Introduction to Quantum Physics

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Abstract

The video channel with the title "Professor M does Science" in YouTube offers a simple step-by-step but all the same very valuable and rigorous introduction into the world of quantum physics. This script covers the physics of identical particles and helps to digest the topic covered by a group of those videos but is not meant as a replacement for them.

7 Creation and Annihilation of Identical Particles

7.1 Identical Particles

Particles are identical if they have the same name. Thus, all electrons are identical but electrons and photons are different particles. Exchanging any two identical particles in a system leads to exactly the same physics. In classical physics identical particles are distinguishable but in quantum physics they are not. More formal, two particles are *identical* if their defining intrinsic properties are the same. Intrinsic properties are mass, charge, spin, magnetic moment and so on. All electrons are identical because they have the same mass, charge and spin. Similarly, all muons are identical because they have the same mass, charge and spin. However, electrons and muons are not the same because the have the same charge and spin but not the same mass. Also the electron and the positron are not the same because they have the same mass and spin but not the same charge. The definition of identical particles does not only apply to elementary particles but also to protons consisting of quarks and hydrogen atoms consisting of quarks and electrons.

The fact that two electrons are identical does not mean that they are in the same quantum state. Two electrons, for example, may move with different momenta, or one may be bound in a hydrogen atom while the other is free. Exchanging two identical particles does not affect the properties of the system.

In classical physics two identical particles are distinguishable because one knows the exact paths of them such that one can say where each particle is at any point in time. In quantum physics the situation is different because it is impossible to know the exact trajectories of particles. Two wave packets initially separated in space overlap during a collision. If a detector detects one of them moving in one direction then the other must move in the opposite direction in the center of mass frame. However, one does not know which particle is which because after an overlap they are no longer distinguishable. This is a fundamental result and not a limitation of the measuring equipment.

7.2 Tensor Products

If one wants to describe more than one particle in three dimensions, tensor products of vector spaces are needed. The *tensor product* of the vector spaces $\mathcal{V}_1$ and $\mathcal{V}_2$ is written as $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ and states that for every vector $|\psi\rangle \in \mathcal{V}_1$ and every vector $|\varphi\rangle \in \mathcal{V}_2$ there is a vector $|\psi\rangle_1 \otimes |\varphi\rangle_2 \in \mathcal{V}$ where the tensor product obeys the properties:

(1) It is linear with respect to scalar multiplication such that
$a(|\psi\rangle_1 \otimes |\varphi\rangle_2) = (a\,|\psi\rangle_1) \otimes |\varphi\rangle_2 = |\psi\rangle_1 \otimes (a\,|\varphi\rangle_2)$ for $a \in \mathbb{C}$.
(2) It is distributive with respect to vector addition such that
$(|\psi_1\rangle_1 + |\psi_2\rangle_1) \otimes |\varphi\rangle_2 = |\psi_1\rangle_1 \otimes |\varphi\rangle_2 + |\psi_2\rangle_1 \otimes |\varphi\rangle_2$ and
$|\psi\rangle_1 \otimes (|\varphi_1\rangle_2 + |\varphi_2\rangle_2) = |\psi\rangle_1 \otimes |\varphi_1\rangle_2 + |\psi\rangle_1 \otimes |\varphi_2\rangle_2$.

(Note that $|\psi\rangle_1 \otimes |\varphi\rangle_2 = |\varphi\rangle_2 \otimes |\psi\rangle_1$ because of the indices.)

Given a basis $\{|u_j\rangle\}$ in $\mathcal{V}_1$ of dimension N_1 and a basis $\{|v_k\rangle\}$ in $\mathcal{V}_2$ of dimension N_2, $\{|u_j\rangle_1 \otimes |v_k\rangle_2\}$ is a basis in $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ of dimension $N_1 \cdot N_2$. A general vector $|\psi\rangle_1 \otimes |\varphi\rangle_2 \in \mathcal{V}$ becomes

$$\left.\begin{aligned} |\psi\rangle &= \sum_j c_j\,|u_j\rangle \\ |\varphi\rangle &= \sum_k d_k\,|v_k\rangle \end{aligned}\right\} \Rightarrow \qquad |\psi\rangle_1 \otimes |\varphi\rangle_2 = \left(\sum_j c_j\,|u_j\rangle_1\right) \otimes \left(\sum_k d_k\,|v_k\rangle_2\right) = \sum_{jk} c_j\,d_k\,|u_j\rangle_1 \otimes |v_k\rangle_2$$

where $c_j\,d_k$ are the expansion coefficients. An arbitrary vector $|\chi\rangle \in \mathcal{V}$ can be written as

$$|\chi\rangle = \sum_{jk} a_{jk}\,|u_j\rangle_1 \otimes |v_k\rangle_2$$

and the question arises whether $|\chi\rangle$ can always be decomposed as a product $|\psi\rangle_1 \otimes |\varphi\rangle_2$ where $|\psi\rangle \in \mathcal{V}_1$ and $|\varphi\rangle \in \mathcal{V}_2$. The equality $a_{jk} = c_j\,d_k$ for the coefficients would have to be satisfied. The answer is no as

$$\left.\begin{aligned} |\psi\rangle &= c_1\,|u_1\rangle + c_2\,|u_2\rangle \\ |\varphi\rangle &= d_1\,|v_1\rangle + d_2\,|v_2\rangle \end{aligned}\right\} \qquad |\psi\rangle_1 \otimes |\varphi\rangle_2 = \left\{\begin{array}{l} c_1d_1\,|u_1\rangle_1 \otimes |v_1\rangle_2 + c_1d_2\,|u_1\rangle_1 \otimes |v_2\rangle_2 + \\ c_2d_1\,|u_2\rangle_1 \otimes |v_1\rangle_2 + c_2d_2\,|u_2\rangle_1 \otimes |v_2\rangle_2 \end{array}\right.$$

with

$$\begin{aligned} |\chi\rangle &= a_{11}\,|u_1\rangle_1 \otimes |v_1\rangle_2 + a_{12}\,|u_1\rangle_1 \otimes |v_2\rangle_2 + a_{21}\,|u_2\rangle_1 \otimes |v_1\rangle_2 + a_{22}\,|u_2\rangle_1 \otimes |v_2\rangle_2 \\ &\stackrel{?}{=} \frac{1}{\sqrt{2}}\Big(\,|u_1\rangle_1 \otimes |v_1\rangle_2 - |u_2\rangle_1 \otimes |v_2\rangle_2\Big) \end{aligned}$$

shows because $a_{11} = c_1d_1 = 1/\sqrt{2}$, $a_{12} = c_1d_2 = a_{21} = c_2d_1 = 0$, $a_{22} = c_2d_2 = -1/\sqrt{2}$ is not possible as two values among c_1, c_2, d_1, d_2 must be zero. States like $1/\sqrt{2}\,(|u_1\rangle_1 \otimes |v_1\rangle_2 - |u_2\rangle_1 \otimes |v_2\rangle_2)$ are called *entangled* and play an important role in quantum mechanics.

The scalar product of $|\psi\rangle_1 \otimes |\varphi\rangle_2\,, |\psi'\rangle_1 \otimes |\varphi'\rangle_2 \in \mathcal{V}$ with $|\psi\rangle\,, |\psi'\rangle \in \mathcal{V}_1$ and $|\varphi\rangle\,, |\varphi'\rangle \in \mathcal{V}_2$ is defined as

$$\big(\,{}_1\langle\psi| \otimes {}_2\langle\varphi|\,\big)\big(\,|\psi'\rangle_1 \otimes |\varphi'\rangle_2\,\big) = \big(\,{}_1\langle\psi|\psi'\rangle_1\,\big)\big(\,{}_2\langle\varphi|\varphi'\rangle_2\,\big)$$

and with $\{|u_j\rangle\} \in \mathcal{V}_1$ such that $\langle u_j|u_m\rangle = \delta_{jm}$ and with $\{|v_k\rangle\} \in \mathcal{V}_2$ such that $\langle v_k|v_n\rangle = \delta_{kn}$

$$\big(\,{}_1\langle u_j| \otimes {}_2\langle v_k|\,\big)\big(\,|u_m\rangle_1 \otimes |v_n\rangle_2\,\big) = \big(\,{}_1\langle u_j|u_m\rangle_1\,\big)\big(\,{}_2\langle v_k|v_n\rangle_2\,\big) = \delta_{jm}\delta_{kn}$$

proves that the basis $\{|u_j\rangle_1 \otimes |v_k\rangle_2\}$ is also orthonormal.

The next question is how the tensor product $\hat{A}_1 \otimes \hat{B}_2$ of an operator $\hat{A}_1$ acting on $\mathcal{V}_1$ and an operator $\hat{B}_2$ acting on $\mathcal{V}_2$ act on $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$. Defining

$$\big(\hat{A}_1 \otimes \hat{B}_2\big)\big(\,|\psi\rangle_1 \otimes |\varphi\rangle_2\,\big) = \big(\hat{A}_1\,|\psi\rangle_1\,\big) \otimes \big(\hat{B}_2\,|\varphi\rangle_2\,\big) \tag{7.1}$$

such that the operators only act on the states in their own state space does not yet cover entangled states but

$$\begin{aligned} \big(\hat{A}_1 \otimes \hat{B}_2\big)\,|\chi\rangle = \big(\hat{A}_1 \otimes \hat{B}_2\big) \sum_{jk} a_{jk}\,|u_j\rangle_1 \otimes |v_k\rangle_2 &= \sum_{jk} a_{jk}\big(\hat{A}_1 \otimes \hat{B}_2\big)\,|u_j\rangle_1 \otimes |v_k\rangle_2 \\ &= \sum_{jk} a_{jk}\big(\hat{A}_1\,|u_j\rangle_1\,\big) \otimes \big(\hat{B}_2\,|v_k\rangle_2\,\big) \end{aligned}$$

covers all states $|\chi\rangle = \sum_{jk} a_{jk} |u_j\rangle_1 \otimes |v_k\rangle_2$ in $\mathcal{V}_1 \otimes \mathcal{V}_2$. An operator $\hat{A}_1$ acting on $\mathcal{V}_1$ acts on $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ as $\hat{A}_1 \otimes \mathbb{I}_2$ such that

$$\big(\hat{A}_1 \otimes \mathbb{I}_2\big) |u_j\rangle_1 \otimes |v_k\rangle_2 = \big(\hat{A}_1 |u_j\rangle_1\big) \otimes \big(\mathbb{I}_2 |v_k\rangle_2\big) = \big(\hat{A}_1 |u_j\rangle_1\big) \otimes |v_k\rangle_2$$

and $|v_k\rangle_2$ is left untouched. Similarly, an operator $\hat{B}_2$ acting on $\mathcal{V}_2$ acts on $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ as $\mathbb{I}_1 \otimes \hat{B}_2$ and leaves vectors in $\mathcal{V}_1$ untouched.

Notation is often simplified. Instead of $|\psi\rangle_1 \otimes |\varphi\rangle_2$ one simply writes $|\psi\rangle_1 |\varphi\rangle_2$ or even $|\psi\rangle |\varphi\rangle$ and $|\psi, \varphi\rangle$ where it is assumed that the first vector belongs to the first vector space and the second to the second one. As an example, the three vector spaces $\mathcal{V}_1$ for x, $\mathcal{V}_2$ for y, $\mathcal{V}_3$ for z as the tensor product $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2 \otimes \mathcal{V}_3$ should contain vectors $|x\rangle_1 \otimes |y\rangle_2 \otimes |z\rangle_3$ but they are usually written in one of the forms $|x\rangle_1 |y\rangle_2 |z\rangle_3$, $|x\rangle |y\rangle |z\rangle$, $|x, y, z\rangle$ or $|\underline{r}\rangle$. Similarly for operators, one uses $\hat{A}_1 \hat{B}_2$ instead of $\hat{A}_1 \otimes \hat{B}_2$ and $\hat{A}_1 \mathbb{I}_2$ or $\hat{A}_1$ instead of $\hat{A}_1 \otimes \mathbb{I}_2$.

7.3 Eigenvalues and Eigenstates in Tensor Product State Spaces

Given the eigenvalue equations $\hat{A} |\psi\rangle = \lambda |\psi\rangle$ in $\mathcal{V}_1$ and $\hat{B} |\varphi\rangle = \mu |\varphi\rangle$ in $\mathcal{V}_2$ the operator $\hat{C}$ acting on $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ is assumed to be $\hat{C} = \hat{A}_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes \hat{B}$ as the sum of two tensor products and to satisfy the eigenvalue equation $\hat{C} |\chi\rangle = \omega |\chi\rangle$. This special form of $\hat{C}$ occurs in physical systems such as

(i) particles moving in three dimensions with the example $\hat{H} = \hat{H}_x \otimes \mathbb{I}_y \otimes \mathbb{I}_z + \mathbb{I}_x \otimes \hat{H}_y \otimes \mathbb{I}_z + \mathbb{I}_x \otimes \mathbb{I}_y \otimes \hat{H}_z$ of the three-dimensional harmonic oscillator,
(ii) multi-particle systems with the example $\hat{H} = \hat{H}_{\mathrm{CoM}} \otimes \mathbb{I}_{\mathrm{rel}} + \mathbb{I}_{\mathrm{CoM}} \otimes \hat{H}_{\mathrm{rel}}$ of two particles interacting via a potential that depends on their relative position in the center-of-mass coordinates.

The ket $|\psi\rangle_1 \otimes |\varphi\rangle_2 \in \mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ is an eigenstate of $\hat{C}$ as

$$\begin{aligned}\hat{C} |\psi\rangle_1 \otimes |\varphi\rangle_2 &= \big(\hat{A}_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes \hat{B}\big) |\psi\rangle_1 \otimes |\varphi\rangle_2 = \big(\hat{A}_1 |\psi\rangle_1\big) \otimes \big(\mathbb{I}_2 |\varphi\rangle_2\big) + \big(\mathbb{I}_1 |\psi\rangle_1\big) \otimes \big(\hat{B}_2 |\varphi\rangle_2\big) \\ &= \lambda |\psi\rangle_1 \otimes |\varphi\rangle_2 + |\psi\rangle_1 \otimes \mu |\varphi\rangle_2 = \lambda\big(|\psi\rangle_1 \otimes |\varphi\rangle_2\big) + \mu\big(|\psi\rangle_1 \otimes |\varphi\rangle_2\big) = (\lambda + \mu) |\psi\rangle_1 \otimes |\varphi\rangle_2\end{aligned}$$

shows using (7.1). This proves that $|\chi\rangle = |\psi\rangle_1 \otimes |\varphi\rangle_2$ is an eigenstate of $\hat{C}$ with eigenvalue $\omega = \lambda + \mu$.

7.4 Permutation Operators

Permutation operators exchange particles. The mathematics need these operators to capture the symmetry of identical particles, and permutations are the tools to rearrange ordered elements. A permutation $P : 123 \to 312$ is written as P_{312} because the initial state is assumed to be the ordered state 123. For N elements there are $N!$ permutations.

As an example, $N = 3$ particles are assumed and the state space is therefore $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2 \otimes \mathcal{V}_3$ with the basis $\{|u_i\rangle_1 |u_j\rangle_2 |u_k\rangle_3\} \in \mathcal{V}$. There are $3! = 6$ permutations P_{123}, P_{312}, P_{231}, P_{132}, P_{213}, P_{321}. The permutation operator acts as

$$\hat{P}_{mnp} |u_i\rangle_1 |u_j\rangle_2 |u_k\rangle_3 = |u_i\rangle_m |u_j\rangle_n |u_k\rangle_p$$

on the basis states, and this moves the particle associated with state space $\mathcal{V}_1$ to the state space $\mathcal{V}_m$ and so on for the other two particles.

A transposition is a permutation that exchanges two elements and leaves the rest invariant. Transpositions are Hermitian $P_{21} = P_{21}^\dagger$, involutory $P_{21}^2 = \mathbb{I}$ and unitary $P_{21}^\dagger = P_{21}^{-1}$ as one can easily show for $N = 2$ but can also be generalized to any transpositions. Every permutation can be written as the product of transpositions. The parity of any permutation is even or odd depending on the number of transpositions needed.

When writing P_α for a general permutation and T_β for a general transposition one can show that also permutations are unitary but that not all permutations are Hermitian because transpositions do not commute in general. A further property is that the adjoint of a permutation has the same parity as the permutation because the adjoint is just the same sequence of transpositions but in reverse order.

All permutations for a given N form a group. The identity is the permutation that does not change anything. The product of two group elements gives another group element because two permutations one after the other just reorder the elements in a way one can achieve with one permutation. Finally, the inverse is the permutation that undoes the permutation.

The rearrangement theorem states that if $\hat{P}_1$, $\hat{P}_2$, ... , $\hat{P}_{N!}$ is a list of all permutations and P_α is one of them then $P_\alpha \hat{P}_1$, $P_\alpha \hat{P}_2$, ... , $P_\alpha \hat{P}_{N!}$ contains each element of the permutation group exactly once. Thus, this reorders the elements but does not duplicate some of them.

7.5 Symmetric and Antisymmetric States of Many Quantum Particles

In quantum systems of identical particles exchanging any two particles does not change the physics. Symmetric states do not change at all when two particles are exchanged, and antisymmetric states change only a sign when two particles are exchanged. This captures the key difference between bosons and fermions.

In an N-particle system $\mathcal{V} = \mathcal{V}_1 \otimes ... \otimes \mathcal{V}_N$ with the $N!$ permutation operators $\hat{P}_\alpha$ is the state ψ_+ totally symmetric if $\hat{P}_\alpha \psi_+ = \psi_+$ for every permutation $\hat{P}_\alpha$. Totally symmetric states exist in a subspace $\mathcal{V}_+$ of $\mathcal{V}$. If $\hat{P}_\alpha \psi_- = \eta_\alpha \psi_-$ for any permutation $\hat{P}_\alpha$ where $\eta_\alpha = \pm 1$ depending on whether $\hat{P}_\alpha$ is even or odd then ψ_- is a totally antisymmetric state. Totally antisymmetric states exist in a subspace $\mathcal{V}_-$ of $\mathcal{V}$.

With the definition of the two operators

$$\hat{S}_+ = \frac{1}{N!} \sum_\alpha \hat{P}_\alpha \qquad\qquad \hat{S}_- = \frac{1}{N!} \sum_\alpha \eta_\alpha \hat{P}_\alpha \tag{7.2}$$

where the sum goes over all permutations any state can be projected onto $\mathcal{V}_+$ with $\hat{S}_+$ called symmetrizer and onto $\mathcal{V}_-$ with $\hat{S}_-$ called antisymmetrizer. To prove this the property $\hat{P}_\alpha \hat{S}_+ = \hat{S}_+ \hat{P}_\alpha = \hat{S}_+$ and the property $\hat{P}_\alpha \hat{S}_- = \hat{S}_- \hat{P}_\alpha = \eta_\alpha \hat{S}_-$ both following from the rearrangement theorem are needed. These two properties allow to show $\hat{S}_+^2 = \hat{S}_+$ and $\hat{S}_-^2 = \hat{S}_-$. Thus, the symmetrizer and the antisymmetrizer operators are projection operators.

Further, one can prove $\hat{S}_+ \hat{S}_- = 0$ such that they project to orthogonal subspaces. Finally, $\hat{S}_+ + \hat{S}_- \neq \mathbb{I}$ for $N > 2$ shows that the two operators do not project to complementary subspaces except for $N = 2$. The last point to show is that $|\psi'\rangle = \hat{S}_+ |\psi\rangle$ is a totally symmetric state, and this follows from $\hat{P}_\alpha |\psi'\rangle = \hat{P}_\alpha \hat{S}_+ |\psi\rangle = \hat{S}_+ |\psi\rangle = |\psi'\rangle$. It also follows that any permutation of a ket projects to the same totally symmetric state because $\hat{S}_+ \big(\hat{P}_\alpha |\psi\rangle\big) = \hat{S}_+ |\psi\rangle$, and that any permutation of a ket projects to the same antisymmetric state possibly up to a sign.

If $\hat{A}_1$ and $\hat{A}_2$ are two observables with $\hat{A}_1 |u_j\rangle = a_j |u_j\rangle$ such that $\{|u_j\rangle\} \subset \mathcal{V}_1$ and $\hat{A}_2 |u_k\rangle = a_k |u_k\rangle$ such that $\{|u_k\rangle\} \subset \mathcal{V}_2$ then $\hat{A}_1 \otimes \mathbb{I}_2 \to \hat{A}_1$ and $\mathbb{I}_1 \otimes \hat{A}_2 \to \hat{A}_2$. The permutation operator $\hat{P}_{21}$ acts as

$$\begin{aligned}
\hat{P}_{21} \hat{A}_1 \hat{P}_{21}^\dagger |u_j\rangle_1 |u_k\rangle_2 &= \hat{P}_{21} \hat{A}_1 |u_j\rangle_2 |u_k\rangle_1 = a_k \hat{P}_{21} |u_j\rangle_2 |u_k\rangle_1 \\
&= a_k |u_j\rangle_1 |u_k\rangle_2 \\
\hat{A}_2 |u_j\rangle_1 |u_k\rangle &= a_k |u_j\rangle_1 |u_k\rangle_2
\end{aligned}$$

such that $\hat{P}_{21} \hat{A}_1 \hat{P}_{21}^\dagger = \hat{A}_2$ and $\hat{P}_{21} \hat{A}_2 \hat{P}_{21}^\dagger = \hat{A}_1$. This is true for any observable $\hat{O}_{12}$ such that one can write $\hat{P}_{21} \hat{O}_{12} \hat{P}_{21}^\dagger = \hat{O}_{21}$ where $\hat{O}_{12}$ could be $\hat{O}_{12} = \hat{A}_1 + \hat{B}_2 = \hat{A}_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes \hat{B}_2$ and $\hat{O}_{21} = \hat{B}_1 + \hat{A}_2$, for example.

A symmetric observable is an observable for which $\hat{O}_{12} = \hat{O}_{21}$. This is equivalent to the statement that the observable commutes with the permutation operator because from $\hat{P}_{21} \hat{O}_{12} \hat{P}_{21}^\dagger = \hat{O}_{21} = \hat{O}_{12}$ follows $\hat{P}_{21} \hat{O}_{12} \hat{P}_{21}^\dagger \hat{P}_{21} = \hat{O}_{12} \hat{P}_{21}$, $\hat{P}_{21} \hat{O}_{12} \mathbb{I} = \hat{O}_{12} \hat{P}_{21}$ and $\hat{P}_{21} \hat{O}_{12} = \hat{O}_{12} \hat{P}_{21}$. Generalizing this to N particles allows to define a totally symmetric observable $\hat{O}_{12...N}$ as an observable satisfying $\big[\hat{O}_{12...N}, \hat{P}_\alpha\big] = 0$ for all permutations $\hat{P}_\alpha$.

Totally symmetric states and totally antisymmetric states are the only allowed states for systems of identical particles. They are fundamental in areas ranging from condensed matter physics and material science to chemistry because they all involve multi-particle systems.

7.6 Exchange Degeneracy

For systems with two identical particles there is an infinite number of kets describing it. However, if one does predictions using the rules of quantum mechanics different states give different results.

As an example a two-particle system $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2$ is used where the particles have a spin $\frac{1}{2}$ such that

$$\hat{S}_z \left|\uparrow\right\rangle_z = +\frac{1}{2}\hbar \left|\uparrow\right\rangle_z \qquad\qquad \hat{S}_z \left|\downarrow\right\rangle_z = -\frac{1}{2}\hbar \left|\downarrow\right\rangle_z$$

are the eigenvalue equations. The state space $\mathcal{V}$ for both spins has dimension 4 and the basis states are $\{\left|\uparrow\right\rangle_{1z} \otimes \left|\uparrow\right\rangle_{2z}, \left|\uparrow\right\rangle_{1z} \otimes \left|\downarrow\right\rangle_{2z}, \left|\downarrow\right\rangle_{1z} \otimes \left|\uparrow\right\rangle_{2z}, \left|\downarrow\right\rangle_{1z} \otimes \left|\downarrow\right\rangle_{2z}\}$ or simply $\{\left|\uparrow,\uparrow\right\rangle_z, \left|\uparrow,\downarrow\right\rangle_z, \left|\downarrow,\uparrow\right\rangle_z, \left|\downarrow,\downarrow\right\rangle_z\}$. The operators are $\hat{S}_{1z} \otimes \mathbb{I}_2$ and $\mathbb{I}_1 \otimes \hat{S}_{2z}$ simply written as $\hat{S}_{1z}$ and $\hat{S}_{2z}$, respectively.

Assuming that measuring S_z gives $+\hbar/2$ and $-\hbar/2$ then one particles is up and one particle is down but it is not clear which particle is in which state because $\left|\uparrow,\downarrow\right\rangle_z$ and $\left|\downarrow,\uparrow\right\rangle_z$ are possible. The two states are orthogonal ${}_z\langle\uparrow,\downarrow \mid \downarrow,\uparrow\rangle_z = 0$. However, not only these two states are consistent with the measurement but also any linear combination $\alpha\left|\uparrow,\downarrow\right\rangle_z + \beta\left|\downarrow,\uparrow\right\rangle_z$ with normalization $|\alpha|^2 + |\beta|^2 = 1$. This linear combination is a superposition state where α and β determine the probability. This means that there are infinitely many states describing the situation that one particle is up and the other is down, and they all describe the same physical situation. This fact is called *exchange degeneracy.*

This means that all the states $\alpha\left|\uparrow,\downarrow\right\rangle_z + \beta\left|\downarrow,\uparrow\right\rangle_z$ are equivalent similar to a global phase $e^{i\vartheta}\left|\psi\right\rangle$. All physical quantities are independent of a global phase. To understand the problem of exchange degeneracy one can ask the question what the probability is of getting $(+\hbar/2, +\hbar/2)$ if one measures $\hat{S}_{1x}$ and $\hat{S}_{2x}$ in the x-direction. Using $\left|\uparrow\right\rangle_x = 1/\sqrt{2}\left(\left|\uparrow\right\rangle_z + \left|\downarrow\right\rangle_z\right)$ gives

$$\left|\uparrow,\uparrow\right\rangle_x = \left(\frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle_z + \left|\downarrow\right\rangle_z\right)\right) \otimes \left(\frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle_z + \left|\downarrow\right\rangle_z\right)\right) = \frac{1}{2}\Big(\left|\uparrow,\uparrow\right\rangle_z + \left|\uparrow,\downarrow\right\rangle_z + \left|\downarrow,\uparrow\right\rangle_z + \left|\downarrow,\downarrow\right\rangle_z\Big)$$

and the probability becomes

$$\left|\left({}_x\langle\uparrow,\uparrow|\right)\left(\alpha\left|\uparrow,\downarrow\right\rangle_z + \beta\left|\downarrow,\uparrow\right\rangle_z\right)\right|^2 = \left|\left(\frac{1}{2}\left({}_z\langle\uparrow,\uparrow| + {}_z\langle\uparrow,\downarrow| + {}_z\langle\downarrow,\uparrow| + {}_z\langle\downarrow,\downarrow|\right)\right)\Big(\alpha\left|\uparrow,\downarrow\right\rangle_z + \beta\left|\downarrow,\uparrow\right\rangle_z\Big)\right|^2$$
$$= \left|\frac{1}{2}\left(\alpha\,{}_z\langle\uparrow,\downarrow \mid \uparrow,\downarrow\rangle_z + \beta\,{}_z\langle\downarrow,\uparrow \mid \downarrow,\uparrow\rangle_z\right)\right|^2 = \left|\frac{1}{2}(\alpha+\beta)\right|^2$$

such that the result depends on α and β. The situation is therefore different from a global phase factor.

All possible permutations $\hat{P}_\alpha$ applied to a state $\left|\psi\right\rangle \in \mathcal{V}$ in a system with N particles where $\mathcal{V} = \mathcal{V}_1 \otimes ... \otimes \mathcal{V}_N$ gives the set $\{\hat{P}_\alpha\left|\psi\right\rangle\}$. This set spans $\mathcal{V}_\psi$ and each of the states in this set describes the same physical situation if all particles are identical. This is the *exchange degeneracy* for N identical particles. It gives rise to a big problem because all these states describe mathematically the same system but when used for physical predictions using the rules of quantum mechanics result in different answers. The question is which state describes the physical system. The answer is given by the symmetrization postulate added to the initial sets of postulates for quantum mechanics.

7.7 The Symmetrization Postulate

There is an infinite number of states that describe a quantum system with multiple identical particles but depending on the state selected different outcomes of measurement result. This problem consistent with the rules of quantum mechanics introduced so far is called exchange degeneracy. To overcome this problem an additional postulate is needed.

Symmetrization Postulate: For a system of identical particles, the only kets of its state space that can describe physical states are

1. totally symmetric kets with respect to permutations of identical particles or
2. totally antisymmetric kets with respect to permutations of identical particles.

The particles that obey the totally symmetric case are called *bosons* and the particles that obey the totally antisymmetric case are called *fermions.*

The space state of N distinguishable particles is $\mathcal{V} = \mathcal{V}_1 \otimes ... \otimes \mathcal{V}_N$ but the space state of N identical particles is either $\mathcal{V}_+$ for bosons or $\mathcal{V}_-$ for fermions. The question is how does one know whether a given particle is a boson or a fermion. The empirical answer comes from experiments. Particles with integer spins are bosons and particles with half-integer spins are fermions. Elementary particles such as photons are bosons but also composite particles such as mesons and helium-4 belong into this group. Elementary particles such as electrons and muons are fermions but also composite particles such as protons, neutrons and helium-3 belong into this group. The spin is an intrinsic property for elementary particles and for non-elementary particles one has to combine the spins of their elementary components. The relation between spin and the bosonic or fermionic nature of a particle is an empirical fact in elementary quantum mechanics but there is the spin-statistics theorem in quantum field theory such that this relation can be derived from other principles.

As shown above $\{\hat{P}_\alpha |\psi\rangle\}$ span $\mathcal{V}_\psi$ for $|\psi\rangle \in \mathcal{V}$ and this causes exchange degeneracy. On the other hand the symmetrization postulate tells that the physically allowed kets live either in $\mathcal{V}_+$ for bosons or in $\mathcal{V}_-$ for fermions. Thus, one has to show that only one ket in the set $\{\hat{P}_\alpha |\psi\rangle\}$ lives also in $\mathcal{V}_+$ or $\mathcal{V}_-$. The symmetrizer $\hat{S}_+$ and the antisymmetrizer $\hat{S}_-$ both commute with all permutations $\hat{P}_\alpha$ such that all terms are equal to $\hat{S}_+$ respectively equal to $\eta_\alpha \hat{S}_-$. Therefore, symmetrizing $|\psi\rangle$ gives $\hat{S}_+ |\psi\rangle \in \mathcal{V}_+$ and symmetrizing $\hat{P}_\alpha |\psi\rangle$ gives also $\hat{S}_+(\hat{P}_\alpha |\psi\rangle) = \hat{S}_+ |\psi\rangle \in \mathcal{V}_+$. This shows that the symmetrization postulate removes the exchange degeneracy. The single state is $\hat{S}_+ |\psi\rangle$ for bosons and $\hat{S}_- |\psi\rangle$ for fermions, and the remaining question is how this single state is constructed. This is shown for a few examples.

In a two-particle system with $|\varphi\rangle \in \mathcal{V}_1$ and $|\chi\rangle \in \mathcal{V}_2$ the state $|\psi\rangle = |\varphi\rangle_1 \otimes |\chi\rangle_2 = |\varphi\rangle_1 |\chi\rangle_2 \in \mathcal{V}$ is chosen in the first step. The second step is the application of the symmetrizer such that the symmetrized state

$$\hat{S}_+ |\psi\rangle = \frac{1}{2}\big(\hat{P}_{12} + \hat{P}_{21}\big)\big(\,|\varphi\rangle_1 |\chi\rangle_2\,\big) = \frac{1}{2}\big(\,|\varphi\rangle_1 |\chi\rangle_2 + |\chi\rangle_1 |\varphi\rangle_2\,\big)$$

is a boson, or the application of the antisymmetrizer such that the antisymmetrized state

$$\hat{S}_- |\psi\rangle = \frac{1}{2}\big(\hat{P}_{12} - \hat{P}_{21}\big)\big(\,|\varphi\rangle_1 |\chi\rangle_2\,\big) = \frac{1}{2}\big(\,|\varphi\rangle_1 |\chi\rangle_2 - |\chi\rangle_1 |\varphi\rangle_2\,\big)$$

is a fermion. The third step is normalization and one has to distinguish $|\varphi\rangle \neq |\chi\rangle$ with the normalized state $1/\sqrt{2}\big(\,|\varphi\rangle_1 |\chi\rangle_2 \pm |\chi\rangle_1 |\varphi\rangle_2\,\big)$ and $|\varphi\rangle = |\chi\rangle$ with $\frac{1}{2}\big(\,|\varphi\rangle_1 |\varphi\rangle_2 + |\varphi\rangle_1 |\varphi\rangle_2\,\big) = |\varphi\rangle_1 |\varphi\rangle_2$ for bosons. The case $|\varphi\rangle = |\chi\rangle$ for fermions gives $\frac{1}{2}\big(\,|\varphi\rangle_1 |\varphi\rangle_2 - |\varphi\rangle_1 |\varphi\rangle_2\,\big) = 0$ and shows therefore that there is no ket in $\mathcal{V}_-$ that can describe this physical state. This is the *Pauli exclusion principle* stating that two identical fermions cannot be in the same state.

In the three-particle system with $|\varphi\rangle$, $|\chi\rangle$, $|\omega\rangle$ the state $|\psi\rangle$ is select ordered $|\psi\rangle = |\varphi\rangle_1 |\chi\rangle_2 |\omega\rangle_3$ in the first step. The symmetrizer for bosons gives

$$\begin{aligned}\hat{S}_+ |\psi\rangle = \frac{1}{6}\big(\,&|\varphi\rangle_1 |\chi\rangle_2 |\omega\rangle_3 + |\omega\rangle_1 |\varphi\rangle_2 |\chi\rangle_3 + |\chi\rangle_1 |\omega\rangle_2 |\varphi\rangle_3 + \\ &|\varphi\rangle_1 |\omega\rangle_2 |\chi\rangle_3 + |\chi\rangle_1 |\varphi\rangle_2 |\omega\rangle_3 + |\omega\rangle_1 |\chi\rangle_2 |\varphi\rangle_3\,\big)\end{aligned}$$

in the second step. In the last step several different cases have to be distinguished. The result in the case $|\varphi\rangle \neq |\chi\rangle \neq |\omega\rangle$ is

$$|\psi\rangle = \frac{1}{\sqrt{6}}\big(\,|\varphi\rangle_1 |\chi\rangle_2 |\omega\rangle_3 + |\omega\rangle_1 |\varphi\rangle_2 |\chi\rangle_3 + |\chi\rangle_1 |\omega\rangle_2 |\varphi\rangle_3 + |\varphi\rangle_1 |\omega\rangle_2 |\chi\rangle_3 + |\chi\rangle_1 |\varphi\rangle_2 |\omega\rangle_3 + |\omega\rangle_1 |\chi\rangle_2 |\varphi\rangle_3\,\big)$$

and is

$$|\psi\rangle = \frac{1}{\sqrt{3}}\big(\,|\varphi\rangle_1 |\varphi\rangle_2 |\omega\rangle_3 + |\varphi\rangle_1 |\omega\rangle_2 |\varphi\rangle_3 + |\omega\rangle_1 |\varphi\rangle_2 |\varphi\rangle_3\,\big)$$

in case $|\varphi\rangle = |\chi\rangle \neq |\omega\rangle$. The state is $|\psi\rangle = |\varphi\rangle_1 |\varphi\rangle_2 |\varphi\rangle_3$ for $|\varphi\rangle = |\chi\rangle = |\omega\rangle$.

Also in the three-particle system with $|\varphi\rangle$, $|\chi\rangle$, $|\omega\rangle$ and $|\psi\rangle = |\varphi\rangle_1 |\chi\rangle_2 |\omega\rangle_3$ the antisymmetrizer for fermions gives

$$\begin{aligned}\hat{S}_- |\psi\rangle = \frac{1}{6}\big(\,&|\varphi\rangle_1 |\chi\rangle_2 |\omega\rangle_3 + |\omega\rangle_1 |\varphi\rangle_2 |\chi\rangle_3 + |\chi\rangle_1 |\omega\rangle_2 |\varphi\rangle_3 \\ &- |\varphi\rangle_1 |\omega\rangle_2 |\chi\rangle_3 - |\chi\rangle_1 |\varphi\rangle_2 |\omega\rangle_3 - |\omega\rangle_1 |\chi\rangle_2 |\varphi\rangle_3\,\big)\end{aligned}$$

in the second step. State $|\psi\rangle$ in the case $|\varphi\rangle \neq |\chi\rangle \neq |\omega\rangle$ is

$$|\psi\rangle = \frac{1}{\sqrt{6}}\big(|\varphi\rangle_1 |\chi\rangle_2 |\omega\rangle_3 + |\omega\rangle_1 |\varphi\rangle_2 |\chi\rangle_3 + |\chi\rangle_1 |\omega\rangle_2 |\varphi\rangle_3 - |\varphi\rangle_1 |\omega\rangle_2 |\chi\rangle_3 - |\chi\rangle_1 |\varphi\rangle_2 |\omega\rangle_3 - |\omega\rangle_1 |\chi\rangle_2 |\varphi\rangle_3 \big)$$

and the Pauli exclusion principle does not allow the other cases $|\varphi\rangle = |\chi\rangle \neq |\omega\rangle$ and $|\varphi\rangle = |\chi\rangle = |\omega\rangle$.

For a system with N particles $|\varphi_1\rangle, ..., |\varphi_N\rangle$ the state $|\psi\rangle = |\varphi_1\rangle_1, ..., |\varphi_N\rangle_N$ is symmetrized or antisymmetrized by

$$\hat{S}_+ |\psi\rangle = \left(\frac{1}{N!}\sum_\alpha \hat{P}_\alpha\right) |\varphi_1\rangle_1, ..., |\varphi_N\rangle_N \qquad \hat{S}_- |\psi\rangle = \left(\frac{1}{N!}\sum_\alpha \eta_\alpha \hat{P}_\alpha\right) |\varphi_1\rangle_1, ..., |\varphi_N\rangle_N$$

where the left side shows the case for bosons and the right side the case for fermions. When this bosonic state is represented in the position basis in terms of wave functions this object is sometimes called the permanent. When this fermionic state is represented in the position basis in terms of wave functions the signs introduced by η_α obey the same rules as those for the determinant. The corresponding determinants are called Slater determinants.

7.8 Occupation Number Representation

The occupation number representation provides an alternative compact formulation to describe systems of identical particles. It is a more natural way of describing identical particles, forms the basis of what is sometimes called "second quantization", and is a powerful formalism that allows to study advanced topics like quantum field theory or quantum statistical mechanics. Labeling particles in a system of identical particles leads to much redundancy making symmetrizers necessary. Instead of specifying which particles are in a certain state it is enough to specify how many particles are in this state.

If $\{|u_j\rangle\}$ is the basis for one particle then $\{|u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N\}$ is the basis for a system of N identical particles $\mathcal{V} = \mathcal{V}_1 \otimes ... \otimes \mathcal{V}_N$. However, to describe this system a basis for $\mathcal{V}_+$ for bosons or $\mathcal{V}_-$ for fermions is needed. The basis states in $\mathcal{V}_\pm$ are

$$|\psi\rangle \in \mathcal{V} \qquad \Rightarrow \qquad |\psi\rangle = \sum_{jk...p} c_{jk...p} |u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N$$

$$\hat{S}_\pm |\psi\rangle \in \mathcal{V}_\pm \qquad \Rightarrow \qquad \hat{S}_\pm |\psi\rangle = \hat{S}_\pm \sum_{jk...p} c_{jk...p} |u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N = \sum_{jk...p} c_{jk...p}\, \hat{S}_\pm |u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N$$

and this shows that $\{\hat{S}_\pm |u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N\}$ is a basis for $\mathcal{V}_\pm$. There is a lot of redundancy in this basis because $\mathcal{V}_+$ and $\mathcal{V}_-$ are complementary subspaces of $\mathcal{V}$. The repeated states are permutations of each other, and the basis of $\mathcal{V}_\pm$ are equivalence classes of all permutations applied to $\{|u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N\}$.

Because all $\hat{P}_\alpha |u_j\rangle_1 |u_k\rangle_2 ... |u_p\rangle_N$ represent the same state in $\mathcal{V}_\pm$, a quantity which is the same in all permutations is needed to remove the redundancy. Ordering the states as

$$|u_1\rangle_1 |u_1\rangle_2 ... |u_1\rangle_{n_1} |u_2\rangle_{n_1+1} ... |u_2\rangle_{n_1+n_2} + ...$$

such that the individual states are grouped together allows to use the occupation numbers n_1 for $|u_1\rangle$, n_2 for $|u_2\rangle$ and so on as this quantity. In another permutation of this state $|u_1\rangle$ still appears n_1 times, $|u_2\rangle$ appears n_2 times and so on. This leads to the occupation number representation

$$|n_1, n_2, ...\rangle = A_\pm \hat{S}_\pm |u_1\rangle_1 |u_1\rangle_2 ... |u_1\rangle_{n_1} |u_2\rangle_{n_1+1} ... |u_2\rangle_{n_1+n_2} + ...$$

for N identical particles. Any permutation $\hat{P}_\alpha$ of $|u_1\rangle_1 |u_1\rangle_2 ... |u_1\rangle_{n_1} |u_2\rangle_{n_1+1} ... |u_2\rangle_{n_1+n_2} + ...$ results in the same occupation numbers where $A_\pm$ is needed for the normalization of states. Note that the occupation numbers may be zero, and $N = \sum_k n_k$. Note also that in general there is an infinite number of single particle states $|u_j\rangle$.

The normalization of the states in the occupation number representation is

$$|n_1, n_2, ...\rangle = \sqrt{\frac{N!}{n_1! n_2! ...}}\, \hat{S}_+ |u_1\rangle_1 |u_1\rangle_2 ... |u_1\rangle_{n_1} |u_2\rangle_{n_1+1} ... |u_2\rangle_{n_1+n_2} + ...$$

for bosons and

$$|n_1, n_2, ...\rangle = \begin{cases} \sqrt{N!}\,\hat{S}_- \,|u_1\rangle_1 \,|u_1\rangle_2 \,...\, |u_1\rangle_{n_1} \,|u_2\rangle_{n_1+1} \,...\, |u_2\rangle_{n_1+n_2} + ... & \text{if all } u_j \text{ are different} \\ 0 & \text{if two or more } u_j \text{ are equal} \end{cases}$$

for fermions because of the Pauli exclusion principle. For fermions the question is simply whether a state is occupied or not. Examples of states in the occupation number representation are $|0,5,3,0,8,...\rangle$ for bosons and $|1,0,0,1,...\rangle$ for fermions. The order is important because $\hat{P}_\alpha |\psi_-\rangle = \eta_\alpha |\psi_-\rangle$ changes the sign if the permutation is odd. A transposition $|u_j, u_k, ...\rangle = -|u_k, u_j, ...\rangle$ changes the sign.

7.9 Fock Space

So far state spaces for a fixed number of particles have been used. To allow a variable number of particles the state space is a *Fock space* which is the space for quantum field theory.

If one works in a specific single-particle basis $\{|u_k\rangle\}$ a system with N identical particles can be represented using occupation numbers $|n_1, n_2, ...\rangle$ where n_1 particles are in state $|u_1\rangle$, n_2 particles are in state $|u_2\rangle$ and therefore n_j particles are in state $|u_j\rangle$ with $N = \sum_k n_k$. In this case, the different occupation numbers n_j and the total number of particles N are well-defined. These states are called Fock states. The Fock states belong to the totally symmetric $\mathcal{V}_+$ for bosons and to the totally antisymmetric $\mathcal{V}_-$ for fermions. The space for N identical particles is called $\mathcal{F}_N$ independent of whether the identical particles are bosons or fermions. The space $\mathcal{F}_1$, for example, consists of a single particle. Also $\mathcal{F}_0$ containig zero particles is defined.

The Fock space $\mathcal{F}$ is defined as

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus ... = \bigoplus_{k=0}^{\infty} \mathcal{F}_k \tag{7.3}$$

where $\mathcal{V}_P \oplus \mathcal{V}_Q$ is a vector space $\mathcal{V}_{P+Q}$ with dimension $P+Q$ if $\mathcal{V}_P$ is a vector space of dimension P and $\mathcal{V}_Q$ is a vector space of dimension Q and where all linear combinations of $|p\rangle$ and $|q\rangle$ are in $\mathcal{V}_{P+Q}$ for any $|p\rangle \in \mathcal{V}_P$ and any $|q\rangle \in \mathcal{V}_Q$. Thus, the Fock space is the occupation number space for all possible numbers of particles.

The basis of $\mathcal{F}$ is the combination of the bases of all $\mathcal{F}_N$. Two kets in a Fock space with a different number of particles are orthogonal. Because a Fock state has a fixed number of particles any Fock state belongs to a subspace $\mathcal{F}_N \subset \mathcal{F}$. The vacuum state $|0\rangle \in \mathcal{F}_0$ is the Fock state with zero particles.

The Fock space allows states beyond Fock states such as $|0\rangle + |1\rangle + |1,1\rangle$ with superpositions of Fock states with different numbers of particles. This example state is a superposition of the vacuum state, a single-particle state and a two-particle state where the two particles occupy two different states. This state has some amplitude of having zero particles, some of having one particle and some of having two particles. This is an example how Fock spaces allow to treat systems with a variable number of particles, and this is a feature needed in quantum field theory where particles and antiparticle are created and annihilated and quantum statistical mechanics where a system can be in an equilibrium with a particle reservoir with which it exchanges particles.

7.10 Boson Creation and Annihilation Operators

Given a single-particle basis $\{|u_j\rangle\}$ the Fock state $|n_1, n_2, ..., n_j, ...\rangle$ specifies a state with multiple identical particles with n_j particles in state $|u_j\rangle$. The *creation operator* $\hat{a}^\dagger_{u_j}$ for bosons acts as

$$\hat{a}^\dagger_{u_j} |n_1, n_2, ..., n_j, ...\rangle = \sqrt{n_j + 1}\,|n_1, n_2, ..., n_j + 1, ...\rangle \tag{7.4}$$

on the Fock state $|n_1, n_2, ..., n_j, ...\rangle$. In words, it adds a particle to the state $|u_j\rangle$. Another way of looking at the creation operator is that it allows to navigate the Fock space as it leads from $\mathcal{F}_N$ to $\mathcal{F}_{N+1}$. When there is no possible confusion one often uses the simplified form $\hat{a}^\dagger_{u_j} |n_j\rangle = \sqrt{n_j + 1}\,|n_j + 1\rangle$ instead of (7.4) only showing the occupation number that changes while all the other occupation numbers that stay the same are omitted.

The adjoint operator of $\hat{a}^\dagger_{u_j}$ is $(\hat{a}^\dagger_{u_j})^\dagger = \hat{a}_{u_j}$ and acts as

$$\langle n_j+1|\hat{a}^\dagger_{u_j}|n_j\rangle = \sqrt{n_j+1}\,\langle n_j+1|n_j+1\rangle = \sqrt{n_j+1}$$
$$\langle n_j+1|\hat{a}^\dagger_{u_j}|n_j\rangle = \langle n_j|(\hat{a}^\dagger_{u_j})^\dagger|n_j+1\rangle^* = \langle n_j|\hat{a}_{u_j}|n_j+1\rangle^* = \sqrt{n_j+1} \neq 0$$

because Fock states form an orthonormal basis. However, the fact that Fock states form an orthonormal basis also means that $\hat{a}_{u_j}|n_j+1\rangle$ must be proportional to $|n_j\rangle$. This means

$$\hat{a}_{u_j}|n_j+1\rangle = \sqrt{n_j+1}\,|n_j\rangle \qquad \Rightarrow \qquad \hat{a}_{u_j}|n_j\rangle = \sqrt{n_j}\,|n_j-1\rangle$$

such that this operator navigates from $\mathcal{F}_N$ to $\mathcal{F}_{N-1}$ as long as $N \geq 1$ as it annihilates a particle. The *annihilation operator* $\hat{a}_{u_j}$ for bosons acts as

$$\hat{a}_{u_j}|n_1,n_2,...,n_j,...\rangle = \begin{cases} \sqrt{n_j+1}\,|n_1,n_2,...,n_j-1,...\rangle & \text{if } n_j \geq 1 \\ 0 & \text{otherwise} \end{cases} \tag{7.5}$$

on the Fock state $|n_1,n_2,...,n_j,...\rangle$. In words, it removes a particle from state $|u_j\rangle$ if there is at least one.

To determine the commutation relations between creation and annihilation operators the notation is simplified from $\hat{a}^\dagger_{u_j}$ and $\hat{a}_{u_j}$ to $\hat{a}^\dagger_j$ and $\hat{a}_j$, respectively, with the implicit understanding that the basis for single-particle states is always $\{|u_j\rangle\}$. From

$$\hat{a}^\dagger_j\,\hat{a}^\dagger_k\,|n_j,n_k\rangle = \sqrt{n_j+1}\sqrt{n_k+1}\,|n_j+1,n_k+1\rangle = \hat{a}^\dagger_k\,\hat{a}^\dagger_j\,|n_j,n_k\rangle$$

follows that the commutators $[\hat{a}^\dagger_j,\hat{a}^\dagger_k]$ and $[\hat{a}^\dagger_j,\hat{a}^\dagger_k]^\dagger$ vanish independent of $j \neq k$ or $j = k$. Similarly, from

$$\hat{a}_j\,\hat{a}^\dagger_k\,|n_j,n_k\rangle = \sqrt{n_j}\sqrt{n_k+1}\,|n_j-1,n_k+1\rangle = \hat{a}^\dagger_k\,\hat{a}_j\,|n_j,n_k\rangle$$

follows that the commutator $[\hat{a}_j,\hat{a}^\dagger_k]$ vanishes if $j \neq k$. However, from

$$\hat{a}_j\,\hat{a}^\dagger_j\,|n_j\rangle = \sqrt{n_j+1}\,\hat{a}_j\,|n_j+1\rangle = (n_j+1)\,|n_j\rangle \qquad \hat{a}^\dagger_j\,\hat{a}_j\,|n_j\rangle = \sqrt{n_j}\,\hat{a}^\dagger_j\,|n_j-1\rangle = n_j\,|n_j\rangle$$

follows that $[\hat{a}_j,\hat{a}^\dagger_j] = 1$. To summarize, for the bosonic creation and annihilation operators are

$$[\hat{a}_{u_j},\hat{a}_{u_k}] = 0 \qquad [\hat{a}^\dagger_{u_j},\hat{a}^\dagger_{u_k}] = 0 \qquad [\hat{a}_{u_j},\hat{a}^\dagger_{u_k}] = \delta_{jk} \tag{7.6}$$

the commutation relations.

Given a fixed single-particle state the creation operator $\hat{a}^\dagger$ allows to navigate from the vacuum $|0\rangle$ in one step to $|1\rangle$, in another step to $|2\rangle$ and so on up the ladder. In the bosonic case one can add arbitrarily many particles to the same state. The annihilation operator $\hat{a}$ on the other hand allows to navigate down the ladder to $|2\rangle$, from there in one step to $|1\rangle$ and in another step to the vacuum state $|0\rangle$. Because there is no state with less particles than the vacuum state $\hat{a}\,|0\rangle$ kills the state and this is written as $\hat{a}\,|0\rangle = 0$.

Acting with the creation operator on the vacuum state gives $\hat{a}^\dagger_{u_j}|0\rangle = |1\rangle$, $\left(\hat{a}^\dagger_{u_j}\right)^2|0\rangle = \hat{a}^\dagger_{u_j}|1\rangle = \sqrt{2}\,|2\rangle$ and so on. Acting n_j times with the creation operator for $|u_j\rangle$ on the vacuum state gives

$$\sqrt{n_j!}\,|n_j\rangle = \left(\hat{a}^\dagger_{u_j}\right)^{n_j}|0\rangle \qquad |n_j\rangle = \frac{1}{\sqrt{n_j!}}\left(\hat{a}^\dagger_{u_j}\right)^{n_j}|0\rangle$$

and this generalizes to

$$|n_1,n_2,...,n_j,...\rangle = \frac{1}{\sqrt{n_1!n_2!...,n_j!...}}\left(\hat{a}^\dagger_{u_1}\right)^{n_1}\left(\hat{a}^\dagger_{u_2}\right)^{n_2}...\left(\hat{a}^\dagger_{u_j}\right)^{n_j}...|0\rangle$$

for an arbitrary state $|n_1,n_2,...,n_j,...\rangle$. Thus, to get the occupation number n_j one acts n_j times with $\hat{a}^\dagger_{u_j}$ on the vacuum state $|0\rangle$. Comparing this with

$$|n_1,n_2,...,n_j,...\rangle = \sqrt{\frac{N!}{n_1!n_2!...,n_j!...}}\hat{S}_+\,|u_1\rangle_1...|u_1\rangle_{n_1}|u_2\rangle_{n_1+1}...|u_2\rangle_{n_1+n_2}...$$

shows the relation

$$\frac{1}{\sqrt{n_1!n_2!...,n_j!...}}\left(\hat{a}_{u_1}^\dagger\right)^{n_1}\left(\hat{a}_{u_2}^\dagger\right)^{n_2}...\left(\hat{a}_{u_j}^\dagger\right)^{n_j}...|0\rangle$$
$$=\sqrt{\frac{N!}{n_1!n_2!...,n_j!...}}\hat{S}_+|u_1\rangle_1...|u_1\rangle_{n_1}|u_2\rangle_{n_1+1}...|u_2\rangle_{n_1+n_2}...$$

with the expression in terms of the symmetrizer.

The occupation number operator is defined as $\hat{n}_{u_j}=\hat{a}_{u_j}^\dagger\hat{a}_{u_j}$ and acts as

$$\hat{n}_{u_j}|n_1,n_2,...,n_j,...\rangle=\hat{a}_{u_j}^\dagger\hat{a}_{u_j}|n_1,n_2,...,n_j,...\rangle=\hat{a}_{u_j}^\dagger\sqrt{n_j}|n_1,n_2,...,n_j-1,...\rangle=n_j|n_1,n_2,...,n_j,...\rangle$$

showing that the Fock states are the eigenstates of the occupation number operator and that the eigenvalues n_j tell how many particles are in that state. The operator $\hat{N}$ counts

$$\hat{N}=\sum_j\hat{n}_{u_j}=\sum_j\hat{a}_{u_j}^\dagger\hat{a}_{u_j}$$

the total number of particles.

7.11 Fermion Creation and Annihilation Operators

Given a single-particle basis $\{|u_j\rangle\}$ the Fock state is written as $|u_k,u_\ell,...,u_p,...\rangle$ listing only the states with one particle because there is either no particle or one particle in a state such that the states with zero particles can be ignored. The *creation operator* $\hat{c}_{u_j}^\dagger$ for fermions acts as

$$\hat{c}_{u_j}^\dagger|u_k,u_\ell,...,u_p,...\rangle=|u_j,u_k,u_\ell,...,u_p,...\rangle\qquad\qquad\hat{c}_{u_j}^\dagger|u_k,u_\ell,...,u_j,...,u_p,...\rangle=0\tag{7.7}$$

on the Fock state $|u_k,u_\ell,...,u_p,...\rangle$. In words, the creation operator creates a particle in the given state if and only if there is no particle in this state. This follows from the Pauli exclusion principle. The creation operator allows to navigate from $\mathcal{F}_N$ to $\mathcal{F}_{N+1}$. Because the order in which the states appear is critical the new state is added at the beginning of the list.

The adjoint operator of $\hat{c}_{u_j}^\dagger$ is $(\hat{c}_{u_j}^\dagger)^\dagger$ and acts as

$$\langle u_j,u_k,u_\ell,...|\hat{c}_{u_j}^\dagger|u_k,u_\ell,...\rangle=\langle u_j,u_k,u_\ell,...|u_j,u_k,u_\ell,...\rangle=1$$
$$\langle u_j,u_k,u_\ell,...|\hat{c}_{u_j}^\dagger|u_k,u_\ell,...\rangle=\langle u_k,u_\ell,...|(\hat{c}_{u_j}^\dagger)^\dagger|u_j,u_k,u_\ell,...\rangle^*=\langle u_k,u_\ell,...|\hat{c}_{u_j}|u_j,u_k,u_\ell,...\rangle^*=1\neq 0$$

because Fock states form an orthonormal basis. However, the fact that Fock states form an orthonormal basis also means $|u_k,u_\ell,...\rangle=\hat{c}_{u_j}|u_j,u_k,u_\ell,...\rangle$ such that the operator $\hat{c}_{u_j}$ has annihilated the fermion in state $|u_j\rangle$. The *annihilation operator* $\hat{c}_{u_j}$ for fermions acts as

$$\hat{c}_{u_j}|u_j,u_k,u_\ell,...\rangle=|u_k,u_\ell,...\rangle\qquad\qquad\hat{c}_{u_j}|u_k,u_\ell,...\rangle=0\tag{7.8}$$

on the Fock state $|u_j,u_k,u_\ell,...\rangle$. In words, it removes a particle from state $|u_j\rangle$ if there is at least one. The annihilation operator navigates from $\mathcal{F}_N$ to $\mathcal{F}_{N-1}$ if possible.

The order in the fermionic Fock states is important because exchanging two fermions introduces a minus sign. The creation operator adds the new state at the beginning of the ordered list, and the annihilation operator removes a state only when it is at the beginning. If a state after creation is needed in another position or if the state to be annihilated is not at the beginning, the states have to be moved but keeping track of the sign changes. Every exchange of two states multiplies with -1. If for example $|u_2\rangle$ should be annihilated in $|u_1,u_2\rangle$ then $\hat{c}_{u_2}|u_1,u_2\rangle=-\hat{c}_{u_2}|u_2,u_1\rangle=-|u_1\rangle$.

The fermionic creation and annihilation operator obey anticommutation relations. To simplify notation $\hat{c}_j^\dagger$ and $\hat{c}_j$ are used instead of $\hat{c}_{u_j}^\dagger$ and $\hat{c}_{u_j}$ assuming implicitly the basis $\{|u_j\rangle\}$. Starting with the creation operators $j\neq k$ and $n_j=n_k=0$ gives

$$\left.\begin{aligned}\hat{c}_j^\dagger\hat{c}_k^\dagger|u_\ell,...\rangle&=\hat{c}_j^\dagger|u_k,u_\ell,...\rangle=|u_j,u_k,u_\ell,...\rangle\\ \hat{c}_k^\dagger\hat{c}_j^\dagger|u_\ell,...\rangle&=\hat{c}_k^\dagger|u_j,u_\ell,...\rangle=|u_k,u_j,u_\ell,...\rangle=-|u_j,u_k,u_\ell,...\rangle\end{aligned}\right\}\qquad\Rightarrow\qquad\{\hat{c}_j^\dagger,\hat{c}_k^\dagger\}=0$$

and this is also the case for $j = k$ because $(\hat{c}_j^\dagger)^2 = 0$ due to the Pauli exclusion principle. A similar calculation shows $\{\hat{c}_j, \hat{c}_k\} = 0$. For $\hat{c}_j$ and $\hat{c}_k^\dagger$ with $n_j = 1$ and $n_k = 0$ the anticommutator is

$$\left.\begin{aligned} \hat{c}_j\hat{c}_k^\dagger |u_j, u_\ell, ...\rangle &= \hat{c}_j |u_k, u_j, u_\ell, ...\rangle = -\hat{c}_j |u_j, u_k, u_\ell, ...\rangle = -|u_k, u_\ell, ...\rangle \\ \hat{c}_k^\dagger\hat{c}_j |u_j, u_\ell, ...\rangle &= \hat{c}_k^\dagger |u_\ell, ...\rangle = |u_k, u_\ell, ...\rangle \end{aligned}\right\} \quad \Rightarrow \quad \{\hat{c}_j, \hat{c}_k^\dagger\} = 0$$

in the case $j \neq k$ but the anticommutator is

$$\left.\begin{aligned} &\left.\begin{aligned} \hat{c}_j\hat{c}_j^\dagger |u_\ell, ...\rangle &= \hat{c}_j |u_j, u_\ell, ...\rangle = |u_\ell, ...\rangle \\ \hat{c}_j^\dagger\hat{c}_j |u_\ell, ...\rangle &= 0 \end{aligned}\right\} \text{ for } n_j = 0 \\ &\left.\begin{aligned} \hat{c}_j\hat{c}_j^\dagger |u_j, u_\ell, ...\rangle &= 0 \\ \hat{c}_j^\dagger\hat{c}_j |u_j, u_\ell, ...\rangle &= \hat{c}_j^\dagger |u_\ell, ...\rangle = |u_j, u_\ell, ...\rangle \end{aligned}\right\} \text{ for } n_j = 1 \end{aligned}\right\} \quad \Rightarrow \quad \{\hat{c}_j, \hat{c}_j^\dagger\} = 1$$

in the case $j = k$. To summarize, for the fermionic creation and annihilation operators are

$$\{\hat{c}_{u_j}, \hat{c}_{u_k}\} = 0 \qquad \{\hat{c}_{u_j}^\dagger, \hat{c}_{u_k}^\dagger\} = 0 \qquad \{\hat{c}_{u_j}, \hat{c}_{u_k}^\dagger\} = \delta_{jk} \tag{7.9}$$

the anticommutation relations.

Acting with the creation operator when the state is already occupied gives zero, and acting with the annihilation operator on a state where there is nothing to annihilate gives also zero. This means

$$\hat{c}_{u_j}^\dagger |u_j\rangle = 0 \qquad \hat{c}_{u_j} |0\rangle = 0$$

and there is no ladder as in the bosonic case because of the Pauli exclusion principle. In general

$$|n_1, n_2, ..., n_j, ...\rangle = \left(\hat{c}_{u_1}^\dagger\right)^{n_1}\left(\hat{c}_{u_2}^\dagger\right)^{n_2} ... \left(\hat{c}_{u_j}^\dagger\right)^{n_j} ... |0\rangle \qquad n_k \in \{0, 1\}$$

for an arbitrary state $|n_1, n_2, ..., n_j, ...\rangle$. Comparing this with

$$|n_1, n_2, ..., n_j, ...\rangle = \sqrt{N!}\,\hat{S}_- |u_1\rangle_1 ... |u_1\rangle_{n_1} |u_2\rangle_{n_1+1} ... |u_2\rangle_{n_1+n_2} ...$$

shows the relation

$$\left(\hat{c}_{u_1}^\dagger\right)^{n_1}\left(\hat{c}_{u_2}^\dagger\right)^{n_2} ... \left(\hat{c}_{u_j}^\dagger\right)^{n_j} ... |0\rangle = \sqrt{N!}\,\hat{S}_- |u_1\rangle_1 ... |u_1\rangle_{n_1} |u_2\rangle_{n_1+1} ... |u_2\rangle_{n_1+n_2} ...$$

with the expression in terms of the antisymmetrizer.

The occupation number operator is defined as $\hat{n}_{u_j} = \hat{c}_{u_j}^\dagger\hat{c}_{u_j}$ and acts as

$$\left.\begin{aligned} \hat{n}_{u_j} |u_k, ...\rangle &= \hat{c}_{u_j}^\dagger\hat{c}_{u_j} |u_k, ...\rangle = 0 & n_j = 0 \\ \hat{n}_{u_j} |u_j, u_k, ...\rangle &= \hat{c}_{u_j}^\dagger\hat{c}_{u_j} |u_j, u_k, ...\rangle = \hat{c}_{u_j}^\dagger |u_k, ...\rangle = |u_j, u_k, ...\rangle & n_j = 1 \end{aligned}\right\} \Rightarrow \quad \hat{n}_{u_j} |u_k, ...\rangle = n_j |u_k, ...\rangle$$

showing that the Fock states are the eigenstates of the occupation number operator and that the eigenvalues n_j tell how many particles are in that state. Note that this is also true if $|u_j\rangle$ is not the first in the list because moving it there in p steps and back again in p steps multiplies the result by $(-1)^{2p} = 1$. The operator $\hat{N}$ counts

$$\hat{N} = \sum_j \hat{n}_{u_j} = \sum_j \hat{c}_{u_j}^\dagger\hat{c}_{u_j}$$

the total number of particles.

To summarize, the commutation and anticommutation relations, respectively, for creation operators and annihilation operators are

$$\begin{aligned} [\hat{a}_{u_j}, \hat{a}_{u_k}] &= 0 & \{\hat{c}_{u_j}, \hat{c}_{u_k}\} &= 0 \\ [\hat{a}_{u_j}^\dagger, \hat{a}_{u_k}^\dagger] &= 0 & \{\hat{c}_{u_j}^\dagger, \hat{c}_{u_k}^\dagger\} &= 0 \\ [\hat{a}_{u_j}, \hat{a}_{u_k}^\dagger] &= \delta_{jk} & \{\hat{c}_{u_j}, \hat{c}_{u_k}^\dagger\} &= \delta_{jk} \end{aligned}$$

on the left side for bosons and on the right side for fermions.

7.12 One-Body Operators

The simplest case of operators are the one-body operators acting on one particle at a time. Examples are the position and the momentum operators. An operator $\hat{f}$ acting on a single particle in $\mathcal{V}_q$ can be written as $\mathbb{I}_1 \otimes \mathbb{I}_2 \otimes ... \otimes \hat{f}_q \otimes ... \otimes \mathbb{I}_N$ acting on the full state space $\mathcal{V} = \mathcal{V}_1 \otimes \mathcal{V}_2 \otimes ... \otimes \mathcal{V}_q \otimes ... \otimes \mathcal{V}_N$. This is simplified to $\hat{f}_q$ by omitting all the $\mathbb{I}_j$. If the N particles are identical then $\mathcal{V} = \mathcal{V}_+$ for bosons and $\mathcal{V} = \mathcal{V}_-$ for fermions, and the operator $\hat{f}$ must by symmetric under particle exchange. In this case

$$\hat{F} = \sum_{q=1}^{N} \hat{f}_q$$

is symmetric and is called a one-body operator. One needs the matrix elements for a given basis and this matrix elements can be written as $\langle \text{state}|\hat{F}|\text{state}\rangle$. However, this expression can become very tedious because creating totally symmetric states by applying the symmetrizer or antisymmetrizer to the tensor product state results in $N!$ terms. With $N!$ terms from the bra, N terms from the sum over $\hat{f}_q$ and $N!$ terms from the ket this means $N(N!)^2$ and makes the calculations very cumbersome.

Using creation and annihilation operators allows a much more compact representation for a one-body operator acting on identical particles. In the basis $\{|u_j\rangle\}$ for $\mathcal{V}_q$ one can write

$$\hat{f} = \sum_{jk} f_{jk}\, |u_j\rangle\langle u_k| \qquad f_{jk} = \langle u_j|\hat{f}|u_k\rangle \qquad \Rightarrow \qquad \hat{f}_q = \sum_{jk} f_{jk}\, |u_j\rangle_q\, {}_q\langle u_k| \qquad f_{jk} = {}_q\langle u_j|\hat{f}|u_k\rangle_q$$

and insert into

$$\hat{F} = \sum_{q=1}^{N} \hat{f}_q = \sum_{q=1}^{N}\sum_{jk} f_{jk}\, |u_j\rangle_q\, {}_q\langle u_k| = \sum_{jk} f_{jk} \sum_{q=1}^{N} |u_j\rangle_q\, {}_q\langle u_k| = \begin{cases} \sum_{jk} f_{jk}\, \hat{a}^\dagger_{u_j}\hat{a}_{u_k} & \text{for bosons} \\ \sum_{jk} f_{jk}\, \hat{c}^\dagger_{u_j}\hat{c}_{u_k} & \text{for fermions} \end{cases} \tag{7.10}$$

to get the symmetrized operator where the last step with the creation and annihilation operators needs a proof. The operator $\hat{a}^\dagger_{u_j}\hat{a}_{u_k}$ respectively $\hat{c}^\dagger_{u_j}\hat{c}_{u_k}$ moves a particle from state $|u_k\rangle$ to state $|u_j\rangle$.

The proof determines how $\hat{F}$ acts on a Fock state

$$|n_r, n_s, ...\rangle = \sqrt{\frac{N!}{n_r!\, n_s! ...}}\hat{S}_\pm\, |u_r\rangle_1 ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ...$$

where only

$$\sum_{q=1}^{N} |u_j\rangle_q\, {}_q\langle u_k| \sqrt{\frac{N!}{n_r!\, n_s! ...}}\hat{S}_\pm\, |u_r\rangle_1 ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ...$$

is needed with $n_j = 0, 1, 2, 3, ...$ for bosons and $n_j = 0, 1$ for fermions. The operator is symmetric, and $[\hat{O}_\text{s}, \hat{P}_\alpha] = 0$ for any symmetric operator $\hat{O}_\text{s}$ and any permutation $\hat{P}_\alpha$ such that also $[\hat{O}_\text{s}, \hat{S}_\pm] = 0$. The operators can therefore be exchanged

$$\sqrt{\frac{N!}{n_r!\, n_s! ...}}\hat{S}_\pm \left(\sum_{q=1}^{N} |u_j\rangle_q\, {}_q\langle u_k|\right) |u_r\rangle_1 ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ...$$

and the sum from 1 to N becomes

$$\begin{aligned} &\left(\sum_{q=1}^{N} |u_j\rangle_q\, {}_q\langle u_k|\right) |u_r\rangle_1\, |u_r\rangle_2 ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ... \\ &= \big(|u_j\rangle_1\, {}_1\langle u_k|u_r\rangle_1\big)\, |u_r\rangle_2 ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ... \\ &\quad + |u_j\rangle_1 \big(|u_j\rangle_2\, {}_2\langle u_k|u_r\rangle_2\big) ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ... + ... \\ &= \big(|u_j\rangle_1\, \delta_{kr}\big)\, |u_r\rangle_2 ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ... \\ &\quad + |u_j\rangle_1 \big(|u_j\rangle_2\, \delta_{kr}\big) ... |u_r\rangle_{n_r}\, |u_s\rangle_{n_r+1} ... |u_s\rangle_{n_r+n_s} ... + ... \end{aligned}$$

showing that only a total of n_k terms will be non-zero. The n_k terms $|u_k\rangle$ are transformed into $|u_j\rangle$ and all these n_k terms are permutations of each other. Thus, the whole expression simplifies to

$$\left(\sum_{q=1}^{N} |u_j\rangle_q \, {}_q\langle u_k|\right)\sqrt{\frac{N!}{n_r!\,n_s!...}}\hat{S}_\pm \, |u_r\rangle_1 \, ... \, |u_r\rangle_{n_r} \, |u_s\rangle_{n_r+1} \, ... \, |u_s\rangle_{n_r+n_s} \, ... \, |u_k\rangle_q \, ...$$
$$= n_k\sqrt{\frac{N!}{n_r!\,n_s!...}}\hat{S}_\pm \, |u_r\rangle_1 \, ... \, |u_r\rangle_{n_r} \, |u_s\rangle_{n_r+1} \, ... \, |u_s\rangle_{n_r+n_s} \, ... \, |u_j\rangle_q \, ...$$

showing the action of $\hat{F}$ on a Fock state. The operator $\hat{F}$ picks a particle in state $|u_k\rangle$ and replaces it by a particle in state $|u_j\rangle$. Thus, $\hat{F}$ acting on a Fock state $|n_r, n_s, ...\rangle$ gives another Fock state $|n_r', n_s', ...\rangle$ both in occupation number representation where $n_k' = n_k - 1$ and $n_j' = n_j + 1$. It follows

$$|n_r', n_s', ...\rangle = \sqrt{\frac{N!}{n_r'!\,n_s'!...}}\hat{S}_\pm \, |u_r\rangle_1 \, ... \qquad \Rightarrow \qquad \hat{S}_\pm \, |u_r\rangle_1 \, ... = \sqrt{\frac{n_r'!\,n_s'!...}{N!}} \, |n_r', n_s', ...\rangle$$

and

$$\left(\sum_{q=1}^{N} |u_j\rangle_q \, {}_q\langle u_k|\right)|n_r, n_s, ..., n_k, ..., n_j, ...\rangle = n_k\sqrt{\frac{N!}{n_r!\,n_s!...}}\sqrt{\frac{n_r'!\,n_s'!...}{N!}} \, |n_r', n_s', ...\rangle$$
$$= n_k\sqrt{\frac{n_j+1}{n_k}} \, |n_r', n_s', ...\rangle = \sqrt{n_k(n_j+1)} \, |n_r, n_s, ..., n_k - 1, ..., n_j + 1, ...\rangle$$

making clear that this is equal to

$$\hat{a}_j^\dagger \hat{a}_k \, |n_r, n_s, ..., n_k, ..., n_j, ...\rangle = \sqrt{n_k}\sqrt{n_j+1} \, |n_r, n_s, ..., n_k - 1, ..., n_j + 1, ...\rangle$$

for the bosonic creation and annihilation operators and analogously for the fermionic case.

The term $f_{jk} \, \hat{a}_{u_j}^\dagger \, \hat{a}_{u_k}$ moves one particle from state $|u_k\rangle$ to state $|u_j\rangle$, and f_{jk} is the amplitude associated with this transition. In the basis of its own eigenstates one gets

$$\hat{f} \, |v_n\rangle = f_n \, |v_n\rangle \qquad \Rightarrow \qquad f_{jk} = \langle v_j|\hat{f}|v_k\rangle = f_k \, \langle v_j|v_k\rangle = f_k \, \delta_{jk}$$
$$\Rightarrow \qquad \hat{F} = \sum_{jk} f_{jk}\hat{a}_{v_j}^\dagger \hat{a}_{v_k} = \sum_{jk} f_k \, \delta_{jk}\hat{a}_{v_j}^\dagger \hat{a}_{v_k} = \sum_j f_j \, \hat{a}_{v_j}^\dagger \hat{a}_{v_j} = \sum_j f_j \, \hat{n}_{v_j}$$

such that the one-body operator $\hat{F}$ in the basis of eigenstates simply counts how many particles there are and multiplies this number for each particle by the eigenvalue corresponding to the single-particle state occupied by this particle.

7.13 Two-Body Operators

Also two-body operators can be written in terms of the creation and annihilation operators. An important example is the Coulomb interaction. The state space of two particles is $\mathcal{V}_q \otimes \mathcal{V}_{q'}$ and the operator $\hat{g}_{qq'}$ acts on this two-particle state space. The space state for N particles is $\mathcal{V} = \mathcal{V}_1 \otimes ... \otimes \mathcal{V}_q \otimes \mathcal{V}_{q'} \otimes ... \otimes \mathcal{V}_N$ and the operator is $\mathbb{I}_1 \otimes ... \otimes \hat{g}_{qq'} \otimes ... \otimes \mathbb{I}_N$ but is simply written as $\hat{g}_{qq'}$. For N identical particles the state space has to take symmetrization into account and the operator acting on all N particles becomes

$$\hat{G} = \frac{1}{2}\sum_{\substack{q,q'=1 \\ q \neq q'}}^{N} \hat{g}_{qq'}$$

because it must be symmetric under particle exchange. Such an operator is called a two-body operator and it is very cumbersome when written in terms of all possible permutations.

Instead of working with symmetrized and antisymmetrized tensor products one can build for the two-body operator on the results obtained for the one-body operator. The commutation relations for bosons and the anticommutation relations for fermions are

$$[\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk} \qquad\qquad \{\hat{c}_j, \hat{c}_k^\dagger\} = \delta_{jk}$$

according to (7.6) and (7.9), respectively. Under the assumption that one is always working in the same basis, $\hat{a}_j$ has been written instead of $\hat{a}_{u_j}$ and similarly for the other operators.

The results in the following are applicable for bosons and fermions but are only developed for bosons, and the commutation and anticommutation relations can be written as

$$\left.\begin{aligned}\hat{a}_j\hat{a}_k^\dagger &= \eta\,\hat{a}_k^\dagger\hat{a}_j + \delta_{jk}\\ \hat{a}_j\hat{a}_k &= \eta\,\hat{a}_k\hat{a}_j\end{aligned}\right\}\qquad\text{with}\qquad \eta = \begin{cases}+1 & \text{for bosons}\\ -1 & \text{for fermions}\end{cases}$$

such that

$$\begin{aligned}\hat{a}_j^\dagger\hat{a}_k\hat{a}_\ell^\dagger\hat{a}_m &= \hat{a}_j^\dagger\left(\eta\,\hat{a}_\ell^\dagger\hat{a}_k + \delta_{k\ell}\right)\hat{a}_m = \eta\,\hat{a}_j^\dagger\hat{a}_\ell^\dagger\hat{a}_k\hat{a}_m + \delta_{k\ell}\,\hat{a}_j^\dagger\hat{a}_m = \eta\,\hat{a}_j^\dagger\hat{a}_\ell^\dagger\left(\hat{a}_k\hat{a}_m\right) + \delta_{k\ell}\,\hat{a}_j^\dagger\hat{a}_m\\ &= \eta\,\hat{a}_j^\dagger\hat{a}_\ell^\dagger\left(\eta\,\hat{a}_m\hat{a}_k\right) + \delta_{k\ell}\,\hat{a}_j^\dagger\hat{a}_m = \eta^2\,\hat{a}_j^\dagger\hat{a}_\ell^\dagger\hat{a}_m\hat{a}_k + \delta_{k\ell}\,\hat{a}_j^\dagger\hat{a}_m = \hat{a}_j^\dagger\hat{a}_\ell^\dagger\hat{a}_m\hat{a}_k + \delta_{k\ell}\,\hat{a}_j^\dagger\hat{a}_m\end{aligned}$$

is as a sample formula used below which is independent of whether the particles are bosons or fermions because the factors η cancel.

A special case is $\hat{g}_{qq'} = \hat{f}_q\,\hat{h}_{q'}$ such that $\hat{G}$ becomes

$$\hat{G} = \frac{1}{2}\sum_{\substack{q,q'=1\\ q\neq q'}}^{N}\hat{g}_{qq'} = \frac{1}{2}\left(\sum_{q=1}^{N}\hat{f}_q\sum_{q'=1}^{N}\hat{h}_{q'} - \sum_{q=1}^{N}\hat{f}_q\,\hat{h}_q\right) = \frac{1}{2}\left(\sum_{q=1}^{N}\hat{f}_q\sum_{q'=1}^{N}\hat{h}_{q'} - \sum_{q=1}^{N}\big(\hat{f}\,\hat{h}\big)_q\right)$$

where $\hat{f}_q\,\hat{h}_q$ acts on the same state and can be written as $\big(\hat{f}\,\hat{h}\big)_q$. Interpreting $\big(\hat{f}\,\hat{h}\big)_q$ as another operator shows that each of the sums are one-body operators such that they can be written in terms of creation and annihilation operators

$$\begin{aligned}\hat{G} &= \frac{1}{2}\left(\sum_{j\ell}f_{j\ell}\,\hat{a}_j^\dagger\hat{a}_\ell\sum_{km}h_{km}\,\hat{a}_k^\dagger\hat{a}_m - \sum_{jm}\big(\hat{f}\,\hat{h}\big)_{jm}\hat{a}_j^\dagger\hat{a}_m\right)\\ &= \frac{1}{2}\left(\sum_{jk\ell m}f_{j\ell}\,h_{km}\,\hat{a}_j^\dagger\hat{a}_\ell\,\hat{a}_k^\dagger\hat{a}_m - \sum_{jm}\big(\hat{f}\,\hat{h}\big)_{jm}\hat{a}_j^\dagger\hat{a}_m\right)\\ &= \frac{1}{2}\left(\sum_{jk\ell m}f_{j\ell}\,h_{km}\,\hat{a}_j^\dagger\hat{a}_k^\dagger\hat{a}_m\hat{a}_\ell + \sum_{jk\ell m}f_{j\ell}\,h_{km}\,\delta_{j\ell}\hat{a}_j^\dagger\hat{a}_m - \sum_{jm}\big(\hat{f}\,\hat{h}\big)_{jm}\hat{a}_j^\dagger\hat{a}_m\right)\end{aligned}$$

according to (7.10) and using the above sample formula with η to distinguish bosons and fermions. The second term is

$$\begin{aligned}\sum_{jk\ell m}f_{j\ell}\,h_{km}\,\delta_{j\ell}\hat{a}_j^\dagger\hat{a}_m &= \sum_{j\ell m}\langle u_j|\hat{f}|u_\ell\rangle\,\langle u_\ell|\hat{h}|u_m\rangle\,\hat{a}_j^\dagger\hat{a}_m = \sum_{jm}\langle u_j|\,\hat{f}\left(\sum_{\ell}|u_\ell\rangle\langle u_\ell|\right)\hat{h}\,|u_m\rangle\,\hat{a}_j^\dagger\hat{a}_m\\ &= \sum_{jm}\langle u_j|\,\hat{f}\hat{h}\,|u_m\rangle\,\hat{a}_j^\dagger\hat{a}_m = \sum_{jm}\langle u_j|\,\hat{f}\hat{h}\,|u_m\rangle\,\hat{a}_j^\dagger\hat{a}_m = \sum_{jm}\big(\hat{f}\,\hat{h}\big)_{jm}\hat{a}_j^\dagger\hat{a}_m\end{aligned}$$

and cancels with the third term such that

$$\hat{G} = \frac{1}{2}\sum_{\substack{q,q'=1\\ q\neq q'}}^{N}\hat{g}_{qq'} = \frac{1}{2}\sum_{jk\ell m}f_{j\ell}\,h_{km}\,\hat{a}_j^\dagger\hat{a}_k^\dagger\hat{a}_m\hat{a}_\ell \qquad\qquad \hat{g}_{qq'} = \hat{f}_q\,\hat{h}_{q'}$$

is the two-body operator for the case where $\hat{g}_{qq'}$ can be factorized as $\hat{f}_q\,\hat{h}_{q'}$ into two one-particle operators.

In the general case the two-body operator $\hat{g}_{qq'}$ can always be written as

$$\hat{g}_{qq'} = \sum_{\alpha\beta}c_{\alpha\beta}\hat{f}_q^{\alpha}\,\hat{h}_{q'}^{\beta}$$

where $\hat{g}_{qq'} = \hat{f}_q\,\hat{h}_{q'}$ is the special case with all expansion coefficients $c_{\alpha\beta}$ being zero except for one of them. The example $(\hat{x}_1 - \hat{x}_2)^2 = \hat{x}_1^2 + \hat{x}_2^2 - \hat{x}_1\hat{x}_2 - \hat{x}_2\hat{x}_1$ illustrates how this can be done. Thus,

$$\begin{aligned}\hat{G} &= \frac{1}{2}\sum_{\substack{q,q'=1\\ q\neq q'}}^{N} \hat{g}_{qq'} = \frac{1}{2}\sum_{\substack{q,q'=1\\ q\neq q'}}^{N}\sum_{\alpha\beta} c_{\alpha\beta}\hat{f}_q^{\alpha}\,\hat{h}_{q'}^{\beta} = \frac{1}{2}\sum_{\alpha\beta} c_{\alpha\beta}\sum_{\substack{q,q'=1\\ q\neq q'}}^{N} \hat{f}_q^{\alpha}\,\hat{h}_{q'}^{\beta}\\ &= \frac{1}{2}\sum_{\alpha\beta} c_{\alpha\beta}\sum_{jk\ell m} \langle u_j|\hat{f}_q^{\alpha}|u_\ell\rangle\,\langle u_k|\hat{h}_{q'}^{\beta}|u_m\rangle\;\hat{a}_j^{\dagger}\hat{a}_k^{\dagger}\hat{a}_m\hat{a}_\ell\end{aligned}$$

using the result for the factorized case. Because

$$g_{jk\ell m} = {}_q\langle u_j|\,{}_{q'}\langle u_k|\hat{g}_{qq'}|u_\ell\rangle\,|u_m\rangle_{q'} = \sum_{\alpha\beta} c_{\alpha\beta}\,\langle u_j|\hat{f}_q^{\alpha}|u_\ell\rangle\,\langle u_k|\hat{h}_{q'}^{\beta}|u_m\rangle$$

the result becomes

$$\hat{G} = \frac{1}{2}\sum_{\substack{q,q'=1\\ q\neq q'}}^{N} \hat{g}_{qq'} = \frac{1}{2}\sum_{jk\ell m} g_{jk\ell m}\,\hat{a}_j^{\dagger}\hat{a}_k^{\dagger}\hat{a}_m\hat{a}_\ell \tag{7.11}$$

with $g_{jk\ell m} = {}_q\langle u_j|\,{}_{q'}\langle u_k|\hat{g}_{qq'}|u_\ell\rangle\,|u_m\rangle_{q'}$ for the general case. This formula is applicable for bosons and fermions. Conceptually, this means that there are initially two particles in states u_ℓ and u_m and finally two particles in states u_j and u_k where $g_{jk\ell m}$ is the transition amplitude.

Note that the order of the indices is important. In $g_{jk\ell m}$ the last two indices are ℓm but the order of the annihilation operators is $\hat{a}_m\hat{a}_\ell$. This order is not relevant for bosons with their commutation relations but is important for fermions with their anticommutation relations.

7.14 Changing Basis of Creation and Annihilation Operators

Choosing a good basis can simplify the mathematics of a problem significantly. This is also the case with creation and annihilation operators. Since states and operators can be written in terms of creation and annihilation operators the question is how they transform under a base change. The single-particle basis is $\{|u_j\rangle\}$ with orthonormality $\langle u_j|u_k\rangle = \delta_{jk}$.

The boson creation operator (7.4) and the boson annihilation operator (7.5) act as

$$\hat{a}_{u_j}^{\dagger}\,|n_j\rangle = \sqrt{n_j+1}\,|n_j+1\rangle \qquad\qquad \hat{a}_{u_j}\,|n_j\rangle = \sqrt{n_j}\,|n_j-1\rangle$$

where only the changing occupation number has been listed showing that n_j particles are initially in state $|u_j\rangle$. The fermion creation operator (7.7) and the fermion annihilation operator (7.8) act as

$$\hat{c}_{u_j}^{\dagger}\,|u_n,\ldots\rangle = |u_j,u_n,\ldots\rangle \qquad\qquad \hat{c}_{u_j}\,|u_j,u_n,\ldots\rangle = |u_n,\ldots\rangle$$

in a similar fashion but written using kets from the basis due to the Pauli exclusion principle because occupation numbers can only be 0 or 1. These operators become $\hat{a}_{v_k}^{\dagger}$ and so on in another basis $\{|v_j\rangle\}$ with orthonormality $\langle v_j|v_k\rangle = \delta_{jk}$.

To see how creation and annihilation operators change from basis $\{|u_j\rangle\}$ to basis $\{|v_j\rangle\}$ one can start from the action of the creation operator on the vacuum

$$\hat{a}_{v_k}^{\dagger}\,|0\rangle = |v_k\rangle = \mathbb{I}\,|v_k\rangle = \left(\sum_j |u_j\rangle\langle u_j|\right)|v_k\rangle = \sum_j \langle u_j|v_k\rangle\,|u_j\rangle = \sum_j \langle u_j|v_k\rangle\,\hat{a}_{u_j}^{\dagger}\,|0\rangle$$

and apply it to the annihilation operator

$$\hat{a}_{v_k} = \left(\hat{a}_{v_k}^{\dagger}\right)^{\dagger} = \left(\sum_j \langle u_j|v_k\rangle\,\hat{a}_{u_j}^{\dagger}\right)^{\dagger} = \sum_j \langle u_j|v_k\rangle^{*}\left(\hat{a}_{u_j}^{\dagger}\right)^{\dagger} = \sum_j \langle v_k|u_j\rangle\,\hat{a}_{u_j}$$

using $\langle u_j|v_k\rangle^\dagger = \langle u_j|v_k\rangle^* = \langle v_k|u_j\rangle$. The result for fermionic operators is the same. Thus, the creation and annihilation operators change as

$$\hat{a}^\dagger_{v_k} = \sum_j \langle u_j|v_k\rangle\, \hat{a}^\dagger_{u_j} \qquad\qquad \hat{a}_{v_k} = \sum_j \langle v_k|u_j\rangle\, \hat{a}_{u_j} \tag{7.12}$$

for bosons and fermions when going from the basis $\{|u_j\rangle\}$ to the basis $\{|v_j\rangle\}$.

As a sanity check one can examine how the commutation relations (7.6) and the anticommutation relations (7.9) behave under a basis change. The commutation relation are

$$\begin{aligned}
[\hat{a}_{v_k}, \hat{a}^\dagger_{v_m}] &= \left[\sum_j \langle v_k|u_j\rangle\, \hat{a}_{u_j}, \sum_\ell \langle u_\ell|v_m\rangle\, \hat{a}^\dagger_{u_\ell}\right] = \sum_{j\ell} \langle v_k|u_j\rangle \langle u_\ell|v_m\rangle\, [\hat{a}_{u_j}, \hat{a}^\dagger_{u_\ell}] = \sum_{j\ell} \langle v_k|u_j\rangle \langle u_\ell|v_m\rangle\, \delta_{j\ell} \\
&= \sum_\ell \langle v_k|u_\ell\rangle \langle u_\ell|v_m\rangle = \langle v_k| \left(\sum_\ell |u_\ell\rangle\langle u_\ell|\right) |v_m\rangle = \langle v_k|\, \mathbb{I}\, |v_m\rangle = \langle v_k|v_m\rangle = \delta_{km}
\end{aligned}$$

in the new basis, and similar calculations for the other three operators show the same.

A last check determines how the particle number operator $\hat{N}$ transforms under a basis change. It is in the new basis

$$\begin{aligned}
\hat{N} &= \sum_k \hat{n}_{v_k} = \sum_k \hat{a}^\dagger_{v_k} \hat{a}_{v_k} = \sum_k \left(\sum_j \langle u_j|v_k\rangle\, \hat{a}^\dagger_{u_j}\right) \left(\sum_\ell \langle v_k|u_\ell\rangle\, \hat{a}_{u_\ell}\right) = \sum_{kj\ell} \langle u_j|v_k\rangle \langle v_k|u_\ell\rangle\, \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} \\
&= \sum_{j\ell} \langle u_j| \left(\sum_k |v_k\rangle\langle v_k|\right) |u_\ell\rangle\, \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} = \sum_{j\ell} \langle u_j|u_\ell\rangle\, \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} = \sum_{j\ell} \delta_{j\ell}\, \hat{a}^\dagger_{u_j} \hat{a}_{u_\ell} = \sum_j \hat{a}^\dagger_{u_j} \hat{a}_{u_j} = \sum_j \hat{n}_{u_j}
\end{aligned}$$

and transforms therefore as expected. The number of particles is conserved under the change of the basis as it is required by physics.