Advanced quantum mechanics (20104301)

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Chapter 2: Identical particles

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Identical particles

2.1 Permutation group

In this section, we make a first contact with quantum many-body systems. We consider a physical system composed of N identical particles. "Identical" means that there is no observable that could distinguish between them. In such a situation, the Hamiltonian operator and in fact any other observable must be symmetric in the coordinates (that is, in the position and spin degrees of freedom). In other words, if A is an arbitrary observable, and P an arbitrary permutation from S_N – so the permutation group with N elements – then we will say that the particles are identical if

$$[A, P] = 0 \tag{2.1}$$

for all $P \in S_N$. We will use the same symbol for the permutation and its representation in Hilbert space. This is a very natural definition: If we could generate an observable effect by simply permuting particles, then we could not call the particles indistinguishable, as we have found a way to distinguish them. For the moment being, this is only a constraint to the involved Hilbert spaces and to their Hamiltonians (as H is also an observable), but we will see in a minute what the consequences are. We will now more closely consider this operator in Hilbert space.

Let ξ_j be the coordinates of the j-th particle, of N particles in total. Say, the state vector of such a particle is from some Hilbert space $\mathcal{H}$. This could in particular be the position of the particle, a situation for which then $\mathcal{H} = L^2(\mathbb{R})$. Or, for a particle with spin, the position and the third component of the spin, with Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}) \otimes \mathbb{C}^2. \tag{2.2}$$

A wave function is then simply a function with values

$$\psi(\xi) = \psi(x, \sigma), \tag{2.3}$$

where $x \in \mathbb{R}^3$ and $\sigma = \{0, 1\}$. How does the entire Hilbert space then look like? Well, we know that this is given by

$$\mathcal{H} \otimes \cdots \otimes \mathcal{H} = \mathcal{H}^{\otimes N}. \tag{2.4}$$

We will now investigate what happens to the wave function when we start permuting particles.

If $\psi(\xi_1, \ldots, \xi_N)$ is the wave function of the system, then the *permutation operator* acts as

$$(P\psi)(\xi_1, \ldots, \xi_N) = \psi(\xi_{P(1)}, \ldots, \xi_{P(N)}). \tag{2.5}$$

It is clear that this really gives rise to a representation of the permutation group, as for two permutations P_1, P_2 we have that

$$((P_2 P_1)\psi)(\xi_1, \ldots, \xi_N) = (P_2(P_1\psi))(\xi_1, \ldots, \xi_N). \tag{2.6}$$

If the function $\psi(\xi_1, \ldots, \xi_N)$ is a solution of the time independent Schrödinger equation,

$$(H\psi)(\xi_1, \ldots, \xi_N) = E\psi(\xi_1, \ldots, \xi_N), \tag{2.7}$$

so is $(P\psi)(\xi_1, \ldots, \xi_N)$ a solution with the same energy E, if

$$[H, P] = 0. \tag{2.8}$$

This is a consequence of the definition. Since for N particles, there exist $N!$ different permutations (this is the cardinality of the symmetric group), we get in this way $N!$ different wave functions. Not all of them will be linearly independent, but usually we will obtain a number of linearly independent solutions of the same energy. That is to say, the energy values of Hamilton operators of identical particles will typically be highly degenerate. This degeneracy is referred to as *exchange degeneracy*.

For an arbitrary observable A, we get

$$\langle\psi|A|\psi\rangle = \langle P\psi|A|P\psi\rangle. \tag{2.9}$$

If $\psi(\xi_1, \ldots, \xi_N; t_0)$ is the wave function at time t_0 and $U(t - t_0)$ is the time evolution operator that for all permutations P satisfies

$$[U(t - t_0), P] = 0 \tag{2.10}$$

(for obvious reasons, since the Hamiltonian P commutes with H)

$$U(t - t_0) = e^{-i(t-t_0)H} \tag{2.11}$$

setting $\hbar = 1$, then also

$$(PU(t - t_0)\psi)(\xi_1, \ldots, \xi_N; t_0) = (U(t - t_0)P\psi)(\xi_1, \ldots, \xi_N; t_0). \tag{2.12}$$

This means that the permuted time evolved wave function is the same as the time evolved permuted wave function. This means no less than that two wave functions that are different only by a permutation, cannot be distinguished by any even sophisticatedly chosen observable. This is hence a property that is preserved under time evolution.

2.2 Completely symmetric and antisymmetric wave functions

It makes a lot of sense to elucidate the situation for a small number of particles. For one particle, the issue is void. Two particles are still quite boring in this respect, as there are only completely symmetric and antisymmetric functions. Or, more precisely, the Hilbert space decomposes int a direct sum of those components. Hence, the most natural first good example is the case of $N = 3$: In fact, for this we see all features we need to know. In order to simplify the notation, we will write j for the coordinates ξ_j. But it is important to stress that this is no number, but just a shortcut for a coordinate. We have the wave function $\psi(i, j, k)$, where $i \neq j \neq l$ can take the values $1, 2, 3$. From these wave functions, one can construct the following functions,

$$\begin{aligned}\psi_S(1,2,3) &= \frac{1}{6^{1/2}}(\psi(1,2,3)+\psi(1,3,2)+\psi(2,3,1)+\psi(2,1,3) \\ &+ \psi(3,1,2)+\psi(3,2,1)), \quad (2.13)\\ \psi_A(1,2,3) &= \frac{1}{6^{1/2}}(\psi(1,2,3)-\psi(1,3,2)+\psi(2,3,1)-\psi(2,1,3) \\ &+ \psi(3,1,2)-\psi(3,2,1)), \quad (2.14)\end{aligned}$$

as well as

$$\begin{aligned}\psi_{M_1}(1,2,3) &= \frac{1}{2\sqrt{3}}(2\psi(1,2,3)-\psi(1,3,2)+2\psi(2,1,3)-\psi(2,3,1) \\ &- \psi(3,1,2)-\psi(3,2,1)), \quad (2.15)\\ \psi_{M_2}(1,2,3) &= \frac{1}{2}(\psi(1,3,2)-\psi(2,3,1)+\psi(3,1,2)-\psi(3,2,1)), \quad (2.16)\\ \psi_{M_1'}(1,2,3) &= \frac{1}{2\sqrt{3}}(2\psi(1,2,3)-\psi(1,3,2)-2\psi(2,1,3)-\psi(2,3,1) \\ &- \psi(3,1,2)+\psi(3,2,1)), \quad (2.17)\\ \psi_{M_2'}(1,2,3) &= \frac{1}{2}(\psi(1,3,2)+\psi(2,3,1)-\psi(3,1,2)-\psi(3,2,1)). \quad (2.18)\end{aligned}$$

The span of these six new wave functions is identical with that of the original functions, needless to say. If $\psi(1, 2, 3)$ already was completely symmetric, then only $\psi_S(1, 2, 3)$ would be non-vanishing. The pre-factors are only normalization constants. It is not difficult to verify that

$$(P\psi_S)(1,2,3) = \psi_S(1,2,3) \quad (2.19)$$

and

$$(P\psi_A)(1,2,3) = \pm\psi_A(1,2,3), \quad (2.20)$$

depending on whether the permutation P is even or odd (so can be generated from an even or odd number of two-entry exchanges). Therefore, as the index indicates, the functions ψ_S and ψ_A are completely symmetric or antisymmetric. There are also the two two-dimensional subspaces spanned by Eqs. (2.15,2.16) and Eqs. (2.17,2.18), respectively. They are again invariant under any permutation $P \in S_3$.

That is to say, the Hilbert space decomposes into a direct sum of four subspaces

$$\mathcal{H}_3 = \mathcal{H}_S \oplus \mathcal{H}_A \oplus \mathcal{H}_M \oplus \mathcal{H}_{M'}. \tag{2.21}$$

This corresponds to a classification of the wave function according to complete symmetry in $\mathcal{H}_S$, antisymmetry $\mathcal{H}_A$, and mixed symmetry in $\mathcal{H}_M \oplus \mathcal{H}_{M'}$. What is more, the representations $\mathcal{H}_M$ und $\mathcal{H}_{M'}$ are equivalent. In this language, we also see why $N = 2$ is a somewhat boring case: Here we simply have

$$\mathcal{H}_2 = \mathcal{H}_S \oplus \mathcal{H}_A. \tag{2.22}$$

The general case of N particles is now clear from basic group theoretic considerations. The Hilbert space decomposes as

$$\mathcal{H}_N = \mathcal{H}_S \oplus \mathcal{H}_A \oplus \mathcal{H}_{\mathcal{S}_1} \oplus \mathcal{H}_{\mathcal{S}_2} \oplus \dots \tag{2.23}$$

each of which is invariant under any permutation $P \in S_N$. In physical system, only the completely symmetric and antisymmetric wave functions can be realized. Why is this so? An argument can be formulated as follows: Let $\{A_1, \dots, A_k\}$ be a complete set of compatible observables (that is, a complete set of observables that are mutually commuting) and $\{a_1, \dots, a_k\}$ the corresponding eigenvalues of $A_1, \dots, A_k$. Then the state vector $|a_1, \dots, a_k\rangle$ is unique, up to a phase. But if $|a_1, \dots, a_k\rangle \in \mathcal{H}_{\mathcal{S}_i}$, then one can find a permutation P so that

$$P|a_1, \dots, a_k\rangle \neq e^{i\alpha}|a_1, \dots, a_k\rangle \tag{2.24}$$

for all $\alpha \in \mathbb{R}$, and still $P|a_1, \dots, a_k\rangle$ is an eigenvector of $A_1, \dots, A_k$ with eigenvalues $a_1, \dots, a_k$. This leads to a contradiction, however, as the subspaces are not one-dimensional. This is the point: The invariant subspaces must be one-dimensional. And, as a representation theoretic consideration shows (which we will not discuss here in detail), this is true only for the completely symmetric and antisymmetric wave functions. All other invariant subspaces are of higher dimension. This leads to an important principle.

Symmetry principle: A state vector of a pure quantum state of a system of identical particles is either completely symmetric or antisymmetric under the exchange of two particles.

One can also derive from considerations in relativistic quantum field theory (which we will not go into at this point), the following important *spin statistics theorem*.

Spin statistics theorem: The pure states of a system of identical particles is completely symmetric, if the spin is integer-values (bosons) and completely antisymmetric, if the spin takes a half-integer value.

Their names originate from the boson and fermion statistics, to which we will come to in a minute. It may be worth stressing – and this is a topic we will get to later – that there are situations of a non-trivial topology that also allow for *frationalized statistics*. Such a situation is encountered, for example, when charged quasi-particles with charge q can strictly move in two spatial dimensions only, in a field of magnetic flux Φ. In this case, the exchange of such quasi-particles leads to a phase factor $e^{i\phi}$, where now $\phi = q\Phi/(\hbar c)$. Only for $\phi = 0$ and $\phi = \pi$ one arrives at the standard statistics.

Important examples of fermions are the usual suspects: Electrons, nuclei ^{3}He are particles with spin $1/2$ are hence fermions. Important examples for bosons are photons in the theory of quantized light, phonons in a body, as quantized excitations of mechanical motion, and ^{4}He. They are all particles with spin 0 or 1. The fermionic *Pauli principle* can be reduced to the antisymmetry of the wave function. It is a cute observation that there are, by the way, additional constraints arising from the antisymmetry of the wave function, except having at most one fermion per mode. In fact, the single-body density operator is constrained to be contained in a polytope. We will later understand what this means. [1]

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[1] At this point, we have all reason in the world to be confused, and presumably this was an origin of confusion even ealier. The universe consists of countless particles, in particular a large number of electrons. If it was necessary, in the light of the previous considerations, to take them all into account and think of completely antisymmetric wave functions, physics was doomed to failure: Physics is concerned with systems, not with describing the entire universe (which would be practically impossible anyway). If we could ever only meaningfully talk about the entire universe, we would not get anywhere, if it was impossible to meaningfully talk about subsystems. Fortunately, one can overcome this dilemma. In fact, to a very good approximation, one can avoid such a radical description of the entire collection of electrons. Let us be more specific: Let us assume we have two electrons that are sufficiently far from each other, so that the overlap of the position part and their interaction can be neglected. If ψ_1 and ψ_2 are the respective normalized wave functions, the approximately normalized antisymmetric wave function is given by

$$\psi(\xi_1, \xi_2) = \frac{1}{\sqrt{2}}(\psi_1(\xi_1)\psi_2(\xi_2) - \psi_1(\xi_2)\psi_2(\xi_1)) \tag{2.25}$$

(it is not strictly normalized for obvious reasons). We can now ask for the particle density in a point $\xi = (x, \sigma)$, that is, in a position in space and a spin component. This density is given by

$$\rho(\xi) = \int d\xi_2 |\psi(\xi, \xi_2)|^2 + \int d\xi_1 |\psi(\xi_1, \xi)|^2, \tag{2.26}$$

where the integral is to be seen as an ordinary integral in space and a sum over the spin components. This gives

$$\rho(\xi) = |\psi_1(\xi)|^2 + |\psi_2(\xi)|^2 - 2\text{re}\left(\psi_1^*(\xi)\psi_2(\xi)\int d\xi_1 \psi_2^*(\xi_1)\psi_1(\xi_1)\right). \tag{2.27}$$

Since ψ_1 and ψ_2 are highly localized in spatially disjoint regions R_1 und R_2, the last term can be neglected, and if $\xi \in R_1$ ist, then

$$\rho(\xi) \approx |\psi_1(\xi)|^2. \tag{2.28}$$

The very same result we would have obtained if we had ignored the second electron altogether. Of course, a similar reasoning holds in generality. The symmetrization and antisymmetrization has to be applied only for particles that are relevant for a physical system. We do not have to include all other particles that do not interact with a given particle. In the classical limit, particles are also highly localized in space, and the influence from symmetry can eb entirely neglected. Hence, we can feel safe again and continue with our argument.

2.3 Non-interacting identical particles

Let us now again turn to systems of N identical particles. But now we do not consider the structure of the underlying Hilbert space, but describe their Hamilton operator. This Hamiltonian – assuming that the particles do not interact – takes the simple form

$$H_0 = \sum_{j=1}^{N} h_j = \sum_{j=1}^{N} \left(\frac{1}{2M} p_j^2 + V_j \right). \tag{2.29}$$

Here, all h_j are the same, but act on the j-th particle only. For simplicity of notation, we will assume that the spectrum of all h_j is discrete, in order to avoid mathematical fine print that is needed for continuous spectra. Let $\psi_1, \psi_2, \dots$ be the normalized one particle wave functions (or "orbitals") of h_j with eigenvalues $E_1, E_2, \dots$, that is, we have

$$h_j \psi_j(\xi_j) = E_j \psi_j(\xi_j). \tag{2.30}$$

The wave function

$$\psi(\xi_1, \dots, \xi_N) = \psi_1(\xi_1) \dots \psi_N(\xi_N) \tag{2.31}$$

is then an eigenfunction of H_0 with eigenvalue

$$E = E_1 + \dots + E_N. \tag{2.32}$$

In the light of the above considerations, the wave function can only be completely antisymmetric or symmetric, depending on whether we are encountering bosons or fermions.

2.3.1 Wave functions of fermions

Wave functions of fermions: The wave functions of fermionic systems are linear combinations of antisymmetric functions of the form

$$\psi_N(\xi_1, \dots, \xi_N) = \frac{1}{(N!)^{1/2}} \sum_{P \in S_N} (-1)^{\pi(P)} \psi_1(\xi_{P(1)}) \dots \psi_N(\xi_{P(N)}). \tag{2.33}$$

This expression can also be written as a determinant, as a so-called *Slater determinant* of an $N \times N$-matrix,

$$\psi_N(\xi_1, \dots, \xi_N) = \frac{1}{(N!)^{1/2}} \begin{vmatrix} \psi_1(\xi_1) & \dots & \psi_1(\xi_N) \\ \psi_2(\xi_1) & \dots & \psi_2(\xi_N) \\ \dots & \dots & \dots \\ \psi_N(\xi_1) & \dots & \psi_N(\xi_N) \end{vmatrix}. \tag{2.34}$$

The exchange of two coordinates is reflected by an exchange of two rows, leading to a sign change of the determinant, concomitant with the desired antisymmetry. The exchange of two orbitals correponds to the exchange of two columns, which again leads to a sign change.

2.3.2 Wave functions of bosons

For bosons we arrive at a similar expression. In the sum (2.35), not all terms are necessarily different. Instead, each term is shown $N_1!N_2!\dots$ many times.

Wave functions of bosons: The wave function of bosonic systems are linear combinations of symmetric functions of the form

$$\psi_N(\xi_1,\dots,\xi_N) = \frac{1}{(N!N_1!N_2\dots)^{1/2}} \sum_{P\in S_N} \psi_1(\xi_{P(1)})\dots\psi_N(\xi_{P(N)}), \quad (2.35)$$

where $N_1, N_2, \dots$ is the number of particles in the orbitals labeled $1, 2, \dots$, with $N_1 + N_2 + \dots = N$.

It should be clear at this point that for both fermions and bosons, it is possible to label the basis states merely by stating the *occupation numbers* $(N_1, N_2, \dots)$, where

$$N_1 + N_2 + \dots = N. \quad (2.36)$$

For fermions these occupation numbers can be 0 or 1. For bosons, in contrast, any non-negative integer is possible. The total energy of such a basis state is given by

$$E = N_1E_1 + N_2E_2 + \dots. \quad (2.37)$$

Again, unsurprisingly, it depends only on the occupation numbers.

2.4 The non-interacting gas of fermions and bosons

A system of N identical particles, for which mutual interactions can be neglected, is called *ideal gas*. We will briefly discuss the situation here, assuming that in statistical mechanics, this type of system will be discussed in more detail. For fermions, we know that the occupation numbers N_j can only take the values 0 and 1. We assume that the concepts of grand canonical ensembles are roughly clear. It is an equilibrium state in quantum statistical mechanics under certain boundary conditions.

In the thermodynamic equilibrium state, the average occupation number of the orbital labeled j is for fermions given by

$$\bar{N}_j = \frac{1}{\exp(-(\mu - E_j)/(k_BT)) + 1}, \quad (2.38)$$

which is the distribution function in the *Fermi-Dirac-statistics*. Here k_B is the *Boltzmann constant*. The chemical potential μ, a real number, depends on the temperature T and the total particle number N via

$$N = \sum_j (\exp(-(\mu - E_j)/(k_BT)) + 1)^{-1}. \quad (2.39)$$

Formally, μ takes the role of a Lagrange multiplier.

For bosons we obtain a very similar expression, only that now the occupation numbers are no longer constrained to be 0 or 1. It turns out that one only finds an equilibrium value if $\exp((\mu - E_j)/(k_B T)) < 1$ for all energies E_j. For this reason, the chemical potential mu cannot be positive. One finds for the occupation numbers in thermal equilibrium

$$\bar{N}_j = \frac{1}{\exp((E_j - \mu)/(k_B T)) - 1}. \tag{2.40}$$

This is the distribution function of the ideal bosonic quantum gas, corresponding to the *Bose-Einstein-statistics* The chemical potential, once again, it determined by

$$N = \sum_j (\exp((E_j - \mu)/(k_B T)) - 1)^{-1}. \tag{2.41}$$

From this, other statistical properties can be derived. Planck's radiation formula, for example, is an immediate consequence thereof. We will briefly come back to it, without anticipating too many topics of quantum statistical physics, which is a course in its own right.