A first look at 2^{nd} quantization

Additional reading

- Sakurai, chapter 7
- Feynman, statistical mechanics, chapter 6
- Bruus and Flensberg, chapter 1
- Altland and Simons, chapters 1 and 2.

A first look at second quantization

The name "second quantization" stands for a different way of writing down the rules of quantum mechanics, that is ideally suited for dealing with a *large number of identical particles*. In quantum mechanics we usually say "which particle is in which state". But for many identical particles, that is too messy. Instead, in second quantization we only specify "*how many* particles are in each state". This is what we call the *occupation number representation*.

Second quantization is the basis of most modern theories in physics, from condensed matter to quantum field theory. It is still quantum mechanics, so everything you learned before continues to hold. What really changes is the way we think about the problem.

Introducing second quantization to a student for the first time is always a bit tricky. I could always try to show you in detail where it all comes from. But that is usually too abstract and not very productive. I therefore propose we do this in 2 steps. In these notes I will give you only the general idea, without rigorous proofs. This will allow us to jump straight to applications. Maybe this introduction will already satisfy you. But maybe it will leave you feeling that the theory is rather mystical. It is not. Second quantization *is* quantum mechanics and can be constructed using only the rules you already know.

To fill this gap, I will also publish an additional set of notes which provide a more rigorous construction. This other set of notes is optional, so if you decide to skip it you will not be penalized in any way.

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Single-particle states

Before we start, I want to clarify the idea of a single-particle state. This means any quantum state $|\alpha\rangle$ which characterizes a single particle. Examples include:

$|n\rangle$ = Particle at site n (tight-binding)

$|k\rangle$ = momentum state

$|k,\sigma\rangle$ = momentum and spin $\sigma = \pm 1$

$|n, \ell, m_\ell, \sigma\rangle$ = Hydrogen orbital

$|x\rangle$ = particle at position x.
Continuous version of $|n\rangle$.

Any of these states completely characterize a single particle. We will write such a general state as $|\alpha\rangle$. And we will assume they span the Hilbert space of a single particle. Moreover, we assume they form an orthonormal basis

$$\langle\alpha|\beta\rangle = \delta_{\alpha\beta} \qquad (1)$$

Bosons and Fermions

Now suppose you have N identical particles. A possible basis to describe your system is the product basis:

$$|\alpha_1, \dots, \alpha_N\rangle = |\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle \tag{2}$$

Thus, the state of the system may be expanded as

$$|\psi\rangle = \sum_{\alpha_1 \dots \alpha_N} c(\alpha_1, \dots, \alpha_N)\, |\alpha_1 \dots \alpha_N\rangle \tag{3}$$

for certain coefficients $c(\alpha_1 \dots \alpha_N)$. For instance, if we have two particles in momentum eigenstates, we could have

$$|\psi\rangle = \sum_{k_1, k_2} c(k_1, k_2)\, |k_1, k_2\rangle \tag{4}$$

Now recall that $c(\alpha_1, \dots, \alpha_N) = \langle \alpha_1 \dots \alpha_N | \psi\rangle$ so

$$\mathrm{Prob}(\alpha_1, \dots, \alpha_N) = |c(\alpha_1, \dots, \alpha_N)|^2 \tag{5}$$

But if the particles are identical, then the probabilities should be invariant under the exchange of any two particles.

$$\mathrm{Prob}(\dots, \alpha_i, \dots, \alpha_j, \dots) = \mathrm{Prob}(\dots, \alpha_j, \dots, \alpha_i, \dots) \tag{6}$$

This means that c may change by at most a phase

$$c(\dots \alpha_i \dots \alpha_j \dots) = e^{i\phi}\, c(\dots \alpha_j \dots \alpha_i \dots) \tag{7}$$

But if we exchange again, we must get back where we started, so $e^{2i\phi} = 1$. Whence we must have $\phi = 0$ or $\phi = \pi$, which means

$$\boxed{c(\ldots, \alpha_i, \ldots, \alpha_j, \ldots) = \pm\, c(\ldots, \alpha_j, \ldots, \alpha_i, \ldots)} \qquad (8)$$

This constraint is a consequence only of the fact that the particles are indistinguishable.

OK! But when should we use "+" and when should we use "−"?

In 1940 Pauli published a paper called "The connection between spin and statistics", where he showed, using only the properties of the Lorentz group, that the choice of "+" or "−" depends only on the spin of the particle in question:

Bosons:	integer spin	: "+" sign
Fermions:	half-integer spin	: "−" sign

(9)

This is a consequence of the invariance of any physical system under Lorentz transformations. We will not derive this result here. Instead, we will take it as a basic postulate.

Bosons

Let us focus on Bosons for a second. Suppose we label our states as $\alpha = 1, 2, 3, 4, \ldots$ We can always do this for any discrete set of states. A possible c coefficient in Eq (3) may then look like

$$c(1, 7, 3, 1, 1, 2, 5, 42, 3, 22, 11, 2, \ldots) \qquad (10)$$

For 10^{23} particles, this will be a complete mess. But for Bosons we are allowed to exchange the order of the indices, so we may regroup the quantum numbers in (10) as

$$c(\underbrace{1, 1, 1, \ldots}_{n_1}, \underbrace{2, 2, 2, \ldots}_{n_2}, \underbrace{3, 3, 3, \ldots}_{n_3}, \ldots) \qquad (11)$$

This introduces us to the idea of describing a state in terms of occupation numbers:

$$\boxed{n_\alpha = \text{number of particles in state } |\alpha\rangle} \qquad (12)$$

The jump to second quantization consists in using the number representation as a basis for the problem. That is, instead of $|\alpha_1, \ldots, \alpha_N\rangle$ in Eq (3), we use

$$|\psi\rangle = \sum_{n_1, n_2, \ldots} f(n_1, n_2, \ldots)\, |n_1, n_2, \ldots\rangle \qquad (13)$$

where the $f(n_1, n_2, \ldots)$ are a new set of coefficients.

Let me clarify what the Fock basis means. For simplicity suppose the single-particle Hilbert space has dimension d. That is, $\alpha = 1, 2, \ldots, d$. This means that there are d possible states a particle may occupy and the Fock basis counts the number of particles in each one. So the Fock basis would look like $|n_1, n_2, \ldots, n_d\rangle$.

The number of Fock states is infinite because there can be as many particles as we want. An important state is that with no particles, which we call the vacuum

$$\boxed{|0\rangle = |0, 0, \ldots, 0\rangle = \text{vacuum} \quad (\text{all } n_\alpha = 0)} \tag{14}$$

Then we have d states with only one particle:

$$|1, 0, 0, \ldots\rangle, \quad |0, 1, 0, \ldots\rangle, \quad \ldots \quad |0, 0, \ldots, 1\rangle$$

the state $|0, 0, 1, 0, \ldots\rangle$ for instance, is the same as the state single particle state $|\alpha = 3\rangle$.

Next we have a bunch of states with 2 particles, such as

$$|2, 0, 0, \ldots\rangle, \quad |1, 1, 0, 0, \ldots\rangle, \quad |0, 2, 0, \ldots\rangle, \quad \text{etc.}$$

It is possible to relate these states to products of single-particle states, like $|\alpha_1, \alpha_2\rangle$. But this is not so trivial and actually not very useful. I do this in the other set of notes, in case you are interested.

At this point, this discussion should start to remind you of the quantum harmonic oscillator. Each single-particle state $|\alpha\rangle$ may have n_α particles in it. So we may now define creation and annihilation operators $a_\alpha^\dagger$ and a_α, which create or destroy particles in state $|\alpha\rangle$. That is

$$\boxed{\begin{aligned} a_\alpha |\ldots, n_\alpha, \ldots\rangle &= \sqrt{n_\alpha}\, |\ldots, n_\alpha - 1, \ldots\rangle \\ a_\alpha^\dagger |\ldots, n_\alpha, \ldots\rangle &= \sqrt{n_\alpha + 1}\, |\ldots, n_\alpha + 1, \ldots\rangle \end{aligned}} \tag{15}$$

In order for this to be true, they must satisfy

$$\boxed{\begin{aligned} [a_\alpha, a_\beta^\dagger] &= \delta_{\alpha\beta} \\ [a_\alpha, a_\beta] &= 0 \end{aligned}} \tag{16}$$

when $\alpha \neq \beta$ (different states), they are completely independent. But when $\alpha = \beta$, they behave exactly like in the quantum harmonic oscillator.

We also naturally define the number operator

$$\boxed{\hat{n}_\alpha = a_\alpha^\dagger a_\alpha} \tag{17}$$

[I always put a hat in it, to avoid confusion with the number n_α]. It satisfies

$$\hat{n}_\alpha |\ldots, n_\alpha, \ldots\rangle = n_\alpha |\ldots, n_\alpha, \ldots\rangle \tag{18}$$

The operator $\hat{n}_\alpha$ therefore counts the number of particles in state $|\alpha\rangle$. If we want to count the total number of particles in the system, we define the operator

$$\boxed{\hat{N} = \sum_\alpha \hat{n}_\alpha} \tag{19}$$

It satisfies

$$\hat{N}\,|n_1, n_2, \dots\rangle = \left(\sum_\alpha n_\alpha\right)|n_1, n_2, \dots\rangle \tag{20}$$

Fermions

Before we continue with the formal development, let's see how all this changes in the case of Fermions. Going back to Eq (8), we now have

$$c(\ldots, \alpha_i, \ldots, \alpha_j, \ldots) = - c(\ldots, \alpha_j, \ldots, \alpha_i, \ldots) \qquad (21)$$

If we happen to choose $\alpha_i = \alpha_j$ then we get $x = -x$, whose only solution is $x = 0$. Thus

$$\boxed{c(\alpha_1, \alpha_2, \ldots, \alpha_N) = 0 \quad \text{if any two } \alpha_i \text{ are equal}} \qquad (22)$$

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

We may continue to use the Fock basis, but now the n_α can only take the values 0 or 1. Thus,

$$\boxed{n_\alpha = \begin{cases} 0, 1, 2, 3, \ldots & \text{for Bosons} \\ 0, 1 & \text{for Fermions} \end{cases}} \qquad (23)$$

We also define creation and annihilation operators $a_\alpha^\dagger$ and a_α. But to ensure that $n_\alpha = 0, 1$, they must now anti-commute

$$\boxed{\begin{aligned} \{a_\alpha, a_\beta^\dagger\} &= \delta_{\alpha\beta} \\ \{a_\alpha, a_\beta\} &= 0 \end{aligned}} \qquad (24)$$

To understand why this must be so, note that if $\alpha = \beta$ we get

$$\boxed{a_\alpha^2 = (a_\alpha^\dagger)^2 = 0} \qquad (25)$$

This is the Pauli principle: try to create twice or annihilate twice and you get zero. Thus, from the vaccum we can only create once

$$a_\alpha^\dagger |0\rangle = |1_\alpha\rangle$$

$$(a_\alpha^\dagger)^2 |0\rangle = a_\alpha^\dagger |1_\alpha\rangle = 0$$

The same is true when you try to annihilate twice.

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Concerning the algebra of Bosons and Fermions, we may write them in a unified way. To do that, define

$$\varepsilon = \begin{cases} +1 & \text{Bosons} \\ -1 & \text{Fermions} \end{cases} \qquad (26)$$

and

$$[A, B]_\varepsilon = AB - \varepsilon BA \qquad (27)$$

Then we may write (16) and (24) as

$$\boxed{\begin{aligned} [a_\alpha, a_\beta^\dagger]_\varepsilon &= \delta_{\alpha\beta} \\ [a_\alpha, a_\beta]_\varepsilon &= 0 \end{aligned}} \qquad (28)$$

Expressing operators in the language of second quantization

In order to make our theory useful, we must be able to write down formulas for any operator we want. Consider, for concreteness, the momentum operator (in 1D, just to make things simple). The momentum operator for a single particle is $\hat{p}$. But if we have N indistinguishable particles, it makes no sense to talk about the momentum of this or that guy. What we need to do is to look at the total momentum

$$\underline{\hat{P}} = \hat{p}_1 + \dots + \hat{p}_N$$

How can we express this in the language of 2nd quantization? Well, we know that the momentum single particle eigenstates are $|k\rangle$. Thus $a_k^\dagger a_k$ is the number operator counting the total number of particles with momentum k. This induces us to define the total momentum operator as

$$\boxed{\underline{\hat{P}} = \sum_k k\, a_k^\dagger a_k} \tag{29}$$

You simply sum each "k" times each number operator $a_k^\dagger a_k$. I know this isn't rigorous, but I think it makes sense

Similarly, let $\hat{T} = \frac{\hat{p}^2}{2m}$ denote the kinetic energy of one particle, and let $\hat{T}$ denote the total kinetic energy. Then we may write

$$\hat{T} = \sum_{k} \frac{k^2}{2m} a_k^\dagger a_k \tag{30}$$

In fact, we can even write a general formula. Let A be any single-particle operator and suppose its eigenstuff Eq reads

$$A|\alpha\rangle = \lambda_\alpha |\alpha\rangle \tag{31}$$

Then its 2^{nd} quantized version may be written as

$$\hat{A} = \sum_{\alpha} \lambda_\alpha a_\alpha^\dagger a_\alpha \tag{32}$$

or, what is better

$$\boxed{\hat{A} = \sum_{\alpha} \langle\alpha|A|\alpha\rangle a_\alpha^\dagger a_\alpha} \tag{33}$$

This is true for any operator written in its diagonal basis.

Next I want to write an operator in a basis where it may not necessarily be diagonal. To do that, let us first remember how to change bases in quantum mechanics. Let $|\alpha\rangle$ and $|i\rangle$ be two orthonormal basis sets. Then, to change from one to the other, we simply write

$$|\alpha\rangle = \sum_i |i\rangle\langle i|\alpha\rangle \tag{34}$$

To make the link with second quantization, we only need to remember that

$$|\alpha\rangle = a_\alpha^\dagger |0\rangle$$
$$|i\rangle = a_i^\dagger |0\rangle$$

Thus (34) becomes

$$\boxed{a_\alpha^\dagger = \sum_i \langle i|\alpha\rangle a_i^\dagger} \tag{35}$$

Conclusion: <u>creation</u> <u>operators</u> <u>transform</u> <u>like</u> <u>kets.</u> Taking the adjoint, we get

$$a_\alpha = \sum_i \langle\alpha|i\rangle a_i \tag{36}$$

Thus, annihilation operators transform like bras.

Now go back to (33) and insert (35), (36):

$$\hat{A} = \sum_{\alpha} \langle \alpha | A | \alpha \rangle \left[\sum_{i} \langle i | \alpha \rangle a_i^{\dagger} \right] \left[\sum_{j} \langle \alpha | j \rangle a_j \right]$$

$$= \sum_{i,j} a_i^{\dagger} a_j \sum_{\alpha} \langle i | \alpha \rangle \langle \alpha | A | \alpha \rangle \langle \alpha | j \rangle$$

The sum over α is

$$\sum_{\alpha} |\alpha\rangle\langle\alpha|A|\alpha\rangle\langle\alpha| = \sum_{\alpha} \lambda_{\alpha} |\alpha\rangle\langle\alpha| = A$$

Thus we conclude that

$$\boxed{\hat{A} = \sum_{ij} \langle i | A | j \rangle a_i^{\dagger} a_j} \qquad (37)$$

This shows how to write down any operator A in the language of second quantization. Notice how it mixes single-particle matrix elements $\langle i | A | j \rangle$ with creation and annihilation operators.

The operator A in Eq (37) is a single-particle operator. Another important class of operators are two-body operators, which describe the interaction between particles.

Two body operators appear when we consider a system of particles interacting via pairwise interactions. Something like

$$H = \sum_i \frac{p_i^2}{2m} + \underbrace{\frac{1}{2}\sum_{i\neq j} v(x_i, x_j)}_{V}$$

then V is a 2-body operator. We will discuss these operators in another set of notes. Right now I just want to mention that, whereas 1-body operators are described by two creation/annihilation operators, 2-body operators will be described by 4 such operators. The general 2-body operator looks like

$$\boxed{V = \sum_{ijkl} \langle ij | V | kl \rangle \, a_i^\dagger a_j^\dagger a_l a_k}$$

For this reason, interacting systems are notoriously more difficult to deal with. Later there will be a full set of notes dedicated to them.

Coordinate representation

An important single-particle ket is the position ket $|x\rangle$. These kets also form a basis, but it is a little delicate since they vary continuously. This means that

$$\langle x|y\rangle = \delta(x-y)$$

$$\int dx\, |x\rangle\langle x| = 1 \qquad (38)$$

Since $|x\rangle$ is a single-particle ket, we can define a corresponding annihilation operator a_x. But for historical reasons, no one writes it like that. They write it as $\psi(x)$. The reason is that, in some sense, this $\psi(x)$ behaves a lot like a wave-function, even though it is actually an operator. I know, it is a bit confusing at first. Simply remember that

$$\boxed{\psi(x) = a_x = \text{annihilates a particle at position } x} \qquad (39)$$

The commutation relations for $\psi(x)$ are a little different since x varies continuously [cf. Eq (38)]. Instead of (28), they read

$$\boxed{\begin{aligned}[\psi(x), \psi^\dagger(x')]_\xi &= \delta(x-x') \\ [\psi(x), \psi(x')]_\xi &= 0\end{aligned}} \qquad (40)$$

The rule is simple to remember; replace Kronecker δ's by Dirac δ's. Also, replace sums by integrals. For instance, the operator $\psi^{+}(x)\psi(x)$ denotes the <u>density of particles</u> at position x. The total number of particles is then

$$\hat{N} = \int dx\, \psi^{+}(x)\psi(x) \tag{41}$$

We can also use (37) to express any single-particle operator in the coordinate representation. It now reads

$$A = \int dx dx' \langle x|A|x'\rangle \psi^{+}(x)\psi(x') \tag{42}$$

For instance, the momentum operator has matrix elements

$$\langle x|\hat{p}|x'\rangle = i\frac{\partial}{\partial x'}\delta(x-x') \tag{43}$$

then the total momentum operator becomes

$$\hat{P} = \int dx dx' \left[i\frac{\partial}{\partial x'}\delta(x-x')\right] \psi^{+}(x)\psi(x')$$

$$= -\int dx dx' \delta(x-x') \left[-i\frac{\partial}{\partial x'}\right] \psi^{+}(x)\psi(x')$$

or

$$\boxed{\hat{P} = \int dx\, \psi^{+}(x)\left[-i\frac{\partial}{\partial x}\right]\psi(x)} \tag{44}$$

This is absolutely identical to the way you compute expectation values $\langle\psi|\hat{p}|\psi\rangle$ in basic quantum mechanics, except that now ψ is an operator.

We can also do the same thing for the Hamiltonian.

The Hamiltonian of a single particle in an external potential $U(x)$ is

$$H = \frac{\hat{p}^2}{2m} + U(x) \qquad (45)$$

Its 2^{nd} quantized version will then be

$$\boxed{\mathcal{H} = \int dx\, \psi^\dagger(x)\left[-\frac{\partial_x^2}{2m} + U(x)\right]\psi(x)} \qquad (46)$$

This is what we call the non-interacting part of the Hamiltonian. Note that it is quadratic in creation and annihilation operators. Quadratic always means "non-interacting".

We can also write (45) in the momentum basis:

$$H = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \sum_{k,k'} \langle k|\hat{U}|k'\rangle a_k^\dagger a_{k'}$$

We can work out $\langle k|V|k'\rangle$ by recalling that $\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{L}}$.

Then

$$\begin{aligned}\langle k|\hat{U}|k'\rangle &= \int dx\, \langle k|\hat{U}|x\rangle\langle x|k'\rangle \\ &= \int dx\, U(x)\, \langle k|x\rangle\langle x|k'\rangle \\ &= \frac{1}{L}\int_0^L dx\, U(x)\, e^{-i(k-k')x}\end{aligned}$$

We define the Fourier transform of the potential as

$$U(q) = \frac{1}{L}\int dx\, U(x)\, e^{-iqx} \tag{47}$$

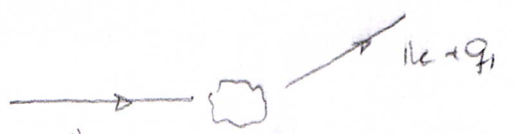
In 3D we would have instead

$$U(\mathbf{q}) = \frac{1}{Vol}\int d^3\mathbf{x}\, U(\mathbf{x})\, e^{-i\mathbf{q}\cdot\mathbf{x}}.$$

then we may write the Hamiltonian more neatly as

$$\boxed{\mathcal{H} = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \sum_{k,q} U(q)\, a_{k+q}^\dagger a_k} \tag{48}$$

the last term describes the effect of the potential $U(q)$ as a series of possible scattering events



It's like $U(\mathbf{x})$ acts as an impurity which scatters a particle of momentum $\mathbf{k}$ into a state of momentum $\mathbf{k}+\mathbf{q}$. In 2nd quantization this is described by first destroying an electron with a_k and subsequently creating another one with $a_{k+q}^\dagger$. Of course, in the process the total number of particles is conserved.

Canonical quantization

I cannot resist to tell you another way to construct 2^{nd} quantization. Recall how first quantization works. We start with a Lagrangian $\mathcal{L}(q, \partial_t q)$ then we define the canonical momentum associated to q as

$$p = \frac{\partial \mathcal{L}}{\partial(\partial_t q)}$$

Next we construct the Hamiltonian as

$$H(q,p) = \dot{q} p - \mathcal{L}$$

and finally we promote q, p to operators satisfying the canonical commutation relation

$$q \to \hat{q} \qquad \text{with} \qquad [\hat{q}, \hat{p}] = i$$
$$p \to \hat{p}$$

$(\hbar = 1)$.

Now consider the Schrödinger Lagrangian

$$\mathcal{L} = i \sum_n \psi_n^* \partial_t \psi_n - \sum_{n,m} H_{n,m} \psi_n^* \psi_m \qquad (49)$$

we repeat the same steps. The canonical momentum associated to ψ_n is

$$\Pi_n = \frac{\partial \mathcal{L}}{\partial(\partial_t \psi_n)} = i \psi_n^* \qquad (49')$$

The momentum associated to ψ_n^* is zero.

Then we construct the Hamiltonian

$$H(\psi_m, \Pi_m) = \sum_n \Pi_n (\partial_t \psi_n) - \mathcal{L}$$

$$= \sum_n i\psi_n^* \partial_t \psi_n - \sum_n i\psi_n^* \partial_t \psi_n + \sum_{n,m} H_{n,m} \psi_n^* \psi_m$$

Thus

$$H(\psi_m, i\psi_n^*) = \sum_{n,m} H_{n,m} \psi_n^* \psi_m \qquad (50)$$

which is, of course, obvious. Finally we promote ψ_n and Π_n to operators satisfying a canonical commutation relation

$$\begin{aligned} \psi_n &\to \hat{\psi}_n \\ \psi_n^* &\to \hat{\psi}_n^\dagger \end{aligned} \qquad (51)$$

with

$$[\hat{\psi}_n, i\hat{\psi}_m^\dagger] = i\delta_{nm} \Rightarrow [\hat{\psi}_n, \hat{\psi}_m^\dagger] = \delta_{nm} \qquad (52)$$

voilà! change the symbol

$$\begin{aligned} \hat{\psi}_n &\to a_n \\ \hat{\psi}_n^\dagger &\to a_n^\dagger \end{aligned}$$

and we get from (50)

$$\boxed{\hat{H} = \sum_{n,m} H_{n,m} a_n^\dagger a_m} \qquad (53)$$

This is just like (37), with $A = H$. This is why this is called 2^{nd} quantization. Eq (47) was the first and it led to (48). Now we quantize again and get (53).