Second Quantization

The name "second quantization" stands for a different way of looking at quantum theory, which is particularly suited for dealing with indistinguishable particles. Spins and qubits are distinguishable, so a state like

$$|\sigma_1, \sigma_2\rangle$$

means qubit 1 is in σ_1 and qubit 2 is in σ_2. But when we have indistinguishable particles, we cannot be this precise.

An example that I love are ultra cold atoms in optical lattices. Using standing-wave lasers it is possible to create traps for atoms. For instance, we could create a trap like this double well.

Now suppose we put an atom in this trap. People do this with Rb, Na, Li and so on. We now define the two states $|L\rangle$ and $|R\rangle$ which mean $|L\rangle$ = "atom is on the left" and so on

But now suppose we have two atoms, then we have four possibilities $|L,L\rangle$, $|L,R\rangle$, $|R,L\rangle$ and $|R,R\rangle$. Thus, a general quantum state could be written as

$$|\psi\rangle = \sum_{i,j=L,R} \psi(i,j)\,|i,j\rangle = \psi(L,L)\,|L,L\rangle + \psi(L,R)\,|L,R\rangle + \psi(R,L)\,|R,L\rangle + \psi(R,R)\,|R,R\rangle \qquad (1)$$

But now comes the catch: the atoms are indistinguishable particles (unless they were different isotopes, whose possibility we neglect). Thus if an alien were to come and exchange the two atoms (using advanced alien technology) we would never know. This means that

$$|\psi(i,j)|^2 = |\psi(j,i)|^2 \qquad (2)$$

The amplitudes don't have to be equal: but the probabilities do.

Hence we find that

$$\psi(i,j) = e^{i\phi}\,\psi(j,i) \qquad (3)$$

for some phase ϕ. This is a fundamental constraint of Nature, imposed only by the indistinguishability of identical particles

In certain exotic situations it is possible to have systems where the phase ϕ does not have a well defined value. These particles are called anyons (a very creative name). However, particles in Nature usually have a well defined ϕ. And they are divided into two categories, depending on their total spin value

- Bosons : $\phi = 0$: $\psi(i,j) = \psi(j,i)$ (4)

  Integer spin: $0, 1, 2, \dots$

  Photons, Rb, Na, ...

- Fermions : $\phi = \pi$: $\psi(i,j) = -\psi(j,i)$ (5)

  Half-integer spin: $1/2, 3/2, \dots$

  Protons, neutrons, electrons, Li, ...

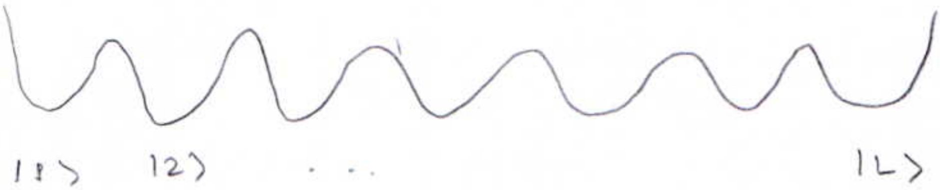
The connection with spin was established in 1940 by W. Pauli in a paper entitled "The connection between spin and statistics". It is a fundamental result of quantum field theory and relativity.

In the particular case of Fermions we see that if $i = j$ we get $\psi(i,i) = -\psi(i,i)$, so that we must have

$$\psi(i,i) = 0 \quad \text{for Fermions} \tag{6}$$

This is the Pauli exclusion principle: two Fermions can never occupy the same quantum state.

Now I want you to start appreciating the big impact that this has on systems containing a large number of particles. So let's suppose we have an optical lattice with L sites where the atoms may reside



Suppose we have N=3 atoms and they are bosons. then a possible quantum state would read

$$|\psi\rangle = \sum_{i_1, i_2, i_3 = 1}^{L} \psi(i_1, i_2, i_3) \, |i_1, i_2, i_3\rangle \qquad (4)$$

For instance.

$\psi(7,7,42)$ = amplitude that
atom 1 is @ site 7
atom 2 is @ site 7
atom 3 is @ site 42.

But the atoms are indistinguishable so this cannot be different from $\psi(7,42,7)$ or $\psi(42,7,7)$. So you see, describing a state like in (4) entails a <u>huge</u> <u>redundancy</u>, which increases <u>exponentially</u> as we increase the number of particles.

It is precisely the goal of 2^{nd} quantization to handle this redundancy in a smart way. In 2^{nd} quantization we take a more laid back approach and focus only on the number of particles in each state.

To do that we introduce the idea of Fock state, or occupation number representation

$$|n_1, n_2, \ldots, n_L\rangle \tag{5}$$

Here n_i represents the number of particles in state $|i\rangle$, where
$i = 1, \ldots, L$. Instead of (4), we then represent states like

$$|\psi\rangle = \sum_{n_1 \ldots n_L} c(n_1, \ldots, n_L)\, |n_1, \ldots, n_L\rangle \tag{6}$$

the coefficients c are different than the ψ in (4): although
it is possible to relate them, the connection is really really
ugly so it is not worth worrying about it. Moreover, the fact
that our state $|\psi\rangle$, in this example, has only $N=3$ particles,
is actually encoded in the c's. For instance, $c(4,0,0,..,0)=0$

The nice thing about Fock states is that they treat on equal footing states having different numbers of particles. First we have one important state which is called the vacuum

$$|0, \dots, 0\rangle = |0\rangle \tag{7}$$

Then we have states with one particle, such as

$$|1, 0, \dots, 0\rangle, \quad |0, 1, 0, \dots, 0\rangle, \quad |0, 0, \dots, 1\rangle \tag{8}$$

A state such as $|0, 1, 0, \dots, 0\rangle$ reads very natural: it is the state where there is one particle at site $i = 2$.

Next we have states with 2 particles. And this is where the distinction between Bosons and Fermions becomes important. States with $N = 2$ include

$$|1, 0, 1, \dots 0\rangle, \quad |0, 2, 0, \dots, 0\rangle \tag{9}$$

and so on. However, whereas for Bosons $|0, 2, 0, \dots, 0\rangle$ would be fine, for Fermions this state is not allowed by the Pauli exclusion principle. Thus, to summarize

$$\boxed{\begin{array}{l} \underline{\text{Occupation numbers}} \\ \text{Bosons: } \; n_i = 0, 1, 2, \dots \\ \text{Fermions: } \; n_i = 0, 1 \end{array}} \tag{10}$$

At this point the connection to the quantum harmonic oscillator starts to become evident for Bosons. We can now define <u>creation</u> <u>and</u> <u>annihilation</u> <u>operators</u>, which literally create and annihilate particles in the quantum states $|i\rangle$. That is

$$\text{(Bosons)} \qquad \boxed{\begin{aligned} a_i \,|n_1, \dots, n_i, \dots, n_L\rangle &= \sqrt{n_i}\,|n_1, \dots, n_i - 1, \dots, n_L\rangle \\ a_i^\dagger \,|n_1, \dots, n_i, \dots, n_L\rangle &= \sqrt{n_i+1}\,|n_1, \dots, n_i + 1, \dots, n_L\rangle \end{aligned}} \qquad (11)$$

these operators, just like in the harmonic oscillator case, satisfy

$$\text{(Bosons)} \qquad \boxed{\begin{aligned} [a_i, a_j^\dagger] &= \delta_{ij} \\ [a_i, a_j] = [a_i^\dagger, a_j^\dagger] &= 0 \end{aligned}} \qquad (12)$$

and, of course, they can be combined to form the <u>number operator</u>

$$\hat{n}_i = a_i^\dagger a_i \qquad \text{(this guy wears a hat!)} \qquad (13)$$

which satisfies

$$\hat{n}_i |n_1, \dots, n_L\rangle = \underbrace{n_i}_{\text{No hat. this is a number}} |n_1, \dots, n_L\rangle \qquad (14)$$

These operators are constructed precisely so as to satisfy the bosonic exchange symmetry (4). For instance, suppose we want to construct a state with one particle at site i and another at site j. We can do this starting from the vacuum and applying $a_i^\dagger$ and then $a_j^\dagger$

$$|1_i, 1_j\rangle = a_j^\dagger a_i^\dagger |0\rangle \tag{15}$$

where 1_i means one particle at site i. But for Bosons the order shouldn't matter: we could have very well have created first in j then in i

$$a_j^\dagger a_i^\dagger |0\rangle = a_i^\dagger a_j^\dagger |0\rangle \tag{16}$$

This is why $[a_i^\dagger, a_j^\dagger] = 0$ [Eq (12)]. So you see, the algebra is a direct reflex of the physical symmetries

Now what about Fermions? Could we similarly construct creation and annihilation operators for them? And if so, what would be the algebra?

Let's call these operators $c_i^\dagger$ and c_i. We have two hints. First, the number operator

$$\hat{n}_i = c_i^\dagger c_i \tag{17}$$

should have eigenvalues 0 and 1 [Eq (10)]. And second, the order we create should obey the Fermionic rule (5):

$$c_i^\dagger c_j^\dagger |0\rangle = -c_j^\dagger c_i^\dagger |0\rangle \tag{18}$$

Thus, for Fermions the operators anti-commute

$$\text{(Fermions)} \qquad \boxed{\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0} \tag{19}$$

where $\{A, B\} = AB + BA$ is the anti-commutator. In particular, this also contemplates the Pauli exclusion principle because $\{A, A\} = 2A$ so if $j = i$ we get

$$c_i^2 = (c_i^\dagger)^2 = 0 \tag{20}$$

(Trying to create 2 particles in the same state is impossible)