

SECOND QUANTIZATION

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- 1) N identical particles (*Identical particles, indistinguishability of identical particles, Slater determinants and permanents, the basis of occupation numbers*)
 - 2) The Fock space (*Creation and destruction operators, the algebra of (anti)commutation relations*)
 - 3) Canonical (anti)-commutation relations (*Field operators*)
 - 4) Second quantization of operators (*one and two-particle operators*)
 - 5) Symmetries (*space translations, rotations, dilations and virial theorem, parity*)
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In quantum mechanics a particle is objectified by a set of observables, i.e. a set of fundamental operators, such as position, momentum and spin, characterized by certain commutation relations. If they are represented irreducibly (i.e. any operator that commutes with them is multiple of the identity), then any other observable of the particle is a function of them. The fundamental operators of different particles commute: this translates the concept of a particle being an autonomous entity. However, two or more identical particles are indistinguishable, and the fundamental operators become unphysical. Only observables that are invariant for permutation of particles, i.e. symmetric functions of the fundamental operators, are meaningful.

A convenient formalism for the quantum description of identical particles is *second quantisation*. There are various ways to introduce it. Here, it is a procedure for rewriting physical operators in a basis of operators $\{\hat{c}_r^\dagger, \hat{c}_r\}_{r=1}^\infty$ that create and destroy a particle in single-particle states $|r\rangle$, with commutation rules that take care of the particle statistics.

Second-quantized operators are defined in Fock spaces for bosons or fermions, that accomodate any number of particles. The formalism is efficient in describing new quantum phenomena, as decays, absorption and emission processes of particles or excitations such as photons, phonons, etc.

The creation and destruction operators with commutation rules (Bose statistics) were introduced by Paul M. A. Dirac (1926, *Quantum theory of light radiation and absorption*). Pascual Jordan extended the formalism to massive bosons (Jordan and Klein, 1927) and to Fermi statistics, with anti-commutation rules (Jordan and Wigner, 1928).

1. N IDENTICAL PARTICLES

The Hilbert space of N particles is $\mathcal{H}(N) = \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_N$, where \mathcal{H}_k is the Hilbert space for the single k -th particle. $\mathcal{H}(N)$ is the closure of the finite linear combinations of factored vectors $|u_1, \dots, u_N\rangle = |u_1\rangle \otimes \dots \otimes |u_N\rangle$, where $|u_k\rangle$ belongs

to \mathcal{H}_k , with the inner product among factored states

$$(1) \quad \langle v_1, \dots, v_N | u_1, \dots, u_N \rangle = \langle v_1 | u_1 \rangle_1 \cdots \langle v_N | u_N \rangle_N$$

where $\langle \cdot | \cdot \rangle_k$ is the inner product in \mathcal{H}_k . The tensor product is linear in each term:

$$|u_1, \dots, \alpha u_i + \beta v_i, \dots, u_N\rangle = \alpha |u_1, \dots, u_i, \dots, u_N\rangle + \beta |u_1, \dots, v_i, \dots, u_N\rangle.$$

An operator \hat{A} on \mathcal{H}_k corresponds to an operator $\hat{A}(k)$ on $\mathcal{H}(N)$ with action $\hat{A}(k)|u_1, \dots, u_k, \dots, u_N\rangle = |u_1, \dots, \hat{A}u_k, \dots, u_N\rangle$. By construction, operators of different particles commute: $[\hat{A}(k), \hat{B}(k')] = 0$.

Example 1.1. A Hilbert space for a spin-less particle is $L^2(\mathbb{R}^3)$. The products $f_1(\mathbf{x}_1) \cdots f_N(\mathbf{x}_N)$ and their linear combinations form a linear space whose closure is the Hilbert space $L^2(\mathbb{R}^{3N})$ of functions with $\int d\mathbf{x}_1 \dots d\mathbf{x}_N |f(\mathbf{x}_1, \dots, \mathbf{x}_N)|^2 < \infty$.

1.1. Identical particles. If the N particles are identical, the spaces $\mathcal{H}_1, \dots, \mathcal{H}_N$ are copies of the same one-particle Hilbert space \mathcal{H} ($\mathcal{H}(N) = \otimes^N \mathcal{H}$). Since the vectors in $|u_1, \dots, u_N\rangle$ belong to the same space, it is possible to introduce the permutation operators. If σ is the permutation $\sigma(1, \dots, N) = (\sigma_1, \dots, \sigma_N)$, the corresponding operator on factored states is

$$(2) \quad \hat{P}_\sigma |u_1, \dots, u_N\rangle = |u_{\sigma_1}, \dots, u_{\sigma_N}\rangle$$

They extend by linearity to unitary operators on the whole space $\mathcal{H}(N)$, and form a representation of the symmetric (non-Abelian) group S_N :

$$(3) \quad \hat{P}_\sigma \hat{P}_{\sigma'} = \hat{P}_{\sigma\sigma'}, \quad \hat{P}_\sigma^\dagger = \hat{P}_{\sigma^{-1}}$$

An important subclass are the exchange operators. The exchange of particles i and j is $\hat{P}_{ij}|u_1 \dots u_i \dots u_j \dots u_N\rangle = |u_1 \dots u_j \dots u_i \dots u_N\rangle$. Since $\hat{P}_{ij}^2 = I$, it follows that \hat{P}_{ij} is self-adjoint with eigenvalues ± 1 .

Any permutation can be factored into exchanges, in various ways. However, the parity of the number of exchanges in any factorization is the same: a permutation is even or odd if the number of exchanges is even or odd¹.

Let's introduce the symmetrization operator $\hat{S}(N)$ (or $\hat{S}(N)_+$) and the antisymmetrization operator $\hat{A}(N)$ (or $\hat{S}(N)_-$) of N particles:

$$(4) \quad \boxed{\hat{S}(N)_\pm = \frac{1}{N!} \sum_{\sigma \in S_N} (\pm 1)^\sigma \hat{P}_\sigma}$$

$(+1)^\sigma = 1$ applies to the symmetrization $\hat{S}(N)$, while $(-1)^\sigma$ applies to $\hat{A}(N)$, and is $+1$ if σ is even, -1 if σ is odd.

We omit the simple proofs of

$$(5) \quad \hat{P}_\sigma \hat{S}(N) = \hat{S}(N) \hat{P}_\sigma = \hat{S}(N), \quad \hat{P}_\sigma \hat{A}(N) = \hat{A}(N) \hat{P}_\sigma = (-1)^\sigma \hat{A}(N)$$

Proposition 1.2. $\hat{S}(N)_\pm$ are projection operators:

$$(6) \quad \hat{S}(N)_\pm^\dagger = \hat{S}(N)_\pm, \quad \hat{S}(N)_\pm^2 = \hat{S}(N)_\pm$$

¹ S_N is represented by $N \times N$ matrices σ_{ij} with elements 0 and a single 1 in each column and row, the determinant may be 1 or -1. There are $N!$ such matrices. The matrix exchanging elements i, j has matrix elements $\sigma_{rs} = \delta_{rs}$ for $r, s \neq i, j$, $\sigma_{ii} = \sigma_{jj} = 0$, $\sigma_{ij} = \sigma_{ji} = 1$. Its determinant is -1 . All factorizations that produce the permutation matrix must give the same value of the determinant.

Proof. In $\hat{S}(N)_\pm^\dagger = \frac{1}{N!} \sum_\sigma (\pm 1)^\sigma \hat{P}_{\sigma^{-1}}$, the sum on σ coincides with the sum on inverse permutations σ^{-1} , and σ has the same parity of σ^{-1} . This gives self-adjointness. The other property follows from (5): $\hat{S}(N)_\pm^2 = \frac{1}{N!} \sum_\sigma (\pm 1)^\sigma \hat{S}(N)_\pm \hat{P}_\sigma = \frac{1}{N!} \sum_\sigma \hat{S}(N)_\pm = \hat{S}(N)_\pm$. \square

Exercise 1.3. Show that $\hat{A}(N)|u_1 \dots u_N\rangle = 0$ if two vectors are equal.

Exercise 1.4. If $|v_k\rangle = \sum_{j=1}^N M_{kj}|u_j\rangle$, $k = 1 \dots N$, show that

$$(7) \quad \boxed{\hat{A}(N)|v_1 \dots v_N\rangle = (\det M)\hat{A}(N)|u_1 \dots u_N\rangle}$$

The projection operators identify two Hilbert (sub)spaces:

$$\mathcal{H}(N)_+ = \hat{S}(N)_+ \mathcal{H}(N), \quad \mathcal{H}(N)_- = \hat{S}(N)_- \mathcal{H}(N)$$

A vector in $\mathcal{H}(N)_+$ is invariant under the action of any exchange operator, while a vector in $\mathcal{H}(N)_-$ changes sign under the action of any exchange operator:

$$\hat{P}_{ij}\Psi_+ = \Psi_+, \quad \hat{P}_{ij}\Psi_- = -\Psi_-, \quad \forall i \neq j$$

In other words, $\mathcal{H}(N)_+$ is the eigenspace with eigenvalue 1 for all exchange operators, while $\mathcal{H}(N)_-$ is the eigenspace with eigenvalue -1 for all exchange operators. Therefore, $\mathcal{H}(N)_+$ and $\mathcal{H}(N)_-$ are orthogonal subspaces of $\mathcal{H}(N)$.

1.2. Indistinguishability of identical particles. In quantum mechanics identical particles are *indistinguishable*. This means that the operators associated to observables are symmetric functions of the fundamental 1-particle operators:

$$\hat{O}(1, 2, \dots, N) = \hat{O}(\sigma_1, \sigma_2, \dots, \sigma_N)$$

where for brevity we put $i = (\mathbf{x}_i, \mathbf{p}_i, \mathbf{s}_i)$. Therefore, they commute with all permutation operators: $[\hat{O}, \hat{P}_\sigma] = 0$.

Proof: $\langle v_1, \dots, v_N | \hat{O}(1, \dots, N) | u_1, \dots, u_N \rangle = \langle v_{\sigma_1}, \dots, v_{\sigma_N} | \hat{O}(\sigma_1, \dots, \sigma_N) | u_{\sigma_1}, \dots, u_{\sigma_N} \rangle = \langle v_1, \dots, v_N | \hat{P}_\sigma^\dagger \hat{O}(1, \dots, N) \hat{P}_\sigma | u_1, \dots, u_N \rangle$ for all factored states and permutations. Since factored states generate the whole space, it is $\hat{P}_\sigma^\dagger \hat{O} \hat{P}_\sigma = \hat{O}$. \square

The only subspaces in $\mathcal{H}(N)$ that are left invariant by the action of the observables, and in particular by the time evolution, are $\mathcal{H}(N)_\pm$. For this reason they are the Hilbert spaces for the physics of N identical particles.

The **spin-statistics connection** is a fundamental result of relativistic quantum field theory, where a violation would correspond to a violation of causality. It states that:

- $\mathcal{H}(N)_+$ is the space for N bosons (integer spin),
- $\mathcal{H}(N)_-$ is the space for N fermions (half-integer spin).

Of particular relevance are the two classes of observables:

- 1-particle operators $\hat{A} = \sum_{i=1}^N a(i)$, (total momentum $\hat{\mathbf{P}} = \sum_{i=1}^N \mathbf{p}_i$, particle density $\hat{n}(\mathbf{x}) = \sum_{i=1}^N \delta_3(\mathbf{x} - \mathbf{x}_i)$), spin density $\hat{\mathbf{S}}(\mathbf{x}) = \sum_{i=1}^N \mathbf{s}_i \delta_3(\mathbf{x} - \mathbf{x}_i)$, ...);
- 2-particle operators $\hat{A} = \sum_{i < j} a(i, j)$, with $a(i, j) = a(j, i)$ (the two-particle interaction energy $\hat{V} = \sum_{i < j} v(\mathbf{x}_i, \mathbf{x}_j)$).

1.3. Slater determinants and permanents. The inner product of two vectors $\hat{S}(N)_\pm|u_1, \dots, u_N\rangle$ and $\hat{S}(N)_\pm|v_1, \dots, v_N\rangle$ is:

$$\begin{aligned}
 \langle u_1, \dots, u_N | \hat{S}(N)_\pm^2 | v_1, \dots, v_N \rangle &= \frac{1}{N!} \sum_{\sigma} (\pm 1)^\sigma \langle u_1, \dots, u_N | \hat{P}_\sigma | v_1, \dots, v_N \rangle \\
 &= \frac{1}{N!} \sum_{\sigma} (\pm 1)^\sigma \langle u_1 | v_{\sigma_1} \rangle \dots \langle u_N | v_{\sigma_N} \rangle \\
 (8) \qquad &= \frac{1}{N!} D_\pm \begin{bmatrix} \langle u_1 | v_1 \rangle & \dots & \langle u_1 | v_N \rangle \\ \vdots & & \vdots \\ \langle u_N | v_1 \rangle & \dots & \langle u_N | v_N \rangle \end{bmatrix}
 \end{aligned}$$

D_+ is the permanent² and D_- is the determinant.

When the inner product is evaluated with the bra $\langle \mathbf{x}_1, m_1; \dots; \mathbf{x}_N, m_N |$, one gets the permanent or the determinant of a matrix whose elements are functions:

$$(9) \qquad D_\pm \begin{bmatrix} v_1(\mathbf{x}_1 m_1) & \dots & v_N(\mathbf{x}_1 m_1) \\ \vdots & & \vdots \\ v_1(\mathbf{x}_N m_N) & \dots & v_N(\mathbf{x}_N m_N) \end{bmatrix}$$

The result is a totally symmetric or antisymmetric N -particle function.

Exercise 1.5. The first N eigenfunctions of the 1D harmonic oscillator are

$$u_k(x) = \frac{1}{\sqrt{2^k k!} \sqrt{\pi}} e^{-\frac{1}{2}x^2} H_k(x)$$

where $H_k(x) = 2^k x^k + \dots$ are the Hermite polynomials. Show that the totally antisymmetric N -particle function is

$$\langle x_1 \dots x_N | \hat{A}(N) | u_1 \dots u_N \rangle = \text{const.} \cdot e^{-\frac{1}{2}(x_1^2 + \dots + x_N^2)} \prod_{i>j} (x_i - x_j).$$

(the product is the Vandermonde determinant).

1.4. The basis of occupation numbers. Given a 1-particle orthonormal complete set of vectors $|r\rangle$, $r = 1, 2, 3, \dots$ the factored vectors $|r_1, r_2, \dots, r_N\rangle$ form an orthonormal basis in $\mathcal{H}(N)$. Their projections $\hat{S}(N)_\pm |r_1, r_2, \dots, r_N\rangle$ span the subspaces $\mathcal{H}(N)_\pm$.

Remark 1.6. Since $\langle r_i | r_j \rangle = \delta_{ij}$, by eq.(8) two vectors $\hat{S}(N)_\pm |r_1, \dots, r_N\rangle$ and $\hat{S}(N)_\pm |r'_1, \dots, r'_N\rangle$ are orthogonal if $|r'_1, \dots, r'_N\rangle$ is not a permutation of $|r_1, \dots, r_N\rangle$.

Bosons. In evaluating the squared norm, the sum on permutations in eq.(8) gives nonzero terms in correspondence of the identity permutation and permutations among vectors that are repeated. Then:

$$\|\hat{S}(N) |r_1, r_2, \dots, r_N\rangle\|^2 = \frac{n_1! n_2! \dots n_\infty!}{N!}$$

where n_r is the number of times that $|r\rangle$ is present in the sequence $|r_1, \dots, r_N\rangle$. Since $n_1 + n_2 + \dots + n_\infty = N$, most occupation numbers n_r are zero.

²The permanent of a matrix is evaluated as a determinant, but omitting the weights ± 1 . Note that $D_+(AB) \neq D_+(A)D_+(B)$.

Consider the normalized and orthogonal vectors

$$(10) \quad |r_1, \dots, r_N\rangle_+ = \sqrt{\frac{N!}{n_1! \dots n_\infty!}} \hat{S}(N) |r_1, \dots, r_N\rangle,$$

Conventionally, 1-particle basis vectors are in ascending order, $r_1 \leq r_2 \leq \dots \leq r_N$, to avoid replicas of the same symmetric vector. These vectors form an orthonormal basis of the space of N bosons $\mathcal{H}(N)_+$.

Fermions. A state $|r\rangle$ cannot appear twice in $|r_1, \dots, r_N\rangle$, therefore $n_r = 0, 1$. In evaluating the norm, only the identity permutation contributes, then $\|\hat{A}(N)|r_1, r_2, \dots, r_N\rangle\|^2 = \frac{1}{N!}$. The vectors

$$(11) \quad |r_1, r_2, \dots, r_N\rangle_- = \sqrt{N!} \hat{A}(N) |r_1, r_2, \dots, r_N\rangle$$

where $r_1 < r_2 < \dots < r_N$, form an orthonormal basis in the space of N fermions $\mathcal{H}(N)_-$.

A vector $|r_1, \dots, r_N\rangle_\pm$ is proportional to the symmetric or the antisymmetric sum on all permutations of $|r_1\rangle, \dots, |r_N\rangle$. Therefore it carries the information that each of the N particles has equal probability in the specified 1-particle states. The information is specified by the occupation number of each state of the basis.

We introduce the equivalent notation:

$$(12) \quad |n_1, n_2, \dots, n_\infty\rangle_\pm \equiv |r_1, r_2, \dots, r_N\rangle_\pm$$

where n_r is the *occupation number* of the single particle state $|r\rangle$, i.e. the number of times that the vector $|r\rangle$ appears in $|r_1, \dots, r_N\rangle$. For bosons $n_r = 0, 1, 2, \dots$, for fermions $n_r = 0, 1$. In any case $n_1 + \dots + n_\infty = N$.

Example 1.7. Let $|1\rangle, |2\rangle, \dots$ denote the vectors of a 1-particle basis.

- The vector for 6 bosons $|2, 3, 3, 5, 5, 8\rangle_+$ (note the ascending order) can be represented as the number state $|0, 1, 2, 0, 2, 0, 0, 1, 0, \dots\rangle_+$.
- The vector for 6 fermions $|2, 3, 4, 5, 6, 8\rangle_-$ (ascending order, no repetitions) is equivalent to the number state $|0, 1, 1, 1, 1, 1, 0, 1, 0, \dots\rangle_-$.
- The number state for fermions $|1, 0, 1, 1, 0, \dots\rangle_-$ describes 3 particles in states $|1\rangle, |3\rangle$ and $|4\rangle$, i.e. the state $|1, 3, 4\rangle_-$.

The orthogonality and completeness relations in $\mathcal{H}(N)_\pm$ are:

$$(13) \quad \pm \langle n_1, n_2, \dots | n'_1, n'_2, \dots \rangle_\pm = \delta_{n_1, n'_1} \delta_{n_2, n'_2} \dots$$

$$(14) \quad \sum_{\substack{n_1, n_2, \dots \\ n_1 + n_2 + \dots = N}} \pm |n_1, n_2, \dots\rangle_\pm \langle n_1, n_2, \dots|_\pm = \hat{I}_N$$

2. THE FOCK SPACE

It is advantageous to immerse the Hilbert space of N bosons or fermions in the larger *Fock spaces* (V. Fock, 1928) for bosons or fermions:

$$\mathcal{F}_\pm = |0\rangle \oplus \mathcal{H}(1) \oplus \mathcal{H}(2)_\pm \oplus \dots \oplus \mathcal{H}(N)_\pm \oplus \dots$$

$|0\rangle$ is the vacuum state (zero particle), $\mathcal{H}(1) = \mathcal{H}$ is the one-particle Hilbert space, ..., $\mathcal{H}(N)_\pm$ is the Hilbert space of N bosons or fermions. In this construction, vectors with different number content are orthogonal. Since \mathcal{H} is separable, the

Fock spaces \mathcal{F}_\pm are separable (i.e. it admits a dense numerable subset).

The vectors $|n_1, \dots, n_\infty\rangle_\pm$ with unrestricted sum $n_1 + \dots + n_\infty$ are a basis for \mathcal{F}_\pm .

In the large ambient of Fock space, operators that change the number of particles may be defined. The basic ones are the operators that create or destroy one boson, \hat{B}^\dagger and \hat{B} , or the operators that create or destroy one fermion \hat{A}^\dagger and \hat{A} . Since many properties can be derived jointly, we often use the single notation \hat{c}^\dagger, \hat{c} (for bosons they act on \mathcal{F}_+ , for fermions they act on \mathcal{F}_-).

2.1. Creation and destruction operators. The creation operator of one particle in a single-particle state $|u\rangle$ is defined through its action on factored vectors:

$$(15) \quad \boxed{\hat{c}_{|u}^\dagger \hat{S}(N)_\pm |u_1, \dots, u_N\rangle = \sqrt{N+1} \hat{S}(N+1)_\pm |u, u_1, \dots, u_N\rangle}$$

It simply adds a new particle in state $|u\rangle$ to the existing N particles, and reshuffles the $N+1$ states. In particular, $\hat{c}_{|u}^\dagger |0\rangle = |u\rangle$.

$$\hat{c}_{|u}^\dagger : \mathcal{H}(N)_\pm \rightarrow \mathcal{H}(N+1)_\pm, \quad N = 0, 1, \dots$$

The action on a generic vector in \mathcal{F}_\pm is defined by linearity, once the vector is expanded into factored vectors.

The destruction operator of a particle in a state $|u\rangle$ is defined as the adjoint of $\hat{c}_{|u}^\dagger$. For reasons that will be clear, it is useful to adopt the notation $\hat{c}_{\langle u|}$.

To find the action of $\hat{c}_{\langle u|}$ on vectors, we consider the matrix element between two factored states $\langle v_1, \dots, v_{N'} | \hat{S}(N')_\pm \hat{c}_{\langle u|} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle$. As $\hat{c}_{\langle u|} = (\hat{c}_{|u}^\dagger)^\dagger$ adds a particle in the bra-vector, the matrix element is zero if $N' \neq N-1$, meaning that $\hat{c}_{\langle u|}$ acts on the ket by removing a particle.

Let's then evaluate the matrix element

$$\langle v_1, \dots, v_{N-1} | \hat{S}(N-1)_\pm \hat{c}_{\langle u|} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle$$

The operator adds a state $|u\rangle$ in the left $N-1$ particle state:

$$\begin{aligned} &= \sqrt{N} \langle u, v_1, \dots, v_{N-1} | \hat{S}(N)_\pm |u_1, \dots, u_N\rangle \\ &= \frac{\sqrt{N}}{N!} D_\pm \begin{bmatrix} \langle u|u_1\rangle & \langle u|u_2\rangle & \dots & \langle u|u_N\rangle \\ \langle v_1|u_1\rangle & \dots & \dots & \langle v_1|u_N\rangle \\ \dots & & & \dots \\ \langle v_{N-1}|u_1\rangle & & & \langle v_{N-1}|u_N\rangle \end{bmatrix} \end{aligned}$$

The permanent or determinant is expanded with respect to the first row:

$$\begin{aligned} &= \frac{\sqrt{N}}{N!} \sum_{j=1}^N (\pm 1)^{j+1} \langle u|u_j\rangle D_\pm [\langle v_i|u_k\rangle]_{k \neq j} \\ &= \frac{1}{\sqrt{N}} \sum_{j=1}^N (\pm 1)^{j+1} \langle u|u_j\rangle \langle v_1, \dots, v_{N-1} | \hat{S}(N-1)_\pm |u_1, \dots, \cancel{u_j}, \dots, u_N\rangle \end{aligned}$$

By the arbitrariness of the bra vector, and being the linear combinations of such vectors a dense set in $\mathcal{H}(N-1)_\pm$, we obtain the final formula:

(16)

$$\hat{c}_{\langle u|} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^N (\pm 1)^{j+1} \langle u|u_j\rangle \hat{S}(N-1)_\pm |u_1, \dots, \cancel{u}_j, \dots, u_N\rangle$$

Destruction operators annihilate the vacuum state: $\hat{c}_{\langle u|} |0\rangle = 0$.

With the definition of the creation operator on factored states, and being the destruction operator its adjoint, the following properties of linearity and anti-linearity follow:

$$(17) \quad \hat{c}_{|\alpha u + \beta v\rangle}^\dagger = \alpha \hat{c}_{|u\rangle}^\dagger + \beta \hat{c}_{|v\rangle}^\dagger, \quad \hat{c}_{\langle \alpha u + \beta v|} = \alpha^* \hat{c}_{\langle u|} + \beta^* \hat{c}_{\langle v|}$$

2.2. The algebra of (anti)commutation rules. Creation and destruction operators obey a simple and important algebra. Consider the creation of two particles in the single particle states $|u\rangle$ and $|v\rangle$

$$\hat{c}_{|u\rangle}^\dagger \hat{c}_{|v\rangle}^\dagger \hat{S}(N)_\pm |u_1, \dots, u_N\rangle = \sqrt{(N+2)(N+1)} \hat{S}(N+2)_\pm |u, v, u_1, \dots, u_N\rangle$$

If the order is exchanged, the boson state with vectors exchanged remains the same, while for fermions an exchange means a minus sign:

$$\hat{c}_{|v\rangle}^\dagger \hat{c}_{|u\rangle}^\dagger \hat{S}(N)_\pm |u_1, \dots, u_N\rangle = \pm \sqrt{(N+2)(N+1)} \hat{S}(N+2)_\pm |u, v, u_1, \dots, u_N\rangle$$

By respectively subtracting and summing, the following exact commutation and anti-commutation properties result³:

$$(18) \quad [\hat{b}_{|u\rangle}^\dagger, \hat{b}_{|v\rangle}^\dagger] = 0, \quad (\text{bosons}) \quad \{\hat{a}_{|u\rangle}^\dagger, \hat{a}_{|v\rangle}^\dagger\} = 0, \quad (\text{fermions})$$

By taking their adjoint, it follows that destruction operators exactly commute or anticommute:

$$(19) \quad [\hat{b}_{\langle u|}, \hat{b}_{\langle v|}] = 0, \quad (\text{bosons}) \quad \{\hat{a}_{\langle u|}, \hat{a}_{\langle v|}\} = 0, \quad (\text{fermions})$$

In particular, $(\hat{a}_{|u\rangle}^\dagger)^2 = 0$ and $(\hat{a}_{\langle u|})^2 = 0$ (Pauli principle).

To obtain the relations among creation and destruction operators, their actions in different order are evaluated:

$$\begin{aligned} \hat{c}_{|v\rangle}^\dagger \hat{c}_{\langle u|} S(N)_\pm |u_1, \dots, u_N\rangle &= \sum_{j=1}^N (\pm 1)^{j+1} \langle u|u_j\rangle S(N)_\pm |v, u_1, \dots, \cancel{u}_j, \dots, u_N\rangle \\ \hat{c}_{\langle u|} \hat{c}_{|v\rangle}^\dagger S(N)_\pm |u_1, \dots, u_N\rangle &= \sqrt{N+1} c_{\langle u|} S(N+1)_\pm |v, u_1, \dots, u_N\rangle = \\ &= \langle u|v\rangle S(N)_\pm |u_1, \dots, u_N\rangle \pm \sum_{j=1}^N (\pm 1)^{j+1} \langle u|u_j\rangle S(N)_\pm |v, u_1, \dots, \cancel{u}_j, \dots, u_N\rangle \end{aligned}$$

By comparing the two expressions one concludes that

$$(20) \quad [\hat{b}_{\langle u|}, \hat{b}_{|v\rangle}^\dagger] = \langle u|v\rangle \quad (\text{bosons}) \quad \{\hat{a}_{\langle u|}, \hat{a}_{|v\rangle}^\dagger\} = \langle u|v\rangle \quad (\text{fermions})$$

³ $[A, B] = AB - BA$, $\{A, B\} = AB + BA$

Symmetric or antisymmetric factored states are obtained by acting with creation operators on the vacuum (the state is not normalized, in general):

$$(21) \quad \hat{S}(N)_\pm |u_1, u_2, \dots, u_N\rangle = \frac{1}{\sqrt{N!}} \hat{c}_{|u_1\rangle}^\dagger \hat{c}_{|u_2\rangle}^\dagger \dots \hat{c}_{|u_N\rangle}^\dagger |0\rangle$$

In the formula bosonic creation operators commute, and may be exchanged. Fermionic operators anticommute, and their exchange may imply a sign change.

3. CANONICAL (ANTI)COMMUTATION RELATIONS

In most applications, creation and destruction operators are introduced in association with a complete orthonormal basis $|r\rangle$, $r = 1, 2, \dots$. For brevity we write $\hat{c}_r = \hat{c}_{|r\rangle}$ and $\hat{c}_r^\dagger = \hat{c}_{|r\rangle}^\dagger$.

- For bosons the canonical commutation relations hold:

$$(22) \quad \boxed{[\hat{b}_r, \hat{b}_s] = 0, \quad [\hat{b}_r^\dagger, \hat{b}_s^\dagger] = 0, \quad [\hat{b}_r, \hat{b}_s^\dagger] = \delta_{rs} \quad (\text{CCR})}$$

- For fermions the canonical anti-commutation relations hold:

$$(23) \quad \boxed{\{\hat{a}_r, \hat{a}_s\} = 0, \quad \{\hat{a}_r^\dagger, \hat{a}_s^\dagger\} = 0, \quad \{\hat{a}_r, \hat{a}_s^\dagger\} = \delta_{rs} \quad (\text{CAR})}$$

A *canonical transformation* of creation and destruction operators is a map to another set of operators, that preserves the CCR or CAR rules. For example, the exchange of \hat{a}_r with \hat{a}_r^\dagger is canonical (particle-hole symmetry).

The action of the operators is simple on the occupation number states $|n_1, \dots, n_\infty\rangle_\pm$ referred to the same basis $|r\rangle$. With eqs.(10) and (12), we obtain

- for Bose operators

$$\begin{aligned} \hat{b}_r^\dagger |n_1 \dots n_r \dots n_\infty\rangle &= \sqrt{\frac{N!}{n_1! \dots n_r! \dots}} \hat{b}_r^\dagger \hat{S}(N) |r_1, r_2, \dots, r_N\rangle \\ &= \sqrt{\frac{(N+1)!}{n_1! \dots n_r! \dots}} \hat{S}(N+1) |r, r_1, r_2, \dots, r_N\rangle \\ (24) \quad &= \sqrt{n_r + 1} |n_1 \dots, n_r + 1, \dots, n_\infty\rangle \\ \hat{b}_r |n_1 \dots n_r \dots n_\infty\rangle &= \sqrt{\frac{N!}{n_1! \dots n_r! \dots}} \frac{1}{\sqrt{N}} \sum_{i=1}^N \delta_{r, r_i} \hat{S}(N-1) |r_1 \dots, r_i', \dots, r_N\rangle \\ (25) \quad &= \sqrt{n_r} |n_1 \dots, n_r - 1, \dots, n_\infty\rangle \end{aligned}$$

- for Fermi operators:

$$\begin{aligned} \hat{a}_r^\dagger |n_1 \dots n_r, \dots, n_\infty\rangle &= \sqrt{N!} \sqrt{N+1} \hat{A}(N+1) |r, r_1, r_2, \dots, r_N\rangle \\ &= \sqrt{(N+1)!} (-1)^{n_1 + \dots + n_{r-1}} \hat{A}(N+1) |r_1, \dots, r, \dots, r_N\rangle \\ (26) \quad &= \begin{cases} (-1)^{n_1 + \dots + n_{r-1}} |n_1 \dots, n_r + 1, \dots, n_\infty\rangle & \text{if } n_r = 0 \\ 0 & \text{if } n_r = 1 \end{cases} \end{aligned}$$

$$(27) \quad \hat{a}_r |n_1 \dots n_r \dots n_\infty\rangle = \begin{cases} 0 & \text{if } n_r = 0 \\ (-1)^{n_1 + \dots + n_{r-1}} |n_1 \dots, n_r - 1, \dots, n_\infty\rangle & \text{if } n_r = 1 \end{cases}$$

$(-1)^{n_1 + \dots + n_{r-1}}$ counts the exchanges that bring the vector $|r, r_1 \dots r_N\rangle$ to the vector with $r_1 < \dots < r < \dots < r_N$.

The operators $\hat{n}_r = \hat{b}_r^\dagger \hat{b}_r$ and $\hat{n}_r = \hat{a}_r^\dagger \hat{a}_r$ are the occupation numbers of state $|r\rangle$:

$$(28) \quad \hat{n}_r |n_1 \dots n_r \dots n_\infty\rangle = n_r |n_1 \dots n_r \dots n_\infty\rangle$$

In the basis $|r\rangle$, the following are normalized occupation number vectors:

$$(29) \quad |n_1, n_2, \dots, n_\infty\rangle = \frac{1}{\sqrt{n_1! \dots n_\infty!}} \hat{b}_1^{\dagger n_1} \dots \hat{b}_\infty^{\dagger n_\infty} |0\rangle \quad (\text{bosons})$$

$$(30) \quad |n_1, n_2, \dots, n_\infty\rangle = \hat{a}_1^{\dagger n_1} \dots \hat{a}_\infty^{\dagger n_\infty} |0\rangle \quad (\text{fermions})$$

For Fermi statistics $n_i = 0, 1$; a change of the order of the operators may produce a sign.

Exercise 3.1. Prove for fermions: the number operators commute, the eigenvalues of \hat{n}_r are 0, 1.

3.1. Field operators. The formalism is extended to operators that create and destroy particles in states belonging to a continuum basis. An important example is the single particle basis of position \mathbf{x} and spin s_z

$$\sum_m \int d\mathbf{x} |\mathbf{x}, m\rangle \langle \mathbf{x}, m| = I, \quad \langle \mathbf{x}, m | \mathbf{x}', m' \rangle = \delta_{mm'} \delta_3(\mathbf{x} - \mathbf{x}')$$

The operators that create or destroy a particle in the (unphysical) states $|\mathbf{x}, m\rangle$ are named *field operators*. In place of the symbols $\hat{c}_{|\mathbf{x}, m\rangle}$ and $\hat{c}_{|\mathbf{x}, m\rangle}^\dagger$, it is customary to use the symbols $\hat{\psi}_m(\mathbf{x})$ and $\hat{\psi}_m^\dagger(\mathbf{x})$.

For bosons:

$$(31) \quad [\hat{\psi}_m(\mathbf{x}), \hat{\psi}_{m'}^\dagger(\mathbf{x}')] = \delta_3(\mathbf{x} - \mathbf{x}') \delta_{m, m'}$$

$$(32) \quad [\hat{\psi}_m(\mathbf{x}), \hat{\psi}_{m'}(\mathbf{x}')] = 0, \quad [\hat{\psi}_m^\dagger(\mathbf{x}), \hat{\psi}_{m'}^\dagger(\mathbf{x}')] = 0$$

For fermions:

$$(33) \quad \{\hat{\psi}_m(\mathbf{x}), \hat{\psi}_{m'}^\dagger(\mathbf{x}')\} = \delta_3(\mathbf{x} - \mathbf{x}') \delta_{m, m'}$$

$$(34) \quad \{\hat{\psi}_m(\mathbf{x}), \hat{\psi}_{m'}(\mathbf{x}')\} = 0, \quad \{\hat{\psi}_m^\dagger(\mathbf{x}), \hat{\psi}_{m'}^\dagger(\mathbf{x}')\} = 0$$

Given the one-particle state $|u\rangle$ and the function $u(\mathbf{x}, m) = \langle \mathbf{x}, m | u \rangle$, one has the expansions

$$(35) \quad \hat{c}_{|u\rangle} = \sum_m \int d\mathbf{x} \langle u | \mathbf{x}, m \rangle \hat{\psi}_m(\mathbf{x}), \quad \hat{c}_{|u\rangle}^\dagger = \sum_m \int d\mathbf{x} \langle \mathbf{x}, m | u \rangle \hat{\psi}_m^\dagger(\mathbf{x})$$

On the other hand, given a single particle basis $|r\rangle$:

$$(36) \quad \hat{\psi}_m(\mathbf{x}) = \sum_r \langle \mathbf{x}, m | r \rangle \hat{c}_r, \quad \hat{\psi}_m^\dagger(\mathbf{x}) = \sum_r \langle r | \mathbf{x}, m \rangle \hat{c}_r^\dagger$$

Let's introduce the operators that create and destroy a particle in eigenstates of \mathbf{p} and s_z : $\mathbf{p}|\mathbf{k}, m\rangle = \hbar\mathbf{k}|\mathbf{k}, m\rangle$ and $s_z|\mathbf{k}, m\rangle = \hbar m|\mathbf{k}, m\rangle$. In a box of volume $V = L^3$ with periodic b.c. the eigenstates form a discrete basis ($\mathbf{k} = (2\pi/L)\mathbf{n}$, $\mathbf{n} \in \mathbb{Z}^3$). We associate them to the canonical operators $\hat{c}_{\mathbf{k}m}^\dagger$ and $\hat{c}_{\mathbf{k}m}$. Then, for example:

$$(37) \quad \hat{c}_{\mathbf{k}m} = \int_V \frac{d\mathbf{x}}{\sqrt{V}} e^{-i\mathbf{k} \cdot \mathbf{x}} \hat{\psi}_m(\mathbf{x}), \quad \hat{\psi}_m(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}} \hat{c}_{\mathbf{k}m}$$

In the infinite volume, the basis $|\mathbf{k}, m\rangle$ is continuous, and we associate to it the field operators $\hat{\psi}_m^\dagger(\mathbf{k})$ and $\hat{\psi}_m(\mathbf{k})$. It is:

$$(38) \quad \hat{\psi}_m(\mathbf{k}) = \int \frac{d\mathbf{x}}{(2\pi)^{3/2}} e^{-i\mathbf{k}\cdot\mathbf{x}} \hat{\psi}_m(\mathbf{x}), \quad \hat{\psi}_m(\mathbf{x}) = \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{\psi}_m(\mathbf{k})$$

4. SECOND QUANTIZATION OF OPERATORS

The action of creation operators on the vacuum state gives factored states, that generate the Fock spaces. For this reason creation and destruction operators associated to a basis, are a basis of operators on \mathcal{F}_\pm .

The operators associated to the observables of identical particles commute with the projectors $S(N)_\pm$, and leave the subspaces $\mathcal{H}(N)_\pm$ invariant. In this section, they are expanded in creation and destruction operators.

The proof of the following identity is left to the reader. If $|u\rangle$ and $|v\rangle$ are any two single-particle states, for any factored state:

$$(39) \quad \hat{c}_{|u\rangle}^\dagger \hat{c}_{|v\rangle} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle = \sum_{j=1}^N \langle v|u_j\rangle \hat{S}(N)_\pm |u_1, \dots, u, \dots, u_N\rangle$$

(in the right-hand side, the vector $|u\rangle$ replaces the vector $|u_j\rangle$). The iteration of the formula with new vectors $|u'\rangle$ and $|v'\rangle$ gives:

$$\begin{aligned} \hat{c}_{|u\rangle}^\dagger \hat{c}_{|v\rangle} \hat{c}_{|u'\rangle}^\dagger \hat{c}_{|v'\rangle} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle &= \sum_{j=1..N} \langle v'|u_j\rangle \hat{c}_{|u\rangle}^\dagger \hat{c}_{|v\rangle} \hat{S}(N)_\pm |u_1, \dots, u', \dots, u_N\rangle \\ &= \langle v|u'\rangle \sum_{j=1..N} \langle v'|u_j\rangle \hat{S}(N)_\pm |u_1, \dots, u, \dots, u_N\rangle \\ &\quad + \sum_{j \neq k} \langle v'|u_j\rangle \langle v|u_k\rangle \hat{S}(N)_\pm |u_1, \dots, u', \dots, u, \dots, u_N\rangle \end{aligned}$$

In the last line u replaces u_k and u' replaces u_j . The term with a single sum is $\langle v|u'\rangle \hat{c}_{|u\rangle}^\dagger \hat{c}_{|v'\rangle} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle$.

An exchange of operators by means of $\langle v|u'\rangle = c_{|v\rangle} c_{|u'\rangle}^\dagger \mp c_{|u'\rangle}^\dagger c_{|v\rangle}$ gives

$$\begin{aligned} &\hat{c}_{|u\rangle}^\dagger \hat{c}_{|u'\rangle}^\dagger \hat{c}_{|v'\rangle} \hat{c}_{|v\rangle} \hat{S}(N)_\pm |u_1, \dots, u_N\rangle \\ &= \pm (\hat{c}_{|u\rangle}^\dagger \hat{c}_{|v\rangle} \hat{c}_{|u'\rangle}^\dagger \hat{c}_{|v'\rangle} - \langle v|u'\rangle \hat{c}_{|u\rangle}^\dagger \hat{c}_{|v'\rangle}) \hat{S}(N)_\pm |u_1, \dots, u_N\rangle \\ &= \pm \sum_{j \neq k} \langle v|u_j\rangle \langle v'|u_k\rangle \hat{S}(N)_\pm |u_1, \dots, u', \dots, u, \dots, u_N\rangle \\ (40) \quad &= \sum_{j \neq k} \langle v|u_j\rangle \langle v'|u_k\rangle \hat{S}(N)_\pm |u_1, \dots, u, \dots, u', \dots, u_N\rangle \end{aligned}$$

In the last line, u and u' replace u_j and u_k .

4.1. One-particle operators. They are sums of N identical operators acting on 1-particle subspaces, $\hat{A} = \sum_{k=1}^N \hat{a}(k)$, where $\hat{a}(\cdot)$ is a function of the fundamental 1-particle operators (e.g. position, momentum and spin).

Upon insertion of two resolutions of the identity (not necessarily with same basis):

$$\begin{aligned}
\hat{A}\hat{S}(N)_\pm|u_1, \dots, u_N\rangle &= \hat{S}(N)_\pm \sum_{k=1..N} |u_1, \dots, \hat{a}u_k, \dots, u_N\rangle \\
&= \hat{S}(N)_\pm \sum_r \sum_{k=1..N} \langle r|\hat{a}|u_k\rangle |u_1, \dots, r, \dots, u_N\rangle \\
&= \sum_{r,s} \langle r|\hat{a}|s\rangle \sum_{k=1..N} \langle s|u_k\rangle S(N)_\pm|u_1, \dots, r, \dots, u_N\rangle
\end{aligned}$$

The last line is compared with (39) and, since the vectors $S(N)_\pm|u_1 \dots u_N\rangle$ generate the Fock spaces:

$$(41) \quad \boxed{\hat{A} = \sum_{r,s} \hat{c}_r^\dagger \langle r|\hat{a}|s\rangle \hat{c}_s}$$

If the basis vectors are eigenvectors of the single particle operator \hat{a} with eigenvalues α_r , the expansion is simple and suggestive: $\hat{A} = \sum_r \alpha_r \hat{n}_r$. $\hat{n}_r = \hat{c}_r^\dagger \hat{c}_r$ is the occupation number operator of the state $|r\rangle$.

In the continuous basis of position-spin, the expansion reads:

$$(42) \quad \hat{A} = \sum_{mm'} \int d\mathbf{x} d\mathbf{x}' \hat{\psi}_m^\dagger(\mathbf{x}) \langle \mathbf{x}m|\hat{a}|\mathbf{x}'m'\rangle \hat{\psi}_{m'}(\mathbf{x}')$$

For local operators it is $\langle \mathbf{x}, m|\hat{a}|\mathbf{x}'m'\rangle = \delta_3(\mathbf{x} - \mathbf{x}') a_{m,m'}(\mathbf{x})$. A notable example is the *particle density* operator:

$$(43) \quad \hat{n}(\mathbf{x}) = \sum_{i=1}^N \delta_3(\mathbf{x} - \mathbf{x}_i) = \sum_m \hat{\psi}_m^\dagger(\mathbf{x}) \hat{\psi}_m(\mathbf{x})$$

In the basis $|\mathbf{k}, m\rangle$ (in a box) the kinetic energy operator is diagonal, while in the basis $|\mathbf{x}, m\rangle$ it recalls a 1-particle expectation value

$$(44) \quad \hat{T} = \sum_{i=1}^N \frac{\hat{\mathbf{p}}_i^2}{2m} = \sum_{\mathbf{k}, m} \frac{\hbar^2 k^2}{2m} \hat{c}_{\mathbf{k}, m}^\dagger \hat{c}_{\mathbf{k}, m} = -\frac{\hbar^2}{2m} \sum_m \int d\mathbf{x} \hat{\psi}_m^\dagger(\mathbf{x}) \nabla^2 \hat{\psi}_m(\mathbf{x})$$

4.2. Two-particle operators. The operators are the sum of identical two-particle operators: $\hat{V} = \frac{1}{2} \sum_{i \neq j} v(i, j)$ where $v(i, j) = v(j, i)$. The symmetry implies the exchange symmetry of matrix elements on 2-particle states

$$\langle 1, 2|v|1', 2'\rangle = \langle 2, 1|v|2', 1'\rangle$$

Let us evaluate

$$\begin{aligned}
\hat{V}\hat{S}(N)_\pm|u_1, \dots, u_N\rangle &= \frac{1}{2} \hat{S}(N)_\pm \sum_{i \neq j} v(i, j) |u_1, \dots, u_i, \dots, u_j, \dots, u_N\rangle \\
&= \frac{1}{2} \sum_{r,s;r',s'} \langle r, s|v|r', s'\rangle \sum_{i \neq j} \langle r'|u_i\rangle \langle s'|u_j\rangle S(N)_\pm|u_1, \dots, r, \dots, s, \dots, u_N\rangle
\end{aligned}$$

After using (40) we obtain the following expression:

$$(45) \quad \boxed{\hat{V} = \frac{1}{2} \sum_{r,s,r',s'} \hat{c}_r^\dagger \hat{c}_s^\dagger \langle r, s|v|r', s'\rangle \hat{c}_{s'} \hat{c}_{r'}}$$

(note the order of the destruction operators, which is opposite to that of the ket states in the matrix element). If field operators are used:

$$(46) \quad \hat{V} = \frac{1}{2} \sum_{m_i} \int d\mathbf{x}_1 \dots d\mathbf{x}_4 \hat{\psi}_{m_1}^\dagger(\mathbf{x}_1) \hat{\psi}_{m_2}^\dagger(\mathbf{x}_2) \langle \mathbf{x}_1 m_1, \mathbf{x}_2 m_2 | v | \mathbf{x}_3 m_3, \mathbf{x}_4 m_4 \rangle \hat{\psi}_{m_4}(\mathbf{x}_4) \hat{\psi}_{m_3}(\mathbf{x}_3)$$

The notation can be significantly simplified:

$$\hat{V} = \frac{1}{2} \int d(1234) \hat{\psi}^\dagger(1) \hat{\psi}^\dagger(2) \langle 1, 2 | v | 3, 4 \rangle \hat{\psi}(4) \hat{\psi}(3)$$

If v only depends on the positions of the two particles:

$$\begin{aligned} \langle \mathbf{x}_1 m_1, \mathbf{x}_2 m_2 | v | \mathbf{x}_3 m_3, \mathbf{x}_4 m_4 \rangle &= v(\mathbf{x}_3, \mathbf{x}_4) \langle \mathbf{x}_1 m_1, \mathbf{x}_2 m_2 | \mathbf{x}_3 m_3, \mathbf{x}_4 m_4 \rangle = \\ &= v(\mathbf{x}_3, \mathbf{x}_4) \delta_3(\mathbf{x}_1 - \mathbf{x}_3) \delta_3(\mathbf{x}_2 - \mathbf{x}_4) \delta_{m_1, m_3} \delta_{m_2, m_4} \end{aligned}$$

The operator gains a form similar to a first-quantized expectation value:

$$(47) \quad \boxed{\hat{V} = \frac{1}{2} \sum_{m, m'} \int d\mathbf{x} d\mathbf{x}' \hat{\psi}_m^\dagger(\mathbf{x}) \hat{\psi}_{m'}^\dagger(\mathbf{x}') v(\mathbf{x}, \mathbf{x}') \hat{\psi}_{m'}(\mathbf{x}') \hat{\psi}_m(\mathbf{x})}$$

Remark 4.1. In second-quantized form, operators share some general properties:

- there is no dependence on the total number N of particles: the operators act on the Fock space, and have the same expression for any N ;
- if the numbers of creation and destruction operators are the same, they leave the subspaces of N identical particles invariant;
- they are normally ordered, with destruction operators at the right of creation operators. As a consequence, the expectation value of the operator on the vacuum state (zero particle) is zero.

Exercise 4.2. Given $\hat{H} = \sum_{rs} h_{rs} \hat{c}_r^\dagger \hat{c}_s$, which is the transformation that diagonalizes the Hamiltonian? Study the Hamiltonian $\hat{H} = -t \sum_r (\hat{c}_r^\dagger \hat{c}_{r+1} + \hat{c}_r^\dagger \hat{c}_{r-1})$.

5. SYMMETRIES

A unitary operator \mathbf{u} on one-particle states in \mathcal{H} defines a unitary operator on $\mathcal{H}(N)$: $\hat{\mathbf{U}}_N = \mathbf{u} \otimes \mathbf{u} \otimes \dots \otimes \mathbf{u}$. $\hat{\mathbf{U}}_N$ commutes with exchange operators and leaves the subspaces $\mathcal{H}(N)_\pm$ invariant. The unitary operator on Fock spaces is $\hat{\mathbf{U}} = \mathbf{I} \oplus \mathbf{u} \oplus \hat{\mathbf{U}}_2 \oplus \dots \oplus \hat{\mathbf{U}}_N \oplus \dots$

Proposition 5.1. A one-particle unitary operator \mathbf{u} induces a canonical transformation on creation and destruction operators:

$$(48) \quad \hat{\mathbf{U}}^\dagger \hat{c}_{|v}^\dagger \hat{\mathbf{U}} = \hat{c}_{|\mathbf{u}^\dagger v}^\dagger, \quad \hat{\mathbf{U}}^\dagger \hat{c}_{|v} \hat{\mathbf{U}} = \hat{c}_{\langle \mathbf{u}^\dagger v |}$$

Proof. $\hat{\mathbf{U}}^\dagger \hat{c}_{|v}^\dagger \hat{\mathbf{U}} \hat{S}(N)_\pm |v_1, \dots, v_N\rangle = \hat{\mathbf{U}}^\dagger \hat{c}_{|v}^\dagger \hat{S}(N)_\pm |u v_1, \dots, u v_N\rangle$
 $= \sqrt{N+1} \hat{\mathbf{U}}^\dagger \hat{S}(N+1)_\pm |v, u v_1, \dots, u v_N\rangle = \sqrt{N+1} \hat{S}(N+1)_\pm |u^\dagger v, v_1, \dots, v_N\rangle$
 $= \hat{c}_{|\mathbf{u}^\dagger v}^\dagger \hat{S}(N)_\pm |v_1, \dots, v_N\rangle.$

The second relation follows by adjunction. \square

We present the unitary representations of space translations, rotations, dilations and parity on Fock space. They are important in the study of correlators.

5.1. Space translations. For one particle, translations are represented by the unitary group $u(\mathbf{a})$ with the following action on position, momentum and spin operators:

$$u^\dagger(\mathbf{a})\mathbf{x}u(\mathbf{a}) = \mathbf{x} + \mathbf{a}, \quad u^\dagger(\mathbf{a})\mathbf{p}u(\mathbf{a}) = \mathbf{p}, \quad u^\dagger(\mathbf{a})\mathbf{s}u(\mathbf{a}) = \mathbf{s}$$

They imply $u(\mathbf{a}) = \exp(-\frac{i}{\hbar}\mathbf{a} \cdot \mathbf{p})$ and the following transformations of eigenvectors

$$(49) \quad u(\mathbf{a})|\mathbf{x}, m\rangle = |\mathbf{x} + \mathbf{a}, m\rangle, \quad u(\mathbf{a})|\mathbf{k}, m\rangle = e^{-i\mathbf{k} \cdot \mathbf{a}}|\mathbf{k}, m\rangle$$

On \mathcal{F}_\pm translations are represented by the unitary operators

$$(50) \quad \hat{U}(\mathbf{a}) = \exp(-\frac{i}{\hbar}\mathbf{a} \cdot \mathbf{P}), \quad \mathbf{P} = \sum_{\mathbf{k}, m} \hbar \mathbf{k} \hat{c}_{\mathbf{k}m}^\dagger \hat{c}_{\mathbf{k}m}$$

with action:

$$(51) \quad \hat{U}(\mathbf{a})^\dagger \hat{\psi}_m^\dagger(\mathbf{x}) \hat{U}(\mathbf{a}) = \hat{\psi}_m^\dagger(\mathbf{x} - \mathbf{a}), \quad \hat{U}(\mathbf{a})^\dagger \hat{\psi}_m(\mathbf{x}) \hat{U}(\mathbf{a}) = \hat{\psi}_m(\mathbf{x} - \mathbf{a})$$

$$(52) \quad \hat{U}(\mathbf{a})^\dagger \hat{c}_{\mathbf{k}m}^\dagger \hat{U}(\mathbf{a}) = e^{i\mathbf{k} \cdot \mathbf{a}} \hat{c}_{\mathbf{k}m}^\dagger, \quad \hat{U}(\mathbf{a})^\dagger \hat{c}_{\mathbf{k}m} \hat{U}(\mathbf{a}) = e^{-i\mathbf{k} \cdot \mathbf{a}} \hat{c}_{\mathbf{k}m}.$$

5.2. Rotations. On the Hilbert space of a particle with spin, space rotations act as unitary operators specified by the vector transformation of the fundamental operators:

$$u(R)^\dagger x_i u(R) = R_{ij} x_j, \quad u(R)^\dagger p_i u(R) = R_{ij} p_j, \quad u(R)^\dagger s_i u(R) = R_{ij} s_j$$

The infinitesimal transformations yield the commutation rules of \mathbf{x} , \mathbf{p} , \mathbf{s} with the generator (angular momentum) $j_k = \epsilon_{ijk} x_i p_j + s_k$. The action on basis vectors is

$$u(R)|\mathbf{x}, m\rangle = \sum_{m'} D(R)_{m'm} |R\mathbf{x}, m'\rangle, \quad u(R)|\mathbf{k}, m\rangle = \sum_{m'} D(R)_{m'm} |R\mathbf{k}, m'\rangle$$

where $D(R)$ is a unitary representation of rotations, of dimension $2s+1$, generated by the spin matrices.

To the single-particle representation there corresponds a representation on Fock space, where the generator is the total angular momentum. The field operators transform as follows:

$$(53) \quad \hat{U}(R)^\dagger \hat{\psi}_m^\dagger(\mathbf{x}) \hat{U}(R) = \sum_{m'} \hat{\psi}_{m'}^\dagger(R^{-1}\mathbf{x}) D(R)_{m'm}^\dagger$$

$$(54) \quad \hat{U}(R)^\dagger \hat{\psi}_m(\mathbf{x}) \hat{U}(R) = \sum_{m'} D(R)_{mm'} \hat{\psi}_{m'}(R^{-1}\mathbf{x})$$

The same relations hold for the field operators in the basis of momentum.

5.3. Dilations. Dilations, or scale transformations, are here illustrated in the isotropic case. They form a 1-parameter group of unitary transformations $u(t)$ with the following action on fundamental operators:

$$(55) \quad u(t)^\dagger x_i u(t) = e^t x_i, \quad u(t)^\dagger p_i u(t) = e^{-t} p_i, \quad u(t)^\dagger s_i u(t) = s_i$$

and on position and momentum eigenvectors

$$u(t)|\mathbf{x}, m\rangle = e^{\frac{3}{2}t} |e^t \mathbf{x}, m\rangle, \quad u(t)|\mathbf{k}, m\rangle = e^{-\frac{3}{2}t} |e^{-t} \mathbf{k}, m\rangle$$

With $u(t) = \exp(-itD)$, from (55) one obtains the generator $D = \frac{1}{2\hbar}(\mathbf{x} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{x})$. The representation on Fock space has action:

$$(56) \quad \hat{U}(t)^\dagger \hat{\psi}_m^\dagger(\mathbf{x}) \hat{U}(t) = e^{-\frac{3}{2}t} \hat{\psi}_m^\dagger(e^{-t}\mathbf{x}) \quad \hat{U}(t)^\dagger \hat{\psi}_m(\mathbf{x}) \hat{U}(t) = e^{-\frac{3}{2}t} \hat{\psi}_m(e^{-t}\mathbf{x})$$

$$(57) \quad \hat{U}(t)^\dagger \hat{\psi}_m^\dagger(\mathbf{k}) \hat{U}(t) = e^{\frac{3}{2}t} \hat{\psi}_m^\dagger(e^t \mathbf{k}) \quad \hat{U}(t)^\dagger \hat{\psi}_m(\mathbf{k}) \hat{U}(t) = e^{\frac{3}{2}t} \hat{\psi}_m(e^t \mathbf{k})$$

Theorem 5.2 (Virial theorem). *Let $\hat{H} = \sum_i \hat{H}_i$, where $\hat{U}(t)^\dagger \hat{H}_i \hat{U}(t) = e^{n_i t} \hat{H}_i$. If $|E\rangle$ is an eigenstate of \hat{H} , then*

$$(58) \quad \sum_i n_i \langle E | \hat{H}_i | E \rangle = 0.$$

Proof. From $\hat{U}^\dagger(t) \hat{H} |E\rangle = E \hat{U}^\dagger(t) |E\rangle$ one obtains: $\sum_i e^{n_i t} \hat{H}_i \hat{U}^\dagger(t) |E\rangle = E \hat{U}^\dagger(t) |E\rangle$. A derivative in $t = 0$ gives $\sum_i n_i \hat{H}_i |E\rangle + i \hat{H} \hat{D} |E\rangle = i E \hat{D} |E\rangle$. The inner product with $|E\rangle$ gives the result. \square

Example 5.3 (Coulomb Hamiltonian). $\hat{H} = \hat{T} + \hat{U}$, $\hat{T} = \frac{1}{2m} \sum_{i=1}^n \mathbf{p}_i^2$, $\hat{U} = e^2 \sum_{i < j} |\mathbf{x}_i - \mathbf{x}_j|^{-1}$. For a scale transformation the kinetic term has weight $n_T = -2$ while the Coulomb interaction has weight $n_U = -1$. Then $\langle E | \hat{T} | E \rangle = -\frac{1}{2} \langle E | \hat{U} | E \rangle$.

5.4. Parity. Parity is the unitary self-adjoint operator π defined by the properties: $\pi x_i \pi = -x_i$, $\pi p_i \pi = -p_i$ and $\pi s_i \pi = s_i$. They imply $\pi |\mathbf{x}, m\rangle = |-\mathbf{x}, m\rangle$ and $\pi |\mathbf{k}, m\rangle = |-\mathbf{k}, m\rangle$. The corresponding unitary operator on Fock space is

$$(59) \quad \hat{U}_\pi^\dagger \hat{\psi}_m^\dagger(\mathbf{x}) \hat{U}_\pi = \hat{\psi}_m^\dagger(-\mathbf{x}), \quad \hat{U}_\pi^\dagger \hat{\psi}_m(\mathbf{x}) \hat{U}_\pi = \hat{\psi}_m(-\mathbf{x})$$

$$(60) \quad \hat{U}_\pi^\dagger \hat{\psi}_m^\dagger(\mathbf{k}) \hat{U}_\pi = \hat{\psi}_m^\dagger(-\mathbf{k}), \quad \hat{U}_\pi^\dagger \hat{\psi}_m(\mathbf{k}) \hat{U}_\pi = \hat{\psi}_m(-\mathbf{k}).$$