Kapitel 3

Fermions and bosons

We now turn to the quantum statistical description of many-particle systems. The indistinguishability of microparticles leads to a number of far-reaching consequences for the behavior of particle ensembles. Among them are the symmetry properties of the wave function. As we will see there exist only two different symmetries leading to either Bose or Fermi-Dirac statistics.

Consider a single nonrelativistic quantum particle described by the hamiltonian $\hat{h}$. The stationary eigenvalue problem is given by the Schrödinger equation

$$\hat{h}|\phi_i\rangle = \epsilon_i|\phi_i\rangle, \qquad i = 1, 2, \dots , \tag{3.1}$$

where the eigenvalues of the hamiltonian are ordered, $\epsilon_1 < \epsilon_2 < \epsilon_3 \dots$. The associated single-particle orbitals ϕ_i form a complete orthonormal set of states in the single-particle Hilbert space[1]

$$\begin{aligned} \langle\phi_i|\phi_j\rangle &= \delta_{i,j}, \\ \sum_{i=1}^{\infty} |\phi_i\rangle\langle\phi_i| &= 1. \end{aligned} \tag{3.2}$$

3.1 Spin statistics theorem

We now consider the quantum mechanical state $|\Psi\rangle$ of N identical particles which is characterized by a set of N quantum numbers[2] $j_1, j_2, ..., j_N$, meaning that particle i is in single-particle state $|\phi_{j_i}\rangle$. The states $|\Psi\rangle$ are elements of the N-particle Hilbert space which we define as the direct product of single-particle

[1] The eigenvalues are assumed to be non-degenerate. Also, the extension to the case of a continuous basis is straightforward.

[2] The quantum numbers comprise all orbital and spin quantum numbers of a single particle.

Abbildung 3.1: Example of the occupation of single-particle orbitals by 3 particles. Exchange of identical particles (right) cannot change the measurable physical properties, such as the occupation probability.

Hilbert spaces, $\mathcal{H}_N = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \dots$ (N factors), and are eigenstates of the total hamiltonian $\hat{H}$,

$$\hat{H}|\Psi_{\{j\}}\rangle = E_{\{j\}}|\Psi_{\{j\}}\rangle, \qquad \{j\} = \{j_1, j_2, \dots\}\,. \tag{3.3}$$

The explicit structure of the $N-$particle states is not important now and will be discussed later[3].

Since the particles are assumed indistinguishable it is clear that all physical observables cannot depend upon which of the particles occupies which single particle state, as long as all occupied orbitals, i.e. the set j, remain unchainged. In other words, exchanging two particles k and l (exchanging their orbitals, $j_k \leftrightarrow j_l$) in the state $|\Psi\rangle$ may not change the probability density, cf. Fig. 3.1. The mathematical formulation of this statement is based on the permutation operator P_{kl} with the action

$$\begin{aligned} P_{kl}|\Psi_{\{j\}}\rangle &= P_{kl}|\Psi_{j_1,\dots,j_k,\dots j_l,\dots,j_N}\rangle = \\ &= |\Psi_{j_1,\dots,j_l,\dots j_k,\dots,j_N}\rangle \equiv |\Psi'_{\{j\}}\rangle, \qquad \forall k,l = 1,\dots N, \end{aligned} \tag{3.4}$$

where we have to require

$$\langle\Psi'_{\{j\}}|\Psi'_{\{j\}}\rangle = \langle\Psi_{\{j\}}|\Psi_{\{j\}}\rangle. \tag{3.5}$$

Indistinguishability of particles requires $P_{kl}\hat{H} = \hat{H}$ and $[P_{kl}, \hat{H}] = 0$, i.e. P_{kl} and $\hat{H}$ have common eigenstates. This means P_{kl} obeys the eigenvalue problem

$$P_{kl}|\Psi_{\{j\}}\rangle = \lambda_{kl}|\Psi_{\{j\}}\rangle = |\Psi'_{\{j\}}\rangle. \tag{3.6}$$

[3]Recall that, in this section, we assume that the particles do not interact with each other. The generalization to interacting particles will be discussed in Sec. 3.2.5.

Obviously, $P_{kl}^{\dagger} = P_{kl}$, so the eigenvalue λ_{kl} is real. Then, from Eqs. (3.5) and (3.6) immediately follows

$$\lambda_{kl}^2 = \lambda^2 = 1, \qquad \forall k, l = 1, \ldots N, \tag{3.7}$$

with the two possible solutions: $\lambda = 1$ and $\lambda = -1$. From Eq. (3.6) it follows that, for $\lambda = 1$, the wave function $|\Psi\rangle$ is symmetric under particle exchange whereas, for $\lambda = -1$, it changes sign (i.e., it is "anti-symmetric").

This result was obtained for an arbitrary pair of particles, so we may expect that it is straightforwardly extended to systems with more than two particles. Experience shows that, in nature, there exist only two classes of microparticles – one which has a totally symmetric wave function with respect to exchange of any particle pair whereas, for the other, the wave function is antisymmetric. The first case describes particles with Bose-Einstein statistics ("bosons") and the second, particles obeying Fermi-Dirac statistics ("fermions")[4].

The one-to-one correspondence of (anti-)symmetric states with bosons (fermions) is the content of the spin-statistics theorem. It was first proven by Fierz [Fie39] and Pauli [Pau40] within relativistic quantum field theory. Requirements include 1.) Lorentz invariance and relativistic causality, 2.) positivity of the energies of all particles and 3.) positive definiteness of the norm of all states.

3.2 Symmetric and antisymmetric N-particle wave functions

We now explicitly construct the N-particle wave function of a system of many fermions or bosons.

Case of $N = 2$. For two particles occupying the orbitals $|\phi_{j_1}\rangle$ and $|\phi_{j_2}\rangle$, respectively, there are two possible wave functions: $|\Psi_{j_1,j_2}\rangle$ and $|\Psi_{j_2,j_1}\rangle$ which follow from one another by applying the permutation operator P_{12}. Since both wave functions represent the same physical state it is reasonable to eliminate this ambiguity by constructing a new wave function as a suitable linear combination of the two,

$$|\Psi_{j_1,j_2}\rangle^{\pm} \;=\; C_{12}\left\{|\Psi_{j_1,j_2}\rangle + A_{12}P_{12}|\Psi_{j_1,j_2}\rangle\right\}, \tag{3.8}$$

with an arbitrary complex coefficient A_{12}. Using the eigenvalue property of the permutation operator, Eq. (3.6), we require that this wave function has the

[4]Fictitious systems with mixed statistics have been investigated by various authors, e.g. [MG64, MG65] and obey "parastatistics". For a text book discussion, see Ref. [Sch08], p. 6.

proper symmetry,

$$P_{12}|\Psi_{j_1,j_2}\rangle^{\pm} = \pm|\Psi_{j_1,j_2}\rangle^{\pm}\,, \tag{3.9}$$

which follows from the linearity of $|\Psi\rangle^{\pm}$ in the eigenstates of P. The explicit form of the coefficients in Eq. (3.8) is obtained by acting on this equation with the permutation operator and equating this to $\pm|\Psi_{j_1,j_2}\rangle^{\pm}$, according to Eq. (3.9), and using $P_{12}^2 = \hat{1}$,

$$\begin{aligned} P_{12}|\Psi_{j_1,j_2}\rangle^{\pm} &= C_{12}\left\{|\Psi_{j_2,j_1}\rangle + A_{12}P_{12}^2|\Psi_{j_1,j_2}\rangle\right\} = \\ &= C_{12}\left\{\pm A_{12}|\Psi_{j_2,j_1}\rangle \pm |\Psi_{j_1,j_2}\rangle\right\}, \end{aligned}$$

which leads to the requirement $A_{12} = \lambda$, whereas normalization of $|\Psi_{j_1,j_2}\rangle^{\pm}$ yields $C_{12} = 1/\sqrt{2}$. The final result is

$$\boxed{|\Psi_{j_1,j_2}\rangle^{\pm} = \frac{1}{\sqrt{2}}\{|\Psi_{j_1,j_2}\rangle \pm P_{12}|\Psi_{j_1,j_2}\rangle\} \equiv \Lambda_{12}^{\pm}|\Psi_{j_1,j_2}\rangle} \tag{3.10}$$

where,

$$\Lambda_{12}^{\pm} = \frac{1}{\sqrt{2}}\{1 \pm P_{12}\}, \tag{3.11}$$

denotes the (anti-)symmetrization operator of two particles which is a linear combination of the identity operator and the pair permutation operator.

Case of $N = 3$. The extension of this result to 3 fermions or bosons is straightforward. For 3 particles $(1,2,3)$ there exist $6 = 3!$ permutations: three pair permutations, $(2,1,3), (3,2,1), (1,3,2)$, that are obtained by acting with the permutation operators P_{12}, P_{13}, P_{23}, respectively on the initial configuration. Further, there are two permutations involving all three particles, i.e. $(3,1,2)$ and $(2,3,1)$, which are obtained by applying the operators $P_{13}P_{12}$ and $P_{23}P_{12}$, respectively. Thus, the three-particle (anti-)symmetrization operator has the form

$$\Lambda_{123}^{\pm} = \frac{1}{\sqrt{3!}}\{1 \pm P_{12} \pm P_{13} \pm P_{23} + P_{13}P_{12} + P_{23}P_{12}\}, \tag{3.12}$$

where we took into account the necessary sign change in the case of fermions resulting for any pair permutation.

General case. This result is generalized to N particles where there exists a total of $N!$ permutations, according to[5]

$$|\Psi_{\{j\}}\rangle^{\pm} = \Lambda_{1\ldots N}^{\pm}|\Psi_{\{j\}}\rangle, \tag{3.13}$$

[5]This result applies only to fermions. For bosons the prefactor has to be corrected, cf. Eq. (3.25).

with the definition of the (anti-)symmetrization operator of N particles,

$$\boxed{\Lambda^{\pm}_{1\ldots N} = \frac{1}{\sqrt{N!}} \sum_{P \epsilon S_N} \mathrm{sign}(P) \hat{P}} \tag{3.14}$$

where the sum is over all possible permutations $\hat{P}$ which are elements of the permutation group S_N. Each permutation P has the parity, $\mathrm{sign}(P) = (\pm 1)^{N_p}$, which is equal to the number N_p of successive pair permuations into which $\hat{P}$ can be decomposed (cf. the example $N = 3$ above). Below we will construct the (anti-)symmetric state $|\Psi_{\{j\}}\rangle^{\pm}$ explicitly. But before this we consider an alternative and very efficient notation which is based on the occupation number formalism.

The properties of the (anti-)symmetrization operators $\Lambda^{\pm}_{1\ldots N}$ are analyzed in Problem 1, see Sec. 3.9.

3.2.1 Occupation number representation

The original N-particle state $|\Psi_{\{j\}}\rangle$ contained clear information about which particle occupies which state. Of course, this information is unphysical, as it is in conflict with the indistinguishability of particles. With the construction of the symmetric or anti-symmetric N-particle state, $|\Psi_{\{j\}}\rangle^{\pm}$, this information about the identity of particles is eliminated, and the only information which is retained is *how many particles*, n_p, occupy the single-particle orbital $|\phi_p\rangle$. We thus may use a different notation for the state $|\Psi_{\{j\}}\rangle^{\pm}$ in terms of the *occupation numbers* n_p of the single-particle orbitals,

$$|\Psi_{\{j\}}\rangle^{\pm} = |n_1 n_2 \ldots\rangle \equiv |\{n\}\rangle, \qquad n_p = 0, 1, 2, \ldots, \qquad p = 1, 2, \ldots \tag{3.15}$$

Here $\{n\}$ denotes the total set of occupation numbers of all single-particle orbitals. Since this is the complete information about the N-particle system, these states form a complete system that is orthonormal by construction of the (anti-)symmetrization operators,

$$\begin{aligned} \langle\{n\}|\{n'\}\rangle &= \delta_{\{n\},\{n'\}} \equiv \delta_{n_1,n'_1}\delta_{n_2,n'_2}\ldots \\ \sum_{\{n\}} |\{n\}\rangle\langle\{n\}| &= 1. \end{aligned} \tag{3.16}$$

The attractive feature of this representation is that it is equally applicable to fermions and bosons. The only difference between the two lies in the allowed values of the occupation numbers, as we will see in the next two sections.