the $U(1)$ symmetry.