Chapter 9

Quantum Mechanics of Identical Particles

Up to now we considered only one-body systems. The special success of quantum mechanics can be seen in the prediction of observables of systems consisting of more than two particles, i.e., $N = 3, 4, \cdots$. In this description one has to consider that the particles are identical. The symmetry properties following from the identity of the particles are crucial for the understanding of atomic properties, matter properties, properties of nuclei and even properties of elementary particles.

9.1 General Rules for Describing Several Identical Particles

Analogous to classical mechanics, a quantum mechanical system of N particles is described by a set of fundamental observables for each particle. In non-relativistic physics, those are

$$
\begin{aligned}
\text{position} &\quad \vec{X}_i \\
\text{momentum} &\quad \vec{P}_i \\
\text{spin} &\quad \vec{S}_i
\end{aligned}
$$

$$(9.1)$$

where i describes the corresponding particle, $i = 1, 2, \cdots, N$. The states of each particle are elements of a Hilbert space, in which the operators act. The total system has in

addition

$$\text{total momentum} \quad \vec{P} \;=\; \sum_i \vec{P}_i$$

$$\text{total spin} \quad \vec{S} \;=\; \sum_i S_i \;.$$

$$(9.2)$$

Those operators act in the product space

$$\mathcal{H} \;=\; \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N \;=\; \prod_{i=1}^{N} \otimes \mathcal{H}_i \;. \tag{9.3}$$

For additive observables (9.2), the eigenvalues are obtained by adding the single eigenvalues. Thus, for distinguishable particles, the following **axiom** holds:

The Hilbert space for a system of particles is given by the product of the single Hilbert space.

However, for identical particles, restrictions may apply. Let us consider as simple application of the axiom the hydrogen atom as two-particle system. The index 1 refers to the electron of mass m_e and the index 2 to the proton of mass m_p. The total energy is given by the Hamiltonian

$$H \;=\; \frac{1}{2m_e}\,\vec{P}_1^2 \;+\; \frac{1}{2m_p}\,\vec{P}_2^2 \;+\; V(\mid \vec{X}_1 - \vec{X}_2 \mid, \vec{L}, \vec{S}_1, \vec{S}_2) \;. \tag{9.4}$$

The potential V depends on the relative distance $\mid \vec{X}_1 - \vec{X}_2 \mid \,:=\; \vec{X}$, the orbital angular momentum $\vec{L}$ with respect to the center-of-mass (c.m.) and the spins $\vec{S}_1$ and $\vec{S}_2$ of electron and proton. It contains the following interaction terms:

- The Coulomb attraction $-\frac{e^2}{|\vec{x}|}$

- The spin-orbit coupling of the electron $V_{LS}, \vec{S}_1 \cdot \vec{L}$

- The coupling between the spins of the electron and the proton

$$2\,\frac{\mu_B \mu_N}{\mid \vec{X} \mid^3}\,[\vec{S}_1 \cdot \vec{S}_2 \;-\; \frac{3}{\mid \vec{X} \mid^2}\,\vec{S}_1 \cdot \vec{X}\,\vec{S}_2 \cdot \vec{X}]$$
$$-\; \mu_B \mu_N\,\delta^3(\vec{X})\,\vec{S}_1 \cdot \vec{S}_2\,8\pi \;.$$

The first two contribute to the normal spectrum, the last to the hyperfine splitting. The Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ of the hydrogen atom is spanned by states

$$| \vec{r}_1, \vec{r}_2; \vec{S}_1, \vec{S}_2 \rangle = | \vec{r}_1 \vec{S}_1 \rangle_{(1)} \; | \vec{r}_2 S_2 \rangle_{(2)} \; . \tag{9.5}$$

Since H is translation invariant, one introduces c.m. and relative coordinates

$$\vec{R} = \frac{m_e \vec{r}_1 + M \vec{r}_2}{m_e + M}$$
$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\tag{9.6}$$

and writes

$$| \vec{R}, \vec{r}; \; \vec{S}_1 \vec{S}_2 \rangle$$

for the states. For the wave function

$$\psi(\vec{R}, \vec{r}, \vec{S}_1, \vec{S}_2) = \langle \vec{R}, \vec{r}, S_1, S_2 \mid \psi \rangle \; , \tag{9.7}$$

one introduces the ansatz

$$\psi(\vec{R}, \vec{r}, \vec{S}_1, \vec{S}_2) = \phi(\vec{R}) \; \psi(\vec{r}, \vec{S}_1, \vec{S}_2) \tag{9.8}$$

which separates the physical uninteresting c.m. motion off.

9.2   System of Two Identical Particles

As long as two electrons are separated by a macroscopic distance, they can be considered as distinguishable. However, if they are separated by atomic distances, this is no longer possible since due to the uncertainty principal one cannot follow the separate trajectories.
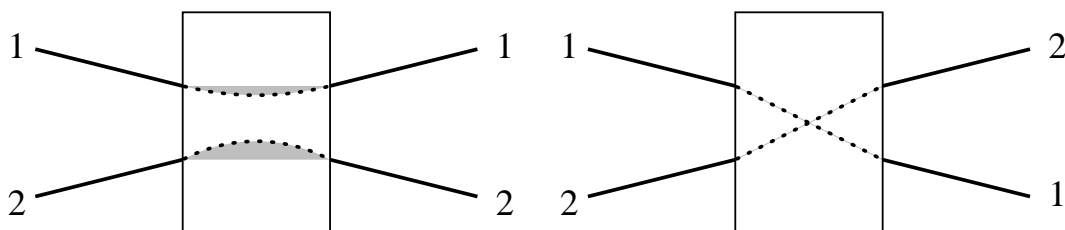

Fig. 9.1 Indistinguishability of Two Electrons

Thus, in quantum mechanics of such systems, only observables $A(1,2)$ can be considered, which are symmetric with respect to the permutation of the indices

$$A(1,2) = A(2,1) . \tag{9.9}$$

The Hamiltonian for two electrons can be written as

$$H = \frac{1}{2m_e} \vec{P}_1^2 + \frac{1}{2m_e} \vec{P}_2^2 + \frac{e^2}{|\vec{X}_1 - \vec{X}_2|} \tag{9.10}$$

which shows explicitly that $H(1,2) = H(2,1)$. We introduce the permutation of two objects as

$$\tau := \begin{pmatrix} 1 & 2 \\ \downarrow & \downarrow \\ 2 & 1 \end{pmatrix} := \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} . \tag{9.11}$$

This "transposition" τ is a symmetry operation and can be represented in a Hilbert space by a unitary operator

$$P := U(\tau) \tag{9.12}$$

with the property

$$P^2 = \mathbf{1} . \tag{9.13}$$

Because of the unitary, we have $P = P^{-1} = P^\dagger$. According to the definition of a symmetry operation, we have

$$A(2,1) = P\, A(1,2) P^{-1} , \tag{9.14}$$

and with (9.9) follows

$$[P, A(1,2)] = 0 . \tag{9.15}$$

Thus, **all** observables of identical particles commute with the permutation operator, especially the Hamiltonian.

Since the preparation of a two-particle state is only possible via observables (which are symmetric with respect to a transposition of the particles), the states $|\psi(1,2)\rangle$ and $P|\psi(1,2)\rangle$ cannot be distinguished. However, this does not mean that one always has a two-fold degeneracy. According to (9.13) P has the eigenvalues $+1$ and -1. Thus each state $|\psi(1,2)\rangle$ can be decomposed into a symmetric piece and an antisymmetric piece:

$$
\begin{aligned}
\sqrt{2}\ |\psi(1,2)\rangle &= \frac{1}{\sqrt{2}} (\mathbf{1} + P)\ |\psi(1,2)\rangle + \frac{1}{\sqrt{2}} (\mathbf{1} - P)\ |\psi(1,2)\rangle \\
&=: \ |\psi_S(1,2)\rangle + \ |\psi_A(1,2)\rangle
\end{aligned}
\tag{9.16}
$$

with

$$P \mid \psi_S \rangle = + \mid \psi_S \rangle$$
$$P \mid \psi_A \rangle = - \mid \psi_A \rangle .$$

$$(9.17)$$

The two components of the decomposition are orthogonal

$$
\begin{aligned}
\langle \psi_S \mid \psi_A \rangle &= \frac{1}{2} \langle \psi \mid (\mathbf{1} + P)(\mathbf{1} - P) \mid \psi \rangle \\
&= \frac{1}{2} \langle \psi \mid \mathbf{1} - P^2 \mid \psi \rangle \\
&= 0 .
\end{aligned}
$$

$$(9.18)$$

Thus (9.16) provides an orthogonal decomposition of the product Hilbert space of the two particles

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_S \otimes \mathcal{H}_A .$$

$$(9.19)$$

Furthermore, the symmetry character of such as a state can neither be changed through measurement (due to (9.15)) nor through time development since

$$\mid \psi_{S,A} \rangle_t = e^{-\frac{i}{\hbar} Ht} \mid \psi_{S,A} \rangle_{t=0} .$$

Thus we can say that the states of a system of two identical particles are either all symmetric or all antisymmetric. When considering a system of identical particles, we are either in $\mathcal{H}_S$ or in $\mathcal{H}_A$. Which of the symmetry properties are realized can only be determined by the initial conditions. W. Pauli showed 1940 via means of quantum field theory that there is a connection between the symmetry properties of a system of identical particles and their spins:

- Identical particles with integer spin (e.g., mesons, photons, α-particles) are described by symmetric state vectors (Bosons).

- Identical particles with half-integer spin (e.g., electrons, nucleons, neutrinos) are described by antisymmetric state vectors (Fermions).

Remark: For $N \geq 3$, Pauli's proof had apart from the principles of quantum field theory to make the additional assumption that the states in either case are either symmetric or antisymmetric.

9.3 Permutation Group for Three Particles

A transposition is given as the interchange of two items in a group. As example take three elements, g_1, g_2, and g_3. There are $3!=6$ possible transpositions in the ordering of these items:

$$
\begin{aligned}
e &: g_1\ g_2\ g_3 \ \rightarrow\ g_1\ g_2\ g_3 \quad \text{(no change)} \\
p &: g_1\ g_2\ g_3 \ \rightarrow\ g_2\ g_3\ g_1 \quad \text{(all one up)} \\
q &: g_1\ g_2\ g_3 \ \rightarrow\ g_3\ g_1\ g_2 \quad \text{(last to front)} \\
r &: g_1\ g_2\ g_3 \ \rightarrow\ g_1\ g_3\ g_2 \quad \text{(interchange 2 and 3)} \\
s &: g_1\ g_2\ g_3 \ \rightarrow\ g_3\ g_2\ g_1 \quad \text{(interchange 1 and 3)} \\
t &: g_1\ g_2\ g_3 \ \rightarrow\ g_2\ g_1\ g_3 \quad \text{(interchange 1 and 2)}
\end{aligned}
\tag{9.20}
$$

This group is called the symmetric group S_3 and has $3!$ elements. In general, the symmetric group S_N has $N!$ elements. The standard representation of the elements of S_3 can be written as

$$
\begin{aligned}
e &\equiv \begin{pmatrix} g_1 & g_2 & g_3 \\ g_1 & g_2 & g_3 \end{pmatrix} &
p &\equiv \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_3 & g_1 \end{pmatrix} &
q &\equiv \begin{pmatrix} g_1 & g_2 & g_3 \\ g_3 & g_1 & g_2 \end{pmatrix} \\[2mm]
r &\equiv \begin{pmatrix} g_1 & g_2 & g_3 \\ g_1 & g_3 & g_2 \end{pmatrix} &
s &\equiv \begin{pmatrix} g_1 & g_2 & g_3 \\ g_3 & g_2 & g_1 \end{pmatrix} &
t &\equiv \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_1 & g_3 \end{pmatrix}
\end{aligned}
\tag{9.21}
$$

Note: The ordering of the items in the e.g the first row is unimportant as long as the type of permutation is preserved, i.e.

$$
r = \begin{pmatrix} g_1 & g_2 & g_3 \\ g_1 & g_3 & g_2 \end{pmatrix} \quad \text{and} \quad r = \begin{pmatrix} g_2 & g_1 & g_3 \\ g_2 & g_3 & g_1 \end{pmatrix}
\tag{9.22}
$$

are the same element of the permutation group, namely r interchanges elements 2 and 3, and leaves 1 alone.

We can consider "multiplication" of permutations, e.g.

$$
p \cdot r = \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_3 & g_1 \end{pmatrix} \odot \begin{pmatrix} g_2 & g_1 & g_3 \\ g_2 & g_3 & g_1 \end{pmatrix} = \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_1 & g_3 \end{pmatrix} = t
\tag{9.23}
$$

which shows that the set of 6 elements in S_3 is **not** independent. In fact, one obtains

$$
\begin{aligned}
p \cdot p &= \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_3 & g_1 \end{pmatrix} \odot \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_3 & g_1 \end{pmatrix} = \begin{pmatrix} g_1 & g_2 & g_3 \\ g_3 & g_1 & g_2 \end{pmatrix} = q \\[2mm]
p \cdot p \cdot r &= q \cdot r = \begin{pmatrix} g_1 & g_2 & g_3 \\ g_3 & g_1 & g_2 \end{pmatrix} \odot \begin{pmatrix} g_1 & g_2 & g_3 \\ g_3 & g_2 & g_1 \end{pmatrix} = s\ .
\end{aligned}
\tag{9.24}
$$

This means, S_3 has only three independent elements. The set of elements $\{e, p, q\}$ forms a sub-group, with the inverse elements $q^{-1} = p$ and $p^{-1} = q$.

9.4 Matrix Representation of a Group

According to Cayley's theorem, every finite group is isomorphic to a sub-group of the permutation group. Thus by discussing matrix representations of a the elements of the permutation group, we investigate matrix representations of finite groups in general.

As example, we consider the matrix representation of S_3. Consider the column vector

$$v = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}. \tag{9.25}$$

Now construct a matrix such that the multiplication of v with this matrix gives the reordering of a given element of S_3:

$$\mathcal{M}_1(e) \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathcal{M}_1(p) \equiv \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

$$\mathcal{M}_1(q) \equiv \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \mathcal{M}_1(r) \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\mathcal{M}_1(s) \equiv \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \mathcal{M}_1(t) \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{9.26}$$

The matrices $\mathcal{M}_1$ under ordinary matrix multiplication form a group that is isomorphic to S_3. This group is known as the matrix representation of S_3. Pay attention to the order of the matrix multiplication:

$$p \cdot r = t \quad \rightarrow \quad \mathcal{M}_1(p \cdot r)v = \mathcal{M}_1(r)\mathcal{M}_1(p)v. \tag{9.27}$$

In general, a set of matrices under matrix multiplication that is either isomorphic or homomorphic to a group G is a matrix representation of G denoted by Γ. If the matrices of the representation are of dimension $N \times N$, then the matrix representation is said to be N-dimensional.

There are many possible matrix representations of a group G, e.g. from a representation Γ one can generate a representation Γ' by similarity transformations U, i.e.

$$\mathcal{M}'(g_i) \equiv U^{-1}\mathcal{M}(g_i)U \tag{9.28}$$

for every $g_i \in G$ forms a representation Γ' of the same dimension. The group representations of Γ and Γ' are identical. As such, Γ and Γ' are said to be **equivalent representations**.

In the representation $\Gamma(G)$ the **character of a group element** $\chi(a)$ of a group element a is defined as the trace of the representation matrix Γ,

$$\chi(a) = Tr(\Gamma) = \sum_i^n \Gamma_{ii}(a). \tag{9.29}$$

The character of the unit element e is given by the dimension n of the representation, $\chi(e) = n$. Since the trace of a matrix is invariant under similarity transformations, the group element a has the same character for equivalent representations. For the characters of the representation $\mathcal{M}_1$ of S_3 are given by:

$$\begin{aligned} \chi(e) &= 3 \\ \chi(r) &= \chi(s) = \chi(t) = 1 \\ \chi(p) &= \chi(q) = 0 \ . \end{aligned} \tag{9.30}$$

9.5 Important Results About Representations of the Permutation Group

In order to generalize the results of the previous section to systems of N particles, we formulate the results in the view of group theory. Let us consider the permutation of two objects:

$$\mathbf{1} := \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix} \ ; \quad \text{Identity}$$

$$\tau := \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \ ; \quad \text{Transposition}$$

$$\tag{9.31}$$

Furthermore, one has $\tau^2 = \mathbf{1}; \tau^{-1} = \tau$. Thus, the set $\{\mathbf{1}, \tau\}$ forms an Abelian group, the symmetric group $\mathbf{S}_2$.

In the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ of two particles, $\mathbf{1}$ and τ are represented by the unitary operators $\mathbf{1}$ and $P = U(\tau)$. Starting from an arbitrary state $|\psi(1,2)\rangle$ from this Hilbert space, the states

$$|\psi(1,2)\rangle \quad \text{and} \quad |\psi(2,1)\rangle = P|\psi(1,2)\rangle \tag{9.32}$$

span the two-dimensional representation of $\mathbf{S}_2$. This space gives only a reducible represen-

tation, which can be reduced by building the symmetric and antisymmetric combinations

$$
\begin{aligned}
| \psi_S \rangle &= \frac{1}{\sqrt{2}} \left(| \psi(1,2) \rangle + | \psi(2,1) \rangle \right) \\
&= \frac{1}{\sqrt{2}} \left(\mathbf{1} + P \right) | \psi(1,2) \rangle \\
| \psi_A \rangle &= \frac{1}{\sqrt{2}} \left(| \psi(1,2) \rangle - | \psi(2,1) \rangle \right) \\
&= \frac{1}{\sqrt{2}} \left(\mathbf{1} - P \right) | \psi(1,2) \rangle .
\end{aligned}
\tag{9.33}
$$

Each of these vectors spans a one-dimensional space, constituting a representation of $\mathbf{S}_2$. These spaces are completely described by giving

$$
\begin{aligned}
(\mathbf{1}, \tau) &\longmapsto (+1, +1) \quad \text{for} \quad | \psi_S \rangle \\
(\mathbf{1}, \tau) &\longmapsto (+1, -1) \quad \text{for} \quad | \psi_A \rangle .
\end{aligned}
\tag{9.34}
$$

We encounter here a special case of the general theorem, stating that irreducible representations of Abelian groups are one-dimensional. For the generalization to N particle systems, we need information about the irreducible representations of the permutation group of N objects, the symmetric group $\mathbf{S}_N$. Only results are given. For details, see, e.g., A. Messiah, *Quantum Mechanics*, Vol. II, Appendix D.

The group $\mathbf{S}_N$ consists of $N!$ permutations of N objects

$$
\begin{pmatrix}
1 & 2 & 3 & \cdots & N \\
\nu_1 & \nu_2 & \nu_3 & \cdots & \nu_N
\end{pmatrix} .
\tag{9.35}
$$

Especially important are **transpositions**, which permute only two objects, e.g.,

$$
\tau := \begin{pmatrix}
1 & 2 & 3 & \cdots & N \\
2 & 1 & 3 & \cdots & N
\end{pmatrix} =: (1 \ 2)
\tag{9.36}
$$

and **cyclic permutations**

$$
\sigma := \begin{pmatrix}
1 & 2 & 3 & 4 & \cdots & N-1 & N \\
2 & 3 & 4 & 5 & \cdots & N & 1
\end{pmatrix} =: (1 \ 2 \ \cdots \ N) .
\tag{9.37}
$$

One can see immediately that

$$
\tau^2 = \mathbf{1} \ ; \quad \sigma^N = \mathbf{1} .
\tag{9.38}
$$

One can further show that any permutation P can be obtained by successive transpositions. A permutation P is called even or odd corresponding to the number of transpositions necessary to obtain P, and one defines

$$
\begin{aligned}
(-1)^P &:= +1 \ , \quad \text{if } P \text{ is even} \\
(-1)^P &:= -1 \ , \quad \text{if } P \text{ is odd} .
\end{aligned}
$$

(9.39)

The set $\mathcal{A}_N$ of all even permutations defines a subgroup of $\mathbf{S}_N$. As example we consider the group $\mathbf{S}_3$ with $3! = 6$ elements. All even permutations can be achieved by cyclic permutations:

$$
\mathbf{1} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} \ ; \quad \sigma = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \ ; \quad \sigma^2 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} .
$$

(9.40)

If one denotes with P_{ij} the permutation of the ith object with the jth object, then

$$
P_{12}P_{23} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \\ - & - & - \\ 2 & 3 & 1 \end{pmatrix} \quad \Rightarrow \quad P_{12}P_{23} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} = \sigma
$$

(9.41)

and

$$
P_{13}P_{23} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \\ - & - & - \\ 3 & 1 & 2 \end{pmatrix} \quad \Rightarrow \quad P_{13}P_{23} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} = \sigma^2 .
$$

(9.42)

The odd elements can be generated by σ and a transposition τ, e.g., $\tau = P_{12}$. Then

$$
\sigma\tau = P_{12}P_{23}P_{12} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} = P_{13}
$$

(9.43)

$$
\sigma^2\tau = P_{13}P_{23}P_{12} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} = P_{23} .
$$

(9.44)

Obviously we have

$$
\mathcal{A}_N = \{\mathbf{1}, \sigma, \sigma^2\} .
$$

(9.45)

Thus, in calculations of three-body systems, it is sufficient to use the operators $\mathbf{1}, \sigma, \sigma^2$ to describe all possible permutations.

In order to construct irreducible representations of $\mathbf{S}_N$, one needs further schemes and definitions.

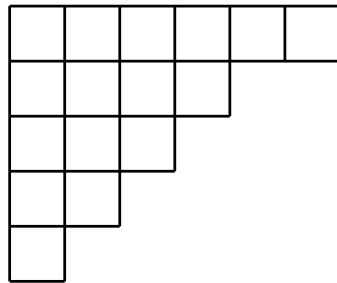An additive decomposition of the number N into natural numbers λ_i

$$N = \lambda_1 + \lambda_2 + \cdots \lambda_r; \quad \lambda_i \in \mathbf{N} \tag{9.46}$$

with

$$\lambda_1 \geq \lambda_1 \geq \cdots \geq \lambda_r \tag{9.47}$$

is called **partition** of N. Obviously, one has for the number r of components $r \leq N$.

Each partition can be represented by a **Young diagram**, which is built up by N squares, ordered in r subsequent rows. The first row consists of λ_1, the second row of λ_2 $\cdots$ the rth row of λ_r squares:

$\lambda_1 = 6$

$\lambda_2 = 4$

$\lambda_3 = 3$

$\lambda_4 = 2$

$\lambda_5 = 1$ **Fig. 9.2** Young-Diagram for the Partition $16 = 6 + 4 + 3 + 2 + 1$

The most important result from the theory of representations of the permutation group can be formulated as follows:

- For each partition of N, i.e., for each Young diagram built out of N squares, there exists an irreducible representation of $\mathbf{S}_N$. Non-equivalent representations correspond to different Young diagrams.

The procedure for constructing the representation is such that first one distributes the N numbers $1, 2, \cdots, N$ in an arbitrary way across the squares of a Young diagram. Each distribution of numbers obtained this way is called **Young Tableau**.

Fig. 9.3 Young Tableau for 16 = 6 + 4 + 3 + 2 + 1.

Especially important are the **standard tableaux**. In those the numbers in each row and column are in ascending order. Fig. 9.3 does not show a standard tableau but Fig. 9.4 does.
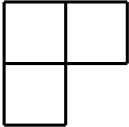

Fig. 9.4 Possible Standard Tableau for 16 = 6 + 4 + 3 + 2 + 1.

The number of all distinguishable standard tableaux, which can be found for a partition of N, gives the dimension of the irreducible representation, which belongs to this partition and its Young diagram.

Example: $N = 3$
The possible partitions and the Young diagrams:

Partition	**abbrev. notation**	**Young diagram**
$3 = 3$	$[\,3\,]$	
$3 = 2 + 1$	$[\,2\,,\,1\,]$	
$3 = 1 + 1 + 1$	$[\,1\,,\,1\,,\,1\,] = [\,1^{3}\,]$	

Standard - Tableaux for N = 3

$[\,3\,]$

1	2	3

$[\,2\,,\,1\,]$

1	2
3	

1	3
2	

$[\,1\,,\,1\,,\,1\,]$

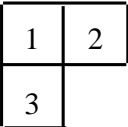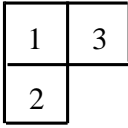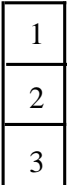| 1 |
|---|
| 2 |
| 3 |
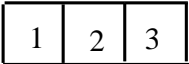
Fig. 9.5 Tableaux for $N = 3$.

As can be seen, there is only one diagram for $[3]$ and $[1^3]$. In both cases the irreducible

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representations are one-dimensional. For $[2, 1]$, there are two standard tableaux, thus the irreducible representation is two-dimensional.

Standard - Tableaux for N = 4
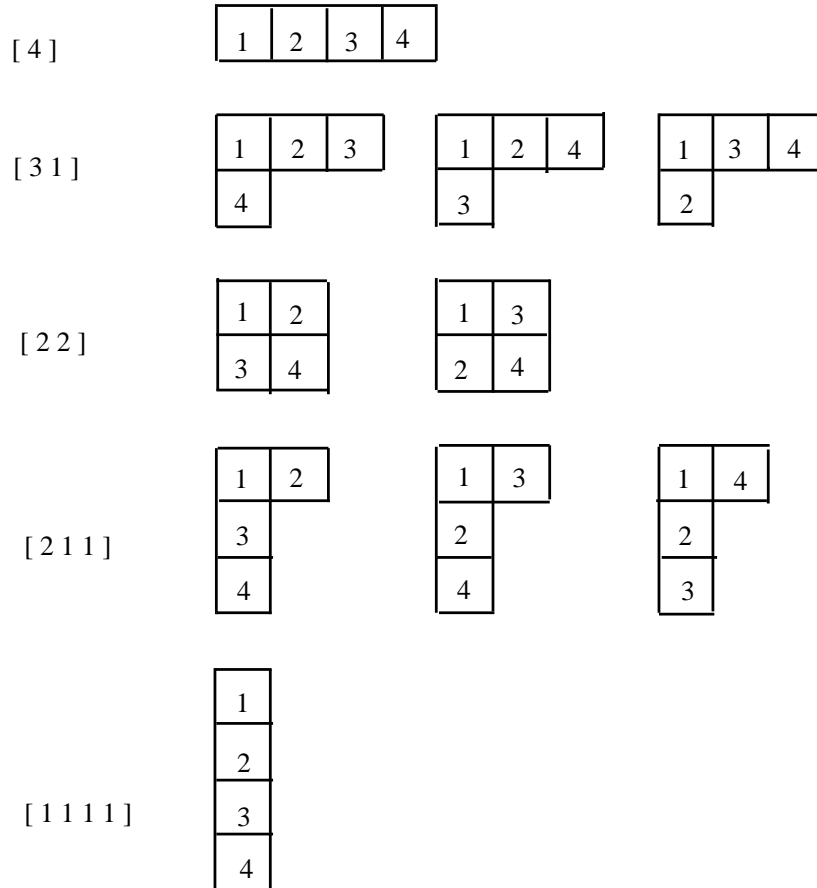
Fig. 9.6 Tableaux for $N = 4$.

The procedure for entering the numbers is to put the number n into that square which, when removed from α_n, gives the Young diagram α_{n-1}. The number $(n-1)$ is put in that square which, when removed, gives the Young diagram α_{n-2}, and so on. By the manner of construction, it is clear that the numbers in the squares of a Young tableau must decrease to the left and upwards. Because of the completeness of this labeling system, it follows immediately that the dimension of the irreducible representation is equal to the number of different tableaux obtainable from the Young diagram α_n.

The explicit construction of a specific representation in the N-particle product Hilbert

space of (9.3) has a general state $|\,\psi(1,2,\cdots,N)\rangle$ from this space and a specific standard tableau. For this tableau, one considers all horizontal permutations P, in which only objects in a specific row are permuted, and all vertical permutations Q, in which only objects in a column are permuted. The set of all P and the set of all Q form a subgroup of $\mathbf{S}_N$. For the specific tableau, one defines the operator

$$E := \left(\sum_{Q} (-1)^Q\, Q\right) \left(\sum_{P} P\right) = \sum_{PQ} (-1)^Q\, QP\ , \tag{9.48}$$

where the sum is taken over all horizontal and vertical permutations. Those are already to be understood as operators in the product Hilbert space. It can be shown that E is a projection operator, i.e.,

$$E^2 = \alpha_E\, E\ ,\quad \alpha_E \in \mathbf{R}\ . \tag{9.49}$$

In addition, one can show that operators E and E' defined from different standard tableaux are orthogonal:

$$E'E = EE' = 0\ . \tag{9.50}$$

The state

$$|\,\psi_E\rangle := E\,|\,\psi(1,2,\cdots,N)\rangle \tag{9.51}$$

belongs to the corresponding irreducible representation. A complete basis can be obtained by building the linear combination

$$\sum_{R} a_R\, R\ ;\quad a_R \in \mathcal{C}\ , \tag{9.52}$$

where R runs over **all** elements of $\mathbf{S}_N$ and a subsequent application on $|\,\psi_E\rangle$:

$$\sum_{R} a_R\, R\,|\,\psi_E\rangle = \sum_{R} a_R\, R\, E\,|\,\psi(1,2,\cdots,N)\rangle\ . \tag{9.53}$$

However, not every state obtained this way is linear independent. The number of linear independent vectors, the dimension of the representation, is given by the number of different standard tableaux of the considered partition.

As examples, we consider the two most simple cases, $N = 2$ and $N = 3$.

For **N = 2** we have to recover the results given in (9.32) - (9.34). The partitions, Young diagrams, standard tableaux and the operators of (9.48) are given below:

[2] ▯▯ | 1 | 2 | E = 1 + P

[1 1] ▯/▯ | 1 |/| 2 | E = 1 - P
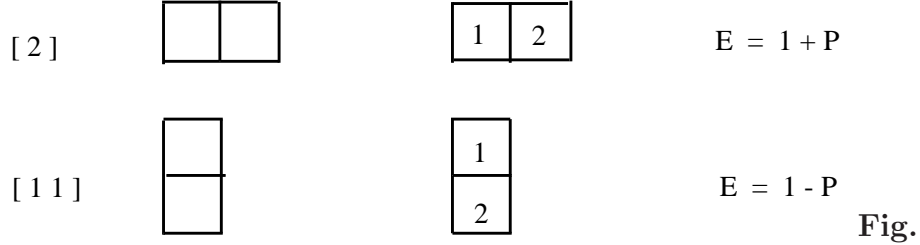
Fig.
9.7 Young diagrams and standard tableau for $N = 2$.

For the partition [2], the vector constructed according to (9.51) gives the symmetric state $\mid \psi_S \rangle$, and for [1 1] we obtain the antisymmetric state $\mid \psi_A \rangle$. If we form operators according to (9.52), we only obtain multiples of the starting vectors, since either $R = \mathbf{1}$ or $R = P$, and those operators change at most the sign.

For $\underline{\mathbf{N} = \mathbf{3}}$ we obtain all Young diagrams and standard tableaux already given in Fig. 9.5. From the tableau corresponding to [3], one obtains via (9.48) the symmetrization operator ("symmetrizer")

$$E_S \; := \; \sum_P \; P \tag{9.54}$$

and from [1 1 1], the anti-symmetrization operator ("anti-symmetrizer")

$$E_A \; := \; \sum_Q \; (-1)^Q \; Q \; . \tag{9.55}$$

In both cases, one has to sum over all elements of $\mathbf{S}_3$. The states $\mid \psi_S \rangle$ and $\mid \psi_A \rangle$ calculated with E_S and E_A, according to (9.48) are

$$\begin{aligned}
\sqrt{6} \mid \psi_S \rangle \; := \; & E_S \mid (1,2,3) \rangle \\
= \; & \mid \psi(1,2,3) \rangle + \; \mid \psi(2,3,1) \rangle + \; \mid \psi(3,1,2) \rangle \\
+ \; & \mid \psi(2,1,3) \rangle + \; \mid \psi(3,2,1) \rangle + \; \mid \psi(1,3,2) \rangle
\end{aligned} \tag{9.56}$$

and

$$\begin{aligned}
\sqrt{6} \mid \psi_A \; := \; & E_A \mid \psi(1,2,3) \rangle \\
= \; & \mid \psi(1,2,3) \rangle + \; \mid \psi(2,3,1) \rangle + \mid \psi(3,1,2) \rangle \\
- \; & \mid \psi(2,1,3) \rangle - \; \mid \psi(3,2,1) \rangle - \; \mid \psi(1,3,2) \rangle \; .
\end{aligned} \tag{9.57}$$

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Here $|\,\psi_S\rangle$ is totally symmetric and applying a permutation P gives

$$P\,|\,\psi_S\rangle \;=\; |\,\psi_S\rangle \;, \tag{9.58}$$

whereas $|\,\psi_A\rangle$ is totally antisymmetric and applying P gives

$$P\,|\,\psi_A\rangle \;=\; (-1)^P\,|\,\psi_A\rangle \;. \tag{9.59}$$

In their generic properties, $|\,\psi_S\rangle$ and $|\,\psi_A\rangle$ correspond to the equivalent states for $N = 2$. New features are obtained from the partition $[2\ \ 1]$ and the corresponding standard tableaux. We consider only the first one as given in Fig. 9.5 and obtain from (9.48)

$$E_M \;:=\; (\mathbf{1} - P_{13})(\mathbf{1} + P_{12}) \;=\; \mathbf{1} + P_{12} - P_{13} - P_{13}P_{12} \;. \tag{9.60}$$

The index M denotes mixed symmetry. (Remember Q are the vertical permutations in (9.48) which enter with $(-1)^Q$.) Applying E_M gives

$$\begin{aligned}
|\,\psi_1^M\rangle \;&:=\; E_M\,|\,\psi(1,2,3)\rangle \\
&=\; |\,\psi(1,2,3)\rangle + |\,\psi(2,1,3)\rangle - |\,\psi(3,2,1)\rangle - |\,\psi(2,3,1)\rangle \;.
\end{aligned} \tag{9.61}$$

Using (9.40), (9.43) and (9.44), it is relatively easy to construct the operators of (9.52). We use the transposition $\tau = P_{12}$ and the cyclic permutation $\sigma = P_{13}P_{12}$. Every other operator is obtained by multiple application of these two:

$$\begin{aligned}
|\,\psi_2^M\rangle \;&:=\; \tau\,|\,\psi_1^M\rangle \\
&=\; |\,\psi(2,1,3)\rangle + |\,\psi(1,2,3)\rangle - |\,\psi(3,1,2)\rangle - |\,\psi(1,3,2)\rangle \;.
\end{aligned} \tag{9.62}$$

The states $|\,\psi_1^M\rangle$ and $|\,\psi_2^M\rangle$ are linear independent and span a two-dimensional space. Because of $\tau^2 = \mathbf{1}$, one has

$$\tau\,|\,\psi_2^M\rangle \;=\; |\,\psi_1^M\rangle \;. \tag{9.63}$$

Furthermore, one finds

$$\begin{aligned}
\sigma\,|\,\psi_1^M\rangle \;&=\; P_{13}P_{12}\big[|\,\psi(1,2,3)\rangle + |\,\psi(2,1,3)\rangle - |\,\psi(3,2,1)\rangle - |\,\psi(2,3,1)\rangle\big] \\
&=\; \big[|\,\psi(2,3,1)\rangle + |\,\psi(3,2,1)\rangle - |\,\psi(1,3,2)\rangle - |\,\psi(3,1,2)\rangle\big] \\
&=\; |\,\psi_2^M\rangle - |\,\psi_1^M\rangle
\end{aligned} \tag{9.64}$$

and

$$\begin{aligned}
\sigma\,|\,\psi_2^M\rangle \;&=\; P_{13}P_{12}\big[|\,\psi(2,1,3)\rangle + |\,\psi(1,2,3)\rangle - |\,\psi(3,1,2)\rangle - |\,\psi(1,3,2)\rangle\big] \\
&=\; \big[|\,\psi(3,2,1)\rangle + |\,\psi(2,3,1)\rangle - |\,\psi(1,2,3)\rangle - |\,\psi(2,1,3)\rangle\big] \\
&=\; -\,|\,\psi_1^M\rangle \;.
\end{aligned} \tag{9.65}$$

Since all other permutations can be built from σ and τ, the application of the general operator (9.52) will always give a linear combination of $|\psi_1^M\rangle$ and $|\psi_2^M\rangle$. Thus the permutations of $\mathbf{S}_3$ mix both these states and leads to the name **"mixed symmetry"**.

A major disadvantage for practical applications in the fact that $|\psi_1^M\rangle$ and $|\psi_2^M\rangle$ are not orthogonal. One can find orthogonal states by finding eigenstates $|\psi_\pm^M\rangle$ of the operator τ with eigenvalues ± 1:

$$\tau \mid \psi_\pm^M\rangle \;=\; \pm \mid \psi_\pm^M\rangle \,. \tag{9.66}$$

One finds

$$\mid \psi_\pm^M\rangle \;=\; \mid \psi_1^M\rangle \pm \mid \psi_2^M\rangle \tag{9.67}$$

or explicitly

$$
\begin{aligned}
\mid \psi_+^M\rangle &= (2 - \sigma^{-1} - \sigma)(1 + \tau)\mid \psi(1,2,3)\rangle \\
\mid \psi_-^M\rangle &= (\sigma^{-1} - \sigma)(1 + \tau)\mid \psi(1,2,3)\rangle
\end{aligned}
\tag{9.68}
$$

(See R.P. Feynman, M. Kislinger and R. Ravndal, *Phys. Rev.* **D3**, 2706 (1971): Current Matrix Elements from a Relativistic Quark Model.)

Starting from the second tableaux for the partition [2 1] in Fig. 9.5, one can analogously construct states $\mid \psi_{1,2}^M\rangle'$ and $\mid \psi_\pm^M\rangle'$. Those give a further representation of $\mathbf{S}_3$, which is equivalent to the above one. Thus, starting from a general state $\mid \psi(1,2,3)\rangle$, one can construct the following representations

$$
\begin{array}{lcc}
S & & d = 1 \\
M & \text{with \; dimension} & d = 2 \\
M' & & d = 2 \\
A & & d = 1
\end{array}
$$

With these representations, obtained by applying the permutation operators on $\mid \psi(1,2,3)\rangle$, the six-dimensional space of $\mathbf{S}_3$ is decomposed according to its irreducible representations.

For a general N-particle system, the manifold of possible representations of $\mathbf{S}_N$, the "symmetry classes" becomes quite large. Only two of the irreducible representations are simple and direct generalizations of the previous considerations. These two cases are represented by tableaux of one row and one column:

$$E_S = \sum_{P\,\varepsilon\,S_N} P$$

$$E_A = \sum_{Q\,\varepsilon\,S_N} (-1)^Q\, Q$$
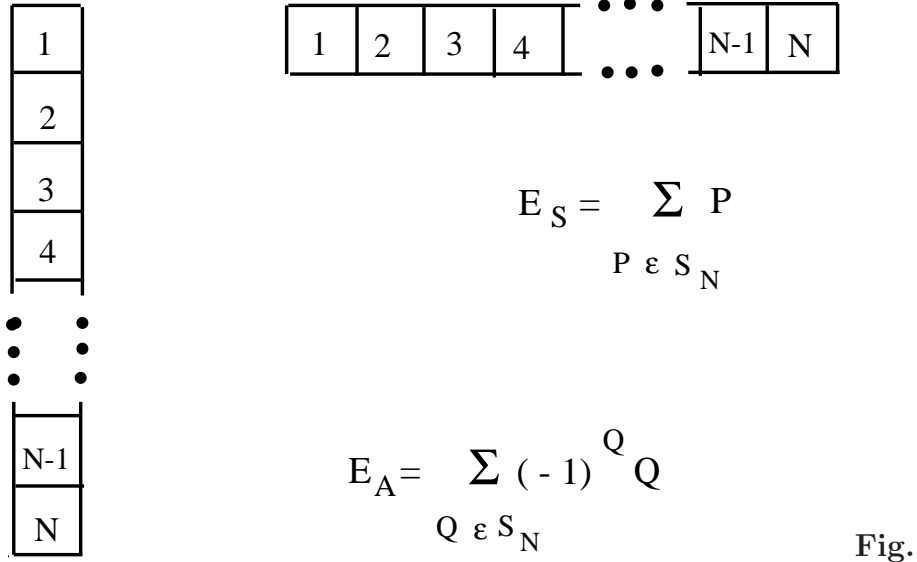
Fig. 9.8 One-Dimensional Representations of $\mathbf{S}_N$.

The operators constructed according to (9.48) are generalizations of symmetrization operator E_S (9.54) and the anti-symmetrization operator E_A (9.55) for the case of $N!$ permutations. The two spaces are given by the vectors

$$
\begin{aligned}
\mid \psi_S(1, 2, \cdots, N)\rangle &:= \frac{1}{\sqrt{N!}} \sum_{P\in S_N} P \mid \psi(1, 2, \cdots, N)\rangle \\
\mid \psi_A(1, 2, \cdots, N)\rangle &:= \frac{1}{\sqrt{N!}} \sum_{Q\in S_N} (-1)^Q\, Q \mid \psi(1, 2, \cdots, N)\rangle \,,
\end{aligned}
$$

$$(9.69)$$

where $\mid \psi_S\rangle$ is a totally symmetric and $\mid \psi_A\rangle$ a totally anti-symmetric state. They are the only one-dimensional representation of $\mathbf{S}_N$, since for every other Young diagram there are several standard tableaux. For this reason those two states play a fundamental role in physics.

9.6   Fermi-, Bose- and Para-Particles

Let us consider a system of N identical particles. According to the considerations of Section 9.2, all observables $A(1, 2, \cdots, N)$ of this system have to be totally symmetric,

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i.e., have to commute with all permutations of $\mathbf{S}_N$:

$$[P, A(1, 2, \cdots, N)] \;=\; 0 \;, \quad P \in \mathbf{S_N} \;. \tag{9.70}$$

This has to be true especially for the Hamiltonian of the system. Therefore, if the state $|\,\psi\,\rangle$ of a system is at some arbitrary time in a particular representation of $\mathbf{S}_N$, then this statement is true for all times. If one introduces the **physical hypothesis**, that one can fix via the measurement of all commuting observables the state of a system – up to a phase factor – then one has, according to the results of the proceeding section, only the symmetric or anti-symmetric representation available to characterize the state. All other symmetry classes are excluded, since they contain permutations which have results other than the multiplication with a factor.

Identical particles with a **totally symmetric** state vector are called **bosons** and identical particles with a **totally anti-symmetric** state vector are called **fermions**. W. Pauli could prove, with means of quantum field theory, the general connection between spin and permutation symmetry:

- Particles with **integer spin** are **bosons**.

- Particles with **half-integer spin** are **fermions**.

Modern proofs of this statement use the so-called micro-causality (field operators either commute or anti-commute for space like distances). (See R.F. Streaker and A.S. Wightman: PCT, Spin and Statistics and All That.)

The above introduced alternatives are, however, not mandatory. In 1953 H.S. Green developed a theory, which is not restricted to one-dimensional representations, and thus allows mixed symmetries (H.S. Green, *Phys. Rev.* **90**, 270 (1953), A Generalized Method of Field Quantization). This theory led to a long discussion and to so-called **Para-Particles**. This term is used for particles for which multi-dimensional representations of the permutation group can occur. For the multitude of possibilities, the following ordering scheme can be used:

- **Para-fermions of rank** r are identical particles for which the state vector of the system has symmetry properties, which are described by Young diagrams with a maximum of r columns.

- **Para-bosons of rank** r are analogously described by Young diagrams with a maximum of r rows.

Obviously, an ordinary fermion is a para-fermion of rank 1, and an ordinary boson a para-boson of rank 1. A generalization of the Pauli Theorem could be proved, namely that para-fermions have half-integer spin and para-bosons have integer spin (R. Haag, Aix-en-Provence Conference 1973, pp. 107-110; The Super-Selection Structure of Particle Physics).

The question is now which of the possible symmetries are realized in nature? To answer this question, the most important **physical consequences of the different symmetries** have to be discussed. For this, we start with the assumption that we can neglect interactions between the particles. (In many systems, this assumption is quite well realized, e.g., for the electrons in an atom, where the Coulomb repulsion between the electrons only leads to a correction term). The Hamiltonian H of such a system can be constructed additively of the single particle Hamiltonians H_j of the N particles

$$H = \sum_{j=1}^{N} H_j \,, \tag{9.71}$$

where H_j only acts on the variables of the jth particle. We choose $\vec{r}_j$ and s_j and define

$$\xi_j := (\vec{r}_j, s_j) \,, \quad j = 1, 2, \cdots, N \,. \tag{9.72}$$

If the index n stands for all eigenvalues, one can write the single particle eigenfunctions of H_j as

$$\phi_n \,|\, \xi_j\rangle := \langle \vec{r}_j, s_j \,|\, n\rangle \,. \tag{9.73}$$

The product function

$$\psi_{n_1, n_2, \cdots, n_N}(\xi_1, \xi_2, \cdots, \xi_n) := \phi_{n_1}(\xi_1) \cdot \phi_{n_2}(\xi_2) \cdots \phi_{n_N}(\xi_N) \tag{9.74}$$

is then eigenfunction of H and gives n basis for the product Hilbert space $\mathcal{H}$ given in (9.3). This result is still valid if one adds to (9.71) an interaction term $V(1, 2, \cdots, N)$, and the functions (9.74) are still a relative good approximation, which is the case for reasonably weak interactions. However, in that case the eigenfunctions usually do not have the desired symmetry properties. Those have to be obtained by applying the operators E constructed according to (9.48). Thus, for **fermions**, one has to use the anti-symmetrizer E_A (9.55), and one obtains

$$\psi_A(\xi_1, \xi_2, \cdots, \xi_N) := \frac{1}{\sqrt{N!}} \sum_{Q} (-1)^Q \, Q[\phi_{n_1}(\xi_1) \cdot \phi_{n_2}(\xi_2) \cdots \phi_{n_N}(\xi_N)] \,, \tag{9.75}$$

where $\frac{1}{\sqrt{N!}}$ is a normalization factor. One has to sum over all permutations of $(\xi_1, \xi_2, \cdots, \xi_N)$, where sequence of indices $n_1, n_2, \cdots, n_N$ remains fixed. According to the definition of a

determinant, one can write

$$
\phi_A(\xi_1, \xi_2, \cdots, \xi_N) \;=\; \frac{1}{\sqrt{N!}}
\begin{vmatrix}
\phi_{n_1}(\xi_1) & \phi_{n_2}(\xi_1) & \cdots & \phi_{n_N}(\xi_1) \\
\phi_{n_1}(\xi_2) & \phi_{n_2}(\xi_2) & \cdots & \phi_{n_N}(\xi_2) \\
\vdots & \vdots & & \\
\phi_{n_1}(\xi_N) & \phi_{n_2}(\xi_2) & \cdots & \phi_{n_N}(\xi_N)
\end{vmatrix} . \tag{9.76}
$$

The right-hand side is known as **Slater determinant**. If two columns are identical, the determinant is zero. This is the case if two of the ϕ_{n_i} are identical, i.e., two of the quantum numbers n_i are identical. From this follows the **Pauli exclusion principle**:

- Identical fermions cannot exist in the same single-particle state.

For **bosons** one has to create a totally symmetric state from (9.74) by applying the symmetrizer E_S (9.54)

$$
\psi_S(\xi_1, \xi_2, \cdots, \xi_N) \;:=\; \frac{1}{\sqrt{N!}} \sum_p P[\phi_{n_1}(\xi_1) \cdot \phi_{n_2}(\xi_2) \cdots \phi_{n_N}(\xi_N)] . \tag{9.77}
$$

The state vector remains unchanged when permitting the particles and

- Identical bosons can occupy the same single-particle state arbitrary many times.

The validity of the Pauli principle for electrons and nucleons has been shown with great success in explaining the structure of atoms and nuclei. It is the main pillar for the periodic system of the elements. The symmetry or anti-symmetry of the wave function plays also an important role in the **statistical behavior** of the particles. A brief summary is given in the following table:

particle	distinguishable	bosons	fermions
wave function	non-symmetric	symmetric	anti-symmetric
statistics	Boltzmann	Bose-Einstein	Fermi-Dirac
number of particles with energy E	$Ae^{\frac{E}{kT}}$	$\dfrac{1}{\frac{1}{A}\,e^{E/kT}-1}$	$\dfrac{1}{\frac{1}{A}\,e^{E/kT}+1}$
valid for	$E \gg kT$	photons (Planck's Law) ^{4}He	electrons in a metal metal
further consequences		Bose-Einstein condensate (super fluidity)	Pauli-principle periodic system nuclei

For considering para-symmetries, we only want to consider **para-fermions**. Here a **generalized Pauli principle** is valid:

- For para-fermions of rank r, only a maximum of r particles can occupy the same quantum state. To understand this, we consider the tableaux in Fig. 9.9.

r colums
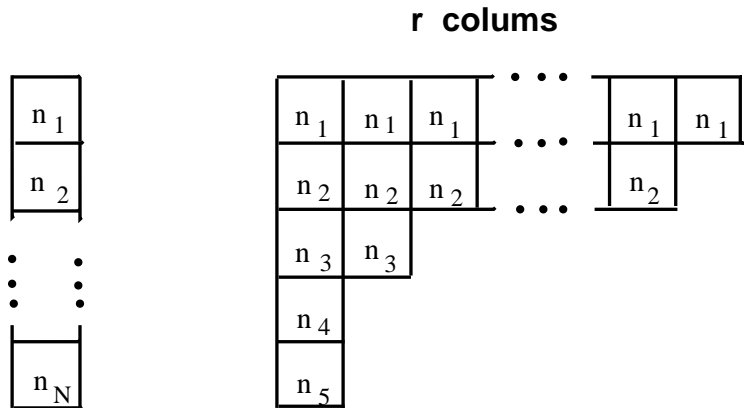
fermions   **para - fermions of rank r** Fig.   9.9

Explanation of the Generalized Pauli Principle for Para-Fermions.

The fermion wave function (9.76) can be represented by distributing the quantum numbers $n_1 \cdots n_N$ into the squares of the Young diagram for fermions. Applying the anti-symmetrizer E_A makes the function vanish as soon as two n_i are identical.

The tableau for para-fermions has r columns. The operator E (9.48) guarantees that the wave function vanishes if quantum numbers are identical within a column. However, in a row a quantum number n_i can occur more than once. The r columns allow that the same quantum number can occur r times, and thus the corresponding single-particle state can be occupied r times.

According to this behavior, one can describe para-fermions in the following way: Introduce a **hidden quantum number** λ, with $\lambda = 1, 2, \cdots, r$. This allows to consider para-fermions of rank r as ordinary fermions with respect to the quantum number (n, λ), which has different values for each pair (n, λ).

The question remains if such particles are realized in nature. For an answer, the following conservation law, which can be generally shown, is helpful:

- Any particle reaction in which, apart from ordinary particles (fermions, bosons) on both sides of the reaction equation only one para-particle appears, is forbidden.

This means a reaction

$$A \; + \; B \; \longrightarrow \; C \; + \; Para \; ,$$

with A, B, C being ordinary particles, is forbidden. The conservation law excludes that any of the many particles in the particle data table (leptons, photons, hadrons) are para-particles.

See O.W. Greenberg and A.M.L. Messiah, *Phys. Rev.* **138B**, 1155 (1965): Selection Rules for Para-Fields and the Absence of Para-Particles in Nature;
O.W. Greenberg in *Conf. Math. Theory of Elementary Particles*, 1965 (ed. by Goodman & Segal).

For non-observed particles and objects, which are in principle not observable as free particle, a para-nature cannot be excluded. There are arguments that quarks are para-fermions of rank 3. In order to explain the hadron spectrum, one has to assume that baryons (like proton and neutron) are composed out of three quarks. The hidden parameter λ is in this context denoted as color degree of freedom. Some references to para-symmetry:

- G. Gentile, *Nuovo Cimento* **17**, 493 (1940)

- M. Dresden, *Branders Lectures*, 1963, p. 377

- S. Duplicher, R. Haag and J.E. Roberts, *Comm. Math. Physics*, 1973.

9.7   The Helium Atom

As demonstration of the important role played by symmetrization principles in the analysis of "two-particle" systems in nature, we consider the helium atom, which has two outer electrons. The theoretical description of the spectrum of this atom was a task at which the semi-classical Bohr description completely failed and only the quantum mechanics of a two-electron system, including the Pauli principle, succeed. The Hamiltonian of helium, in a frame where the nucleus is at rest, is given by

$$\begin{aligned}
H \; &= \; \left(\frac{\vec{P}_1^2}{2m_e} - \frac{2e^2}{|\,\vec{r}_1\,|} \right) \; + \; \left(\frac{\vec{P}_2^2}{2m_e} - \frac{2e^2}{|\,\vec{r}_2\,|} \right) \; + \; \frac{e^2}{|\,\vec{r}_2 - \vec{r}_1\,|} \; + \; H_{SO} \\
&= \; H_0(1) \; + \; H_0(2) \; + \; V_{12} \; + \; H_{SO} \; .
\end{aligned}$$

$$(9.78)$$

The last term, H_{SO}, stands for the spin-orbit interaction between the electrons and the nucleus, while V_{12} is written for the electrostatic interaction between the two electrons.
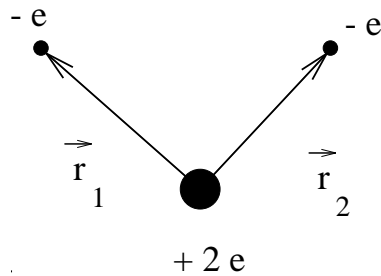

Fig. 9.10 The Coordinates of the Two Electrons in He.

If the electrostatic, as well as spin-orbit terms, are neglected, H reduces to the sum of two hydrogenic Hamiltonians (each with $Z = 2$)

$$H_0 := H_0(1) + H_0(2) .$$ (9.79)

H_0, as well as H, are symmetric with respect to the interchange of the two electrons. For calculating the energy levels, we start from H and consider the other terms as perturbation (actually perturbations in Chapter 10). The eigenvalues of H_0 are sums of the form

$$E = \varepsilon_n + \varepsilon_{n'}$$ (9.80)

with the Coulomb energy

$$\varepsilon_n = -\frac{1}{2} 4\alpha^2 m_e c^2 \frac{1}{n^2} .$$ (9.81)

Due to the large energy difference between ε_1 and ε_2, the most important terms of zeroth order are obtained by assuming that one electron is in the ground state and the other one can occupy all states ε_n. Thus one obtains a level scheme similar to that of hydrogen; however, the levels contain the factor $Z^2 = 4$ and are shifted down by ε_1. Every energy level is occupied by two electrons, and the levels are given as
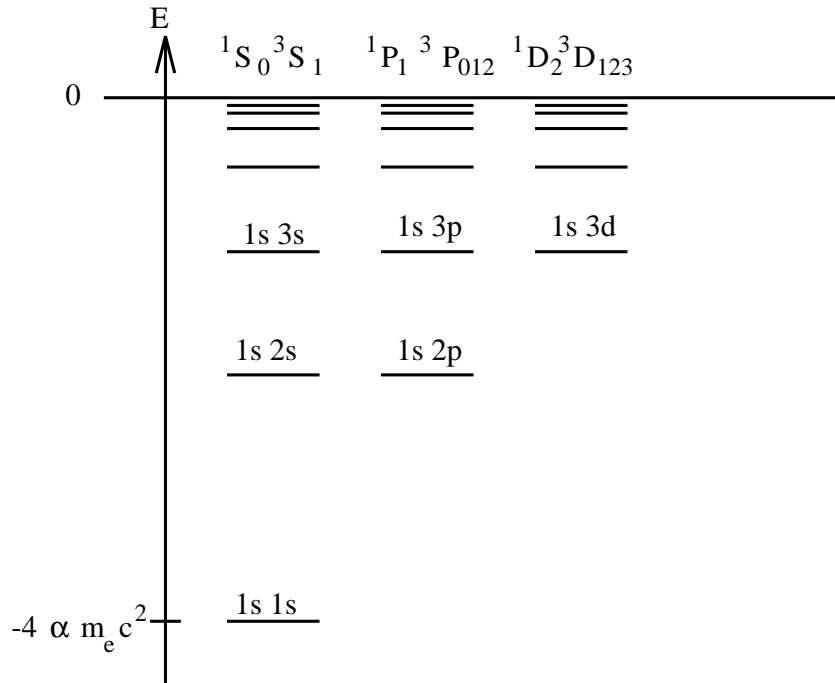
Fig.

9.11 Schematic Representation of the He-Spectrum (0th Order), Without Taking the Pauli Principle into Consideration.

The total orbital angular momentum L is determined by the second electron with $\ell_2 \equiv \ell$ so that the total L is given as

$$L = \ell \; ; \quad \ell = 0, 1, 2, \cdots . \tag{9.82}$$

The corresponding terms are denoted as $S(L = 0), P(L = 1), D(L = 2), \cdots$. The total angular momentum J is composed of the orbital momenta and the spins of the electrons. Since the two spins do not explicitly appear in (9.78), we first couple them separately and obtain $S = 0$ and $S = 1$ for the total spin. From this, we obtain

$$
\begin{aligned}
J &= L \quad \text{for} \;\; S = 0 \\
J &= L \pm 1, L \quad \text{for} \;\; S = 1 .
\end{aligned}
\tag{9.83}
$$

Every energy level can be characterized via the three quantum numbers L, S and J. The conventional notation is

$$^{2S+1}L_J , \tag{9.84}$$

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where the index $2S+1$ gives the spin multiplicity (singlet or triplet).

As next major step, we consider the Pauli principle, leading to an important qualitative change: the $^3S_1$-state cannot exist for the level $(1S\ 1S)$. A qualitative argument is that in the $(1S\ 1S)$ state both electrons are in the same orbital state. If they were in the triplet state, they would have to occupy, in addition, the same spin state, which is not allowed due to the Pauli principle.

Formally we arrive at this result by considering that the eigenfunctions of H_0 are a product of the spatial part $\phi_{1S,n\ell m}(\vec{r}_1, \vec{r}_2)$ and the spin part $\chi_{SM_S}(1,2)$. According to Section 7.32, we have

$$
\begin{aligned}
\chi_{S=0,M_s=0}\ (1,2) &\quad \text{antisymmetric} \\
\chi_{S=1,M_s} = \pm 1, 0\ (1,2) &\quad \text{symmetric .}
\end{aligned}
$$
(9.85)

For the spatial part, we have the product ansatz

$$
\phi_{1S,n\ell m}\ (\vec{r}_1, \vec{r}_2)\ =\ \phi_{1S}\ (\vec{r}_1) \cdot \phi_{n\ell m}\ (\vec{r}_2)
$$
(9.86)

from which we obtain the symmetrized (anti-symmetrized) and normalized expressions

$$
\begin{aligned}
\phi^S_{1S,n\ell m}\ (\vec{r}_1, \vec{r}_2)\ &:=\ \frac{1}{\sqrt{2}}\ [\phi_{1S}(\vec{r}_1)\ \phi_{n\ell m}\ (\vec{r}_2)\ +\ \phi_{1S}\ (\vec{r}_2)\ \phi_{n\ell m}\ (\vec{r}_1)] \\
\phi^A_{1S,n\ell m}\ (\vec{r}_1, \vec{r}_2)\ &:=\ \frac{1}{\sqrt{2}}\ [\phi_{1S}(\vec{r}_1)\ \phi_{n\ell m}\ (\vec{r}_2)\ -\ \phi_{1S}\ (\vec{r}_2)\ \phi_{n\ell m}\ (\vec{r}_1)]\ ,
\end{aligned}
$$
(9.87)

which have to be combined with the corresponding spin parts χ. The general form of the eigenfunctions of H_0 is given by

$$
{}^{2S+1}\psi_{n,JM}(1,2)\ :=\ \sum_{\substack{J-S \le \ell \le J+S \\ m + M_S = M}} \phi^{S,A}_{1S,n\ell m}(\vec{r}_1, \vec{r}_2)\ \chi_{SM_S}(1,2)\ C(\ell SJ, mM_S M)\ .
$$
(9.88)

From this, one obtains for the **singlet function** $(S=0)$:

$$
{}^1\psi_{n,JM}(1,2)\ =\ \phi^S_{1S,nJM}\ (\vec{r}_1, \vec{r}_2)\ \chi_{00}(1,2)
$$
(9.89)

and for the **triplet function** $(S=1)$

$$
{}^3\psi_{n,JM}(1,2)\ =\ \sum_{\substack{J-1 \le \ell \le J+1 \\ m + M_S = M}} \phi^A_{1S,n\ell m}\ (\vec{r}_1, \vec{r}_2)\ \chi_{1M_S}(1,2)\ C(\ell 1J, mM_S M)\ .
$$
(9.90)

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In both cases, the total wave function is anti-symmetric. For the configuration $(1s\ 1s)$, $\phi^A_{1s,n\ell m}(\vec{r}_1, \vec{r}_2) = 0$ in (9.87), so the triplet function vanishes and thus a $^3S_1$ state cannot exist. Further, from the symmetry properties (9.89) and (9.90), one can conclude

- There are no dipole transitions between the singlet and triplet levels.

The dipole moment

$$e(Q_1 + Q_2) \tag{9.91}$$

does not depend on the spin and is a symmetric operator in the two electrons. We have for the transition matrix element from singlet to triplet states:

$$
\begin{aligned}
\langle {}^3\psi_{n,JM} \quad (1,2) \quad &| \ e(Q_1 + Q_2) \ |^1 \ \psi_{n,JM}(1,2) \rangle \\
&= \ \langle \phi^A_{1s,n'\ell'm'}(\vec{r}_1, \vec{r}_2) \ | \ e(Q_1 + Q_2) \ | \ \phi^S_{1s,n\ell m}(\vec{r}_1, \vec{r}_2) \rangle \ \langle \chi_{1M_s}(1,2) \ | \ \chi_{00}(1,2) \rangle \\
&= \ 0 \ .
\end{aligned}
\tag{9.92}
$$

Thus, there are no transitions between singlet and triplet terms. Helium in antisymmetric spin states $(S = 0)$ is called **parahelium**, and helium in symmetric spin states $(S = 1)$ is called **orthohelium**. This distinction is historical since, when first observed, it was thought that there are two different kinds of helium.
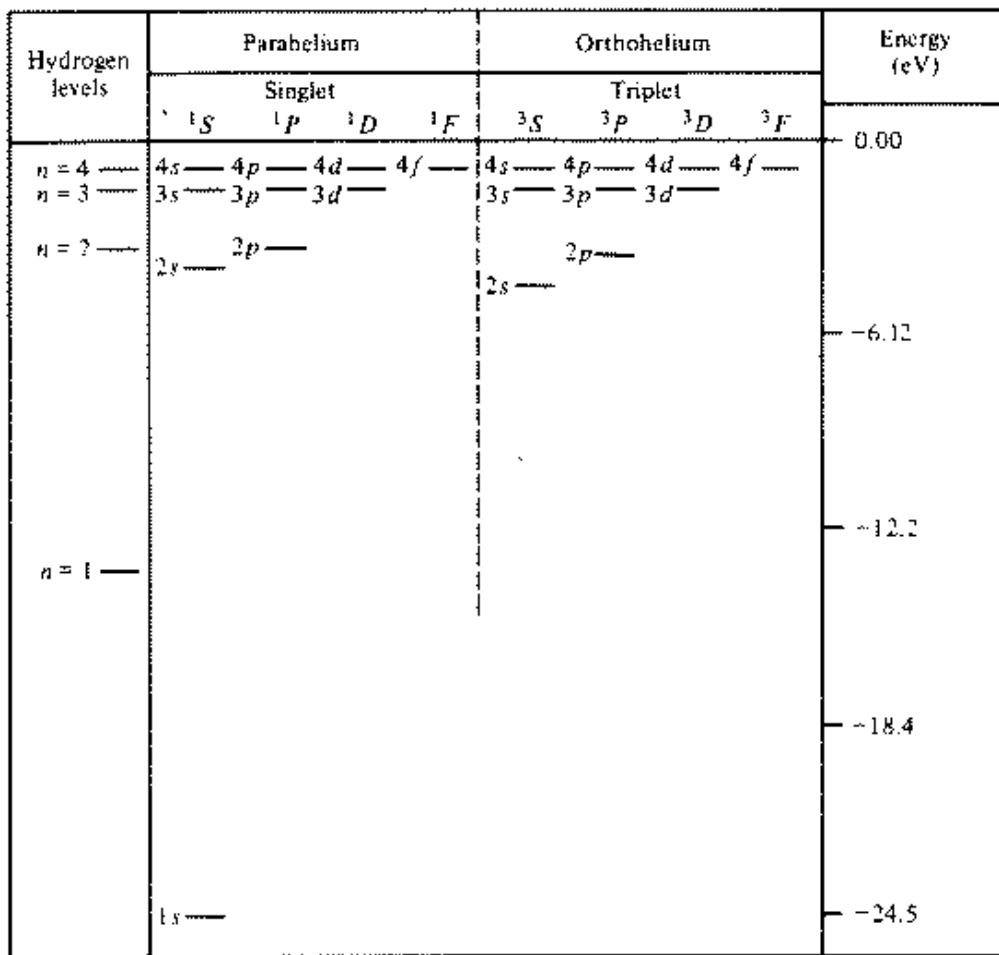
Hydrogen levels	Parahelium				Orthohelium				Energy (eV)
	Singlet				Triplet				
	^1S	^1P	^1D	^1F	^3S	^3P	^3D	^3F	
									0.00
$n=4$	$4s$	$4p$	$4d$	$4f$	$4s$	$4p$	$4d$	$4f$	
$n=3$	$3s$	$3p$	$3d$		$3s$	$3p$	$3d$		
$n=2$	$2s$	$2p$				$2p$			
					$2s$				
									-6.12
									-12.2
$n=1$									
									-18.4
	$1s$								-24.5

Fig. 9.12 Energy Levels of Helium, Illustrating the Singlet and Triplet Series.

For the transition between the two different sets of levels, we have the selection rule

$$\Delta L = \pm 1 \ . \tag{9.93}$$

To see this, we consider the matrix element

$$
\begin{aligned}
\langle {}^1\psi_{n',J'M'} & \mid e(Q_1 + Q_2) \mid {}^1\psi_{n,JM} \rangle \\
&= \langle \phi^S_{1s,n',\ell'm'} \mid e(Q_1 + Q_2) \mid \phi^S_{1s,n\ell m} \rangle \langle \chi_{00} \mid \chi_{00} \rangle
\end{aligned}
\tag{9.94}
$$

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and

$$
\begin{aligned}
\langle {}^3\psi_{n',J'M'} \mid & \; e(Q_1 + Q_2) \mid {}^3\psi_{n,JM} \rangle \\
= & \sum_{\substack{J'-1 \le \ell' \le J'+1 \\ M' + M'_s = M'}} \quad \sum_{\substack{J-1 \le \ell \le J+1 \\ m + M_s = M}} \langle \phi^A_{1s,n'\ell'm'} \mid e(Q_1 + Q_2) \mid \phi^A_{1s,n\ell m} \rangle \\
\times & \; \langle \chi_{1M'_s} \mid \chi_{1M_s} \rangle \; C(\ell'1J', m'M_sM) \; C(\ell 1 J, mM_sM) \; .
\end{aligned}
$$

$$(9.95)$$

According to (7.148), one has as allowed transitions

$$
\Delta L \; = \; \Delta \ell \; = \; \pm, 1, 0 \; .
$$

However, when considering parity selection rules, $\Delta \ell = 0$ is not allowed. The considerations concerning the additional terms in the Hamiltonian (9.78), one postponed to the section on perturbative treatments.

9.8 General Construction of the Anti-Symmetric Wave Function from Spatial and Spin Parts

In the example in the previous section, we saw that the Pauli principle could be fulfilled by combining a symmetric spatial wave function with an anti-symmetric spinor part, and vice versa, to obtain a totally anti-symmetric wave function. The generalization of this procedure to more than two particles is more difficult since complicated mixed symmetries can occur. Using Young diagrams, one can derive rules for the construction of totally anti-symmetric wave functions.

Definition: Given a Young diagram Y. Then the **conjugate diagram Y_c** is obtained from Y by interchanging rows and columns.
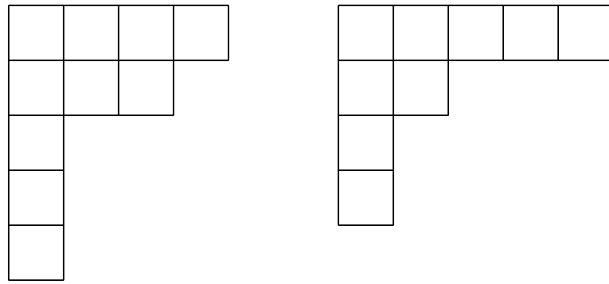
Y   Y$_c$ **Fig. 9.13** Conjugate
Young Diagrams.

For example, the spatial part of a wave function obeys the permutation symmetry of the diagram Y, then it must be multiplied by a spinor part that obeys the permutation symmetry of Y_c so that the total wave function is anti-symmetric. (A proof of this rule is given in M. Hamermesh, *Group Theory and Its Applications to Physical Problems*.) For a system of two fermions, one obtains the following combinations:
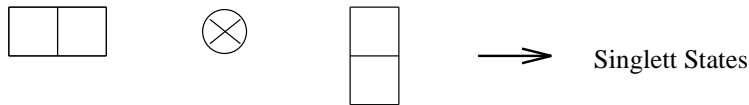

Singlett States

Fig. 9.14

Symmetric spatial part ϕ^s multiplied with an anti-symmetric spin part χ_{00} gives the singlet wave function.
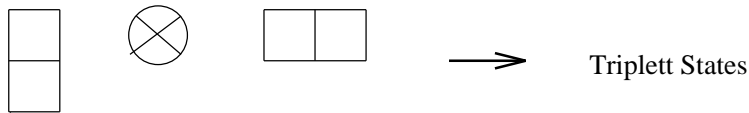

Triplett States

Fig. 9.15

Anti-symmetric spatial part ϕ^A multiplied with symmetric spin Parts gives triplet wave functions.

For a system of three fermions, we obtain the possible symmetries of the spatial part of the wave function from Fig. 9.5. The diagram for [1 1 1] describes a totally anti-symmetric

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spatial part and must be combined with the diagram for [3] for the spin part, i.e., the spin part must be totally symmetric. This can only be the case if all spins are in the same state (parallel), i.e., for total spin $S = \frac{3}{2}$. If the spatial part is of mixed symmetry, i.e., [2 1], then the spin part must also be of mixed symmetry. This can only be realized for total spin $S = \frac{1}{2}$.

A totally symmetric spatial part, according to the diagram for [3], requires a totally anti-symmetric spin part [1 1 1]. Since one has spin-$\frac{1}{2}$ particles, a system of three always has to have two in the same state, and thus a totally anti-symmetric part [1 1 1] does not exist.

The result of the above considerations can be formulated as:

- The spatial part of a system of three spin-$\frac{1}{2}$ particles must be either totally anti-symmetric or of mixed symmetry.