Chapter 4

Identical Particles and Statistics

A curious consequence of the quantum mechanical picture of the world is that elementary particles of the same type (electrons, quarks, *etc.*) naturally come to be thought of as being *fundamentally indistinguishable*. To motivate this consider the following thought experiment (see Figure 1).[28]

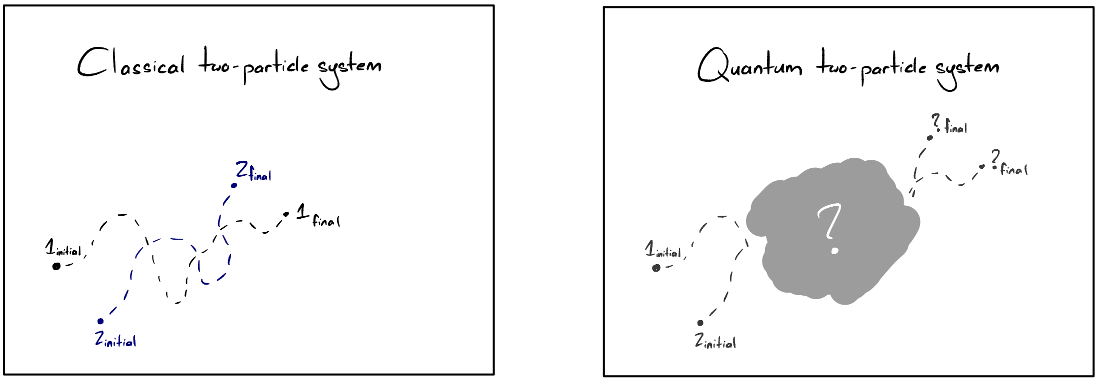

Figure 1. Distinguishable versus indistinguishable elementary particles in classical and quantum physics.

Suppose that at time $t = 0$ you have a pair of electrons whose positions are known well enough to distinguish them (*i.e.*, one is definitely in one half of the room and the other is definitely in the other half). After a period of time elapses, the wave function of the system will have evolved so that both electrons could be anywhere in the room with some probability. At this point, we may make measurements to determine the positions of two electrons, but we will have no way to distinguish the two different electrons. In contrast to the classical case, we can't keep track of "electron one" by following it along its trajectory during the time interval—it had no definite trajectory when it was not being observed!

4.1 Indistinguishable particles and wave functions

We will consider the consequences of indistinguishability on multi-particle wave functions, beginning with the case of two particles. A two particle wave function is a (square-normalisable) function of two positions $\psi(\mathbf{x}_1, \mathbf{x}_2)$. If we now demand that the wave function represent indistinguishable particles, then it should assign the same probability (density) to find "particle one" at $\mathbf{x}_1$ and "particle two" at $\mathbf{x}_2$ as it does to finding "particle one" at $\mathbf{x}_2$ and "particle two" at $\mathbf{x}_1$.[29] In other words, the wave function should obey

$$|\psi(\mathbf{x}_2, \mathbf{x}_1)|^2 = |\psi(\mathbf{x}_1, \mathbf{x}_2)|^2 \quad \Longrightarrow \quad \psi(\mathbf{x}_2, \mathbf{x}_1) = \lambda\psi(\mathbf{x}_1, \mathbf{x}_2) , \tag{4.1}$$

where $\lambda = e^{i\phi}$ is a *phase*. Iterating this relation we see that

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \lambda^2\psi(\mathbf{x}_1, \mathbf{x}_2) , \tag{4.2}$$

so there are just two possibilities: $\lambda = \pm 1$.[30] In the case $\lambda = 1$ we are restricting ourselves to symmetric functions of the two particles' positions, while for $\lambda = -1$ we have anti-symmetric functions.

[28] It also turns out that the indistinguishability of elementary particles is built directly into *quantum field theory*, which is the framework that synthesises quantum theory with the special theory of relativity.

[29] Scare quotes because, of course, there is no unambiguous notion of particle one and particle two; this is just referring to the order of the arguments in the wave function.

[30] There is an oft-mentioned caveat here, which is that in two-dimensions there is a possibility for a more general phase λ, with the corresponding particles referred to as *anyons*. To see the possibility of this more general phase, it is necessary to be a bit more flexible about the description of the Hilbert space for several particles to allow multi-valued functions of positions. We will not pursue this here.

4.1.1 Permutations and Statistics

In the case of many particles, the exchange of the two particle positions generalises to an action of the symmetric group S_n on the space of n-particle wavefunctions,

$$\begin{aligned} \left(S_n, L^2(\mathbb{R}^{n\times d})\right) &\longrightarrow L^2(\mathbb{R}^{n\times d}) \\ (\pi, \psi(\mathbf{x}_1, \ldots, \mathbf{x}_n)) &\longmapsto (\pi \circ \psi)(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \psi(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(n)}) \ . \end{aligned} \tag{4.3}$$

By the same argument we had for the case $n = 2$, indistinguishability implies that this action obeys

$$\psi(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(n)}) = \lambda(\pi)\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ , \tag{4.4}$$

with $\lambda(\pi)$ a (now π-dependent) phase: $\lambda(\pi) = e^{i\phi(\pi)}$. Composing the action of two permutations $\pi, \sigma \in S_n$ we find

$$\begin{aligned} \psi(\mathbf{x}_{(\pi\circ\sigma)(1)}, \ldots, \mathbf{x}_{(\pi\circ\sigma)(n)}) = \lambda(\pi)\psi(\mathbf{x}_{\sigma(1)}, \ldots, \mathbf{x}_{\sigma(n)}) &= \lambda(\pi)\lambda(\sigma)\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ , \\ &= \lambda(\pi \circ \sigma)\psi(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ . \end{aligned} \tag{4.5}$$

So we have the rule $\lambda(\pi \circ \sigma) = \lambda(\pi)\lambda(\sigma)$.

Definition 4.1.1. A *multiplicative character* of a group G is a group homomorphism from G into the circle group $U(1)$ (or more generally into the ring of units $k^\times$ of a field k).

Thus, we have that the map $\lambda : S_n \to \mathbb{C}$ defines a multiplicative character for the permutation group S_n.

It turns out that there are only two inequivalent multiplicative characters for S_n. First observe that any two elements of S_n that are conjugate to each other are mapped to the same value by a multiplicative character,

$$\lambda(\pi \circ \sigma \circ \pi^{-1}) = \lambda(\pi)\lambda(\sigma)\lambda(\pi^{-1}) = \lambda(\pi)\lambda(\sigma)\lambda(\pi)^{-1} = \lambda(\sigma) \ , \tag{4.6}$$

where we have used that $\lambda(\pi^{-1}) = \lambda(\pi)^{-1}$, which follows from the character being a group homomorphism. Now recall that in S_n, a *transposition* is a permutation that just swaps two elements of $\{1, \ldots, n\}$, say r and s, and is denoted $(r\,s)$. Such transpositions are all conjugate to one another:

$$(r\,s) = (1\,r)(2\,s)(1\,2)(2\,s)^{-1}(1\,r)^{-1} \ . \tag{4.7}$$

Thus we have that $\lambda((r\,s)) = \lambda((1\,2)) = \pm 1$, where our previous argument in the two-particle case implies the latter equality.

General permutations are generated by the composition of transpositions, and are unambiguously classified as either being *odd* or *even* according to whether they arise from an odd or even number of transpositions. Thus we have the following

Proposition 4.1.2. Let $\lambda : S_n \to \mathbb{C}$ be a multiplicative character for the symmetric group. Then either $\lambda(\pi) \equiv 1$ or $\lambda(\pi) = \varepsilon(\pi)$, where ε gives the signature of the permutation,

$$\varepsilon(\pi) := \begin{cases} 1 & \text{for } \pi \text{ even} \ , \\ -1 & \text{for } \pi \text{ odd} \ . \end{cases} \tag{4.8}$$

The two possibilities for wave functions of indistinguishable particles are then either *totally symmetric* wave functions ($\lambda \equiv 1$) or *totally antisymmetric* wave functions ($\lambda = \varepsilon$), generalising the two-particle case. For a given species of elementary (indistinguishable) particle, one of these two cases must apply. This leads to a binary classification of indistinguishable particles:

Definition 4.1.3. Indistinguishable particles satisfying (4.4) are called *bosons* if the corresponding group character is the trivial one; these particles are said to obey *Bose–Einstein statistics*. Particles satisfying (4.4) with the nontrivial character (ε) are called *fermions*; these particles are said to obey *Fermi–Dirac statistics*.

The known elementary fermions in nature are electrons, muons, τ-particles, and neutrinos, along with their anti-particles (collectively, *leptons*), as well as quarks. Also composite particles made up of an odd number of elementary fermions, such as protons and neutrons, are fermions. The known elementary bosons in nature are photons, gluons, W- and Z-bosons, gravitons, and the Higgs boson. Also composite particles made up of an even number of elementary fermions, such as *mesons*.

An important fact, whic can be observed empirically in nature, is that the statistics of a particle is correlated with its *spin* (we will give a full treatment of spin in Chapter 5.2.5). In fact, this empirical fact is also a mathematical theorem that can be proven within the context of *relativistic quantum field theory*.

Theorem 4.1.4 (Spin-statistics theorem in three dimensions)**.** In a relativistic quantum theory in three spatial dimension, particles with integer spin must obey Bose–Einstein statistics. Particles with half-integer spin ($n + \frac{1}{2}$ for $n \in \mathbb{N}$) must obey Fermi–Dirac statistics.

An analogous theorem holds in any number of spatial dimensions greater than three, where one must be a bit more precise about the meaning of integer/half-integer spin (spin is no longer characterised by a single number in higher dimensions).

4.2 Bosonic and fermionic wave functions

It is useful to have practical tools for producing and manipulating wave functions for particles obeying appropriate statistics. To this end we can define projection operators onto the subspaces of completely symmetric and completely anti-symmetric (bosonic and fermionic, respectively) wavefunctions. In particular, for a general n-particle wave function ψ, define[31]

$$\Pi_\lambda \psi = \frac{1}{n!} \sum_{\pi \in S_n} \lambda(\pi^{-1}) \psi(\mathbf{x}_{\pi(1)}, \ldots, \mathbf{x}_{\pi(n)}) \,, \tag{4.9}$$

where as before, λ is the identity for Bose–Einstein and is ε for Fermi–Dirac. We can think of this as *averaging over the action of the permutation group*, with the average weighted by the relevant group character. We easily prove the following:

Proposition 4.2.1. For $\sigma \in S_n$ we have

$$(\Pi_\lambda \psi)(\mathbf{x}_{\sigma(1)}, \ldots, \mathbf{x}_{\sigma(n)}) = \lambda(\sigma)(\Pi_\lambda \psi)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \,, \tag{4.10}$$

$\Pi_\lambda^2 = \Pi_\lambda$, and Π_λ is self-adjoint. Thus Π_λ is an orthogonal projection operator onto bosonic/fermionic wave functions.

Proof. For the first result, we proceed by direct calculation:

$$\begin{aligned}
(\Pi_\lambda \psi)(\mathbf{x}_{\sigma(1)}, \ldots, \mathbf{x}_{\sigma(n)}) &= \frac{1}{n!} \sum_{\pi \in S_n} \lambda(\pi^{-1}) \psi(\mathbf{x}_{(\pi\circ\sigma)(1)}, \ldots, \mathbf{x}_{(\pi\circ\sigma)(n)}) \,, \\
&= \frac{1}{n!} \sum_{\pi \in S_n} \lambda(\sigma \circ (\pi \circ \sigma)^{-1}) \psi(\mathbf{x}_{(\pi\circ\sigma)(1)}, \ldots, \mathbf{x}_{(\pi\circ\sigma)(n)}) \,, \\
&= \frac{1}{n!} \sum_{\tilde{\pi} \in S_n} \lambda(\sigma \circ \tilde{\pi}^{-1}) \psi(\mathbf{x}_{\tilde{\pi}(1)}, \ldots, \mathbf{x}_{\tilde{\pi}(n)}) \,, \\
&= \lambda(\sigma)(\Pi_\lambda \psi)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \,.
\end{aligned}$$

To go from the second to the third line, we have used that for fixed $\sigma \in S_n$, as π ranges over S_n, so does $\tilde{\pi} = \pi \circ \sigma$ and so we can replace the latter by the former in the summation.

[31] Since for our multiplicative characters $\lambda(\pi) = \pm 1 = \lambda(\pi^{-1})$, the π^{-1} argument could be replaced with a π. The expression here is the one that generalises to more general finite groups with multiplicative characters that realise more general phase values.

Using this, we then confirm that

$$\begin{aligned}\Pi_\lambda(\Pi_\lambda\psi)(\mathbf{x}_1,\ldots,\mathbf{x}_n) &= \frac{1}{n!}\sum_{\pi\in S_n}\lambda(\pi^{-1})(\Pi_\lambda\psi)(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(n)})\,,\\ &= \frac{1}{n!}\sum_{\pi\in S_n}\lambda(\pi^{-1})\lambda(\pi)(\Pi_\lambda\psi)(\mathbf{x}_1,\ldots,\mathbf{x}_n)\,,\\ &= (\Pi_\lambda\psi)(\mathbf{x}_1,\ldots,\mathbf{x}_n)\,,\end{aligned}$$

where we have used that $|S_n| = n!$. Finally, self-adjointness can be shown by term-by-term change of variables in the inner product. We leave the details to the interested reader. The stated result then follows. ■

4.2.1 Two-particle projections

For the two-particle case ($n = 2$), where the space of distinguishable-particle wave functions is $L^2(\mathbb{R}^d \times \mathbb{R}^d)$, the two projectors we have just defined are just the operations of taking symmetric and antisymmetric combinations, respectively:

$$\Pi_1\psi(\mathbf{x}_1,\mathbf{x}_2) = \frac{\psi(\mathbf{x}_1,\mathbf{x}_2)+\psi(\mathbf{x}_2,\mathbf{x}_1)}{2}\,, \qquad \Pi_\varepsilon\psi(\mathbf{x}_1,\mathbf{x}_2) = \frac{\psi(\mathbf{x}_1,\mathbf{x}_2)-\psi(\mathbf{x}_1,\mathbf{x}_2)}{2}\,. \tag{4.11}$$

In this case, all wave functions can be decomposed into symmetric and antisymmetric parts, so the full space of (distinguishable) two-particle wave functions can be decomposed into bosonic and fermionic wave functions. Alternatively, this can be phrased as the identity

$$\Pi_1 + \Pi_\varepsilon = 1_{L^2(\mathbb{R}^d\times\mathbb{R}^d)}\,, \tag{4.12}$$

which can be re-interpreted as the resolution of the identity for the permutation operator that exchanges $\mathbf{x}_1 \leftrightarrow \mathbf{x}_2$.

Note that this is not the situation for larger values of n; there are wavefunctions that cannot be decomposed into just totally-symmetric and totally-antisymmetric parts. We will make a related observation when we count bosonic and fermionic states associated to finite Hilbert spaces later in this Chapter.

4.2.2 n-particle projections

Though the general projection operator is a little complicated to perform in practice for general wave functions (it involves choosing a sufficiently efficient way to sum over permutations), there is a case where things can be phrased more compactly. This is where we start with a *separable* distinguishable-particle wave function:

$$\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n) = \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)\ldots\psi_n(\mathbf{x}_n)\,. \tag{4.13}$$

This is a particularly natural class of wavefunctions to consider when considering *non-interacting* identical particles, where we might chose the ψ_i to be stationary states of the one-particle Hamiltonian acting on $\mathbf{x}_i$ to get stationary states for the full n-particle system.

The fermionic projection can then be realised in terms of what's called the *Slater determinant* of the single-particle wave-functions.

Definition 4.2.2. The *Slater determinant* of the wave-functions $\{\psi_i(\mathbf{x})\}$ is the determinants

$$\left|\psi_1,\ldots,\psi_n\right\rangle = \frac{1}{\sqrt{n!}}\begin{vmatrix}\psi_1(\mathbf{x}_1) & \psi_2(\mathbf{x}_1) & \ldots & \ldots & \psi_n(\mathbf{x}_1)\\ \psi_1(\mathbf{x}_2) & \psi_2(\mathbf{x}_2) & \ldots & \ldots & \psi_n(\mathbf{x}_2)\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ \psi_1(\mathbf{x}_n) & \ldots & & \ldots\ldots & \psi_n(\mathbf{x}_n)\end{vmatrix}\,. \tag{4.14}$$

The normalisation is such that if the ψ_i are mutually orthonormal, then $\left|\psi_1,\ldots,\psi_n\right\rangle$ is normalised. We then have that

$$\Pi_\varepsilon\left(\psi_1(\mathbf{x}_1)\cdots\psi_n(\mathbf{x}_n)\right) = \frac{1}{\sqrt{n!}}\left|\psi_1,\ldots,\psi_n\right\rangle\,. \tag{4.15}$$

Since arbitrary states can be expressed as (infinite) linear combinations of separable states, all fermionic wave functions can be obtained as (infinite) linear combinations of these types of states.

An analogous construction works in the bosonic case, though this uses the so-called *permanent* of a matrix, which is like the determinant but without the signs,

$$\Pi_1\psi = \frac{1}{n!}\,\mathrm{perm}\begin{pmatrix} \psi_1(\mathbf{x}_1) & \psi_2(\mathbf{x}_1) & \dots & \dots & \psi_n(\mathbf{x}_1) \\ \psi_1(\mathbf{x}_2) & \psi_2(\mathbf{x}_2) & \dots & \dots & \psi_n(\mathbf{x}_2) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \psi_1(\mathbf{x}_n) & \dots & \dots & \dots & \psi_n(\mathbf{x}_n) \end{pmatrix} . \tag{4.16}$$

As in the fermionic case, arbitrary bosonic wave functions can be constructed from these permanent states.

4.3 Symmetric and anti-symmetric tensor products

Though above we focused on fermionic and bosonic *wave functions*, the (anti-)symmetrisation procedure we have developed applies equally well to the case when we are taking tensor powers of some general Hilbert space $\mathcal{H}$ such as the qubit Hilbert space (or even a general vector space, for that matter). Here the n-fold tensor product of $\mathcal{H}$ admits a natural action of the symmetric group S_n just as was the case for wave functions: for $\psi_i \in \mathcal{H}$, we have

$$\begin{aligned} (S_n, \mathcal{H}^{\otimes n}) &\longrightarrow \mathcal{H}^{\otimes n} \\ \left(\pi, \psi_1 \otimes \cdots \otimes \psi_n\right) &\longmapsto \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)} . \end{aligned} \tag{4.17}$$

This action on pure tensors extends by linearity to all of $\mathcal{H}^{\otimes n}$.

We can then define bosonic and fermionic projection operators analogous to the ones we used for wave functions above. Just like we had for separable wave functions, we can define the action of these projection operators on pure tensors in $\mathcal{H}^{\otimes n}$ in terms of the determinants and permanents. We can analogously define bosonic and fermionic states in the n-fold tensor product of identical Hilbert spaces as the ranges of the corresponding orthogonal projectors:

Definition 4.3.1. The *n-fold symmetric tensor product* $\odot^n\mathcal{H}$ of the Hilbert space $\mathcal{H}$ is the subspace of the n-fold tensor product $\mathcal{H}^{\otimes n}$ on which Π_1 acts as the identity, or equivalently,

$$\odot^n \mathcal{H} = \mathrm{Ran}_{\mathcal{H}^{\otimes n}}\Pi_1 . \tag{4.18}$$

This is sometimes also denoted $\mathrm{Sym}^n\mathcal{H}$, and these are states that are compatible with Bose–Einstein statistics.

Definition 4.3.2. The *n-fold antisymmetric tensor product* of the Hilbert space $\mathcal{H}$ is the subspace of the n-fold tensor product $\mathcal{H}^{\otimes n}$ on which Π_ε acts as the identity, or alternatively,

$$\wedge^n \mathcal{H} = \mathrm{Ran}_{\mathcal{H}^{\otimes n}}\Pi_\varepsilon . \tag{4.19}$$

This is sometimes called the *exterior tensor product*, and these states are compatible with Fermi–Dirac statistics.

From the standard properties of determinants, a Slater determinant state will vanish identically if two of the constituent ψ_i are proportional. This means that the basis of n-particle states we get by acting with the fermionic projection operator on a basis of pure tensors all come from states where each of the n particles is in a distinct basis state. This is often phrased in terms of the following,

The Pauli exclusion principle: *Two fermions cannot occupy the same state.*

Indeed, this leads to a significant reduction in the number of fermionic states that can be constructed from a given set of single-particle states. To see this more explicitly, let us count the bosonic and fermionic states that can be built from a given N-dimensional Hilbert space under iterated symmetric and anti-symmetric tensor products.

Lemma 4.3.3. The space of fermionic n-particle states built from an N-dimensional single-particle Hilbert space $\mathcal{H}$ has dimension given by

$$\dim\left(\wedge^n \mathcal{H}\right) = \binom{N}{n} . \tag{4.20}$$

Proof. We choose a basis for $\mathcal{H}$ and build a basis of states for the fermionic n-particle Hilbert space using Slater determinants where the ψ_i are elements of that basis. There are N choices for ψ_1, but since ψ_2 cannot be the same as ψ_1, there are $N-1$ choices for ψ_2 and so on. The final state is independent of the ordering of $\psi_1, \ldots, \psi_n$ so we have

$$\dim\left(\wedge^n \mathcal{H}\right) = \frac{N(N-1)\cdots(N-n+1)}{n!} = \frac{N!}{n!(N-n)!} = \binom{N}{n} . \tag{4.21}$$

■

Which leads to an immediate important observation, which will play an important role when we consider atomic structure in the presence of several electrons.

Corollary 4.3.4. At most N identical, non-interacting fermionic particles can coexist in a given N-dimensional single-particle Hilbert space $\mathcal{H}$.

For completeness, we also consider bosonic multi-particle states built from a given N-dimensional Hilbert space.

Lemma 4.3.5. The space of bosonic n-particle states built from an N-dimensional single-particle Hilbert space $\mathcal{H}$ has dimension given by

$$\dim\left(\odot^n \mathcal{H}\right) = \frac{(N+n-1)!}{(N-1)!\, n!} . \tag{4.22}$$

Proof. In order to prove this we introduce a generating function known as a *partition function* that has much wider applicability. In general a separable bosonic state can be represented as

$$\Pi_1\left(\psi_1^{\otimes k_1} \otimes \psi_2^{\otimes k_2} \cdots \psi_N^{\otimes k_N}\right) , \qquad \sum k_i = n . \tag{4.23}$$

The overall order doesn't matter because of the symmetrisation, so we only pay attention to how many times each basis element appears. We therefore want to count the number of non-negative integer partitions of n, ($\{k_i \in \mathbb{Z}_{\geqslant 0}\}$ such that the $\sum_i k_i = n$). Let us replace the ψ_i by formal variables x_i, whereupon our problem becomes that of counting the number of distinct monomials of the form $x_1^{k_1} x_2^{k_2} \cdots x_N^{k_N}$ of total degree n. If we further multiply each x_i by an additional formal variable s, then the total power of s will be the total degree. Taking the sum over *all* $k_1, \ldots, k_N$, we obtain

$$\sum_{k_1,\ldots,k_N \in \mathbb{N}} (sx_1)^{k_1}(sx_2)^{k_2} \ldots (sx_N)^{k_N} = \prod_{j=1}^{N} \sum_{k_j=0}^{\infty} (sx_j)^{k_j} = \prod_{j=1}^{N} \frac{1}{1-sx_j} . \tag{4.24}$$

If we set all the x_i to one, we obtain $1/(1-s)^N$ and the coefficient of s^n will simply count the number of terms where $\sum k_i = n$. The generalised binomial theorem then gives the following, from which the result follows.

$$\frac{1}{(1-s)^N} = \sum_{n \in \mathbb{N}} \binom{N+n-1}{n} s^n , \tag{4.25}$$

■

One can now observe explicitly that while for $n = 2$ there is an accidental equality

$$\dim \mathcal{H}^{\otimes n} = N^n = \dim \wedge^n \mathcal{H} + \dim \odot^n \mathcal{H} , \qquad n = 2 , \tag{4.26}$$

for more than two particles we have

$$\dim \mathcal{H}^{\otimes n} = N^n > \dim \wedge^n \mathcal{H} + \dim \odot^n \mathcal{H} , \qquad n > 2 . \tag{4.27}$$

So for more than two particles, a general multi-particle state cannot be decomposed into bosonic and fermionic parts.