Second Quantization

2025-04-07

We take a close look at the tedious steps of second quantization, which is a fundamental concept in quantum mechanics and solid state physics. The goal is the put together the basic formalism. We will later use this to study superfluidity and superconductivity..

blog: https://tetraquark.vercel.app/posts/second_quantization/

email: quarktetra@gmail.com

This is a quick review of relatively boring steps of the second quantization formalism. The term "second quantization" refers to a mathematical formalism that extends quantum mechanics from single-particle systems to many-particle systems. The name arises from the historical development of quantum theory: "first quantization" involved replacing classical variables with operators, converting classical mechanics to quantum mechanics for single particles. Second quantization takes this process a step further by promoting quantum wave functions themselves to operators (creation and annihilation operators), effectively quantizing the quantum fields. This approach elegantly handles identical particles and provides the mathematical framework for quantum field theory. While the name might suggest a sequential application of quantization, it's more accurately viewed as a different mathematical representation of the same physical theory, particularly useful for systems with variable particle numbers.

I will closely follow the presentation in [1] with slightly modified notation. I will also use borrowed ideas from [2]. All the credit for the content goes to [1] and [2], while any mistakes or inaccuracies are entirely my own.

Identical Particles

We will look at N identical particles. We will denote the variables of the i^{th} particles as $\zeta_i = (\mathbf{x}_i, \sigma_i)$, which are the position and spin degrees of freedom. The Hamiltonian for the system is given by

$$H = H(\zeta_1, \zeta_2, \ldots, \zeta_N), \tag{1}$$

and it is symmetric in the variables $\zeta_1, \zeta_2, \ldots, \zeta_N$. We write a wave function in the form

$$\psi = \psi(\zeta_1, \zeta_2, \ldots, \zeta_N). \tag{2}$$

Permutation Operator

The permutation operator P_{ij} swaps the variables ζ_i and ζ_j:

$$P_{ij}\psi(\ldots, \zeta_i, \ldots, \zeta_j, \ldots) = \psi(\ldots, \zeta_j, \ldots, \zeta_i, \ldots). \tag{3}$$

Since swapping the variables twice brings them back to their original state, we have $P_{ij}^2 = 1$. This implies that the eigenvalues of P_{ij} are ± 1. Furthermore since the Hamiltonian is invariant under the permutation of the variables, we have

$$[P_{ij}, H] = 0. \tag{4}$$

The permutation group S_N which consists of all permutations of N objects has $N!$ elements. Every permutation P can be represented as a product of transpositions P_{ij}. An element is said to be even (odd) when the number of P_{ij}'s is even (odd).

Properties

(i) Permutation operators do not change the inner product of two states.

$$\begin{aligned}
\langle \varphi | \psi \rangle &= \int dx_1 \cdots dx_i \cdots dx_j \cdots dx_N \varphi^*(\zeta_1, \ldots, \zeta_i, \ldots, \zeta_j, \ldots, \zeta_N)\psi(\zeta_1, \ldots, \zeta_i, \ldots, \zeta_j, \ldots, \zeta_N) \\
&= \int dx_1 \cdots dx_i \cdots dx_j \cdots dx_N P_{ij}\varphi^*(\zeta_1, \ldots, \zeta_j, \ldots, \zeta_i, \ldots, \zeta_N) P_{ij}\psi(\zeta_1, \ldots, \zeta_j, \ldots, \zeta_i, \ldots, \zeta_N) \\
&= \langle P\varphi | P\psi \rangle,
\end{aligned} \tag{5}$$

where we swapped the integration variables.

(ii) P_{ij} is unitary.

Given an operator A, its adjoint $A^\dagger$ is defined as usual by

$$\langle \varphi | A | \psi \rangle = \langle A^\dagger \varphi | \psi \rangle. \tag{6}$$

We will apply this to $P \equiv P_{ij}$:

$$\langle \varphi | P | \psi \rangle = \langle P^{-1} P \varphi | P \psi \rangle = \langle P\varphi | \left(P^{-1}\right)^\dagger | P\psi \rangle = \langle \varphi | \left(P^{-1}\right)^\dagger | \psi \rangle, \tag{7}$$

which implies:

$$P = \left(P^{-1}\right)^{\dagger} \iff P^{\dagger} = P^{-1} \iff PP^{\dagger} = 1 \tag{8}$$

(iii) Any symmetric operator S commutes with the permutation operator P_{ij}.

$$[P_{ij}, S] = 0 \tag{9}$$

Proof:

$$\langle \psi_i | S | \psi_j \rangle = \langle P\psi_i | S | P\psi_j \rangle = \langle \psi_i | P^{\dagger} S P | \psi_j \rangle \iff P^{\dagger} S P = S \implies [P, S] = 0, \tag{10}$$

where we renamed the integration variables as we did in Eq. (5).

This shows that the matrix elements of S are the same in the states ψ_i and in the permutated states $P\psi_i$. The states ψ and $P\psi$ are experimentally indistinguishable.

Completely Symmetric and Antisymmetric States

The *totally symmetric* and *totally antisymmetric* states ψ_s and ψ_a are special states:

$$P_{ij}\psi_a(\ldots, \zeta_i, \ldots, \zeta_j, \ldots) = \pm\psi_a(\ldots, \zeta_i, \ldots, \zeta_j, \ldots) \tag{11}$$

for all P_{ij}. We will construct the basis states of the N-particle system by taking the tensor product of the single-particle states $|i\rangle$: $|1\rangle$, $|2\rangle$, $\cdots$. We will further label the states with the particle label $\alpha \in [1, N]$: $|i\rangle_\alpha \equiv |i_\alpha\rangle$, which means that the α-th particle is in state $|i\rangle$. With this notation, the basis states of the N-particle system are:

$$|i_1, \cdots, i_\alpha, \cdots, i_N\rangle. \tag{12}$$

If the set of states $\{|i\rangle\}$ is a complete and orthonormal one, the product states are also complete orthonormal in the space of N-particle states.

The fully symmetrized/antisymmetrized basis states are then defined by

$$S_{\pm}|i_1, i_2, \cdots, i_N\rangle \equiv \frac{1}{\sqrt{N!}} \sum_P (\pm 1)^P P |i_1, i_2, \cdots, i_N\rangle. \tag{13}$$

Fock Space

Imagine that there are n_1 particles in state 1, n_2 particles in state 2, so and so forth. The total number of particles is N:

$$\sum_{i=1}^{\infty} n_i = N. \tag{14}$$

We now construct the state for N particles in the fully symmetrized basis:

$$|n_1, n_2, ...\rangle = S_+|i_1, i_2, ..., i_N\rangle \cdot \frac{1}{\sqrt{n_1!n_2!\cdots}} \tag{15}$$

The factor $(n_1!n_2!\cdots)^{-1/2}$ acccounts for the combinations in each state. This serves as a complete set of completely symmetric N-particle states. The orthonormality and completeness relations are given by

$$\begin{aligned} \langle n_1, n_2, \cdots | n_1', n_2', \cdots\rangle &= \delta_{n_1,n_1'}\delta_{n_2,n_2'}\cdots \\ \sum_{n_1,n_2,\cdots} |n_1, n_2, \cdots\rangle\langle n_1, n_2, \cdots| &= \mathbb{1} \end{aligned} \tag{16}$$

The *direct sum* of vacuum state $|0\rangle$, i.e., 0 particles, one particle, etc is called the *Fock space*.

It is important to note that all of these operators live in a space of fixed number of particles. They preserve the number of particles. We will now define particle creation and annihilation operators, which will allow us to move between different particle number states.

a_i and $a_i^\dagger$

Let us define a state[2]:

$$|\Psi\rangle = \sum_{n_1,n_2,\cdots} c_{n_1,n_2,\cdots} |n_1, n_2, \cdots, n_i, \cdots, n_j, \cdots\rangle. \tag{17}$$

We will define the creation and annihilation operators as objects that raise or lower the number of particles in a given state:

$$a_j^\dagger |n_1, n_2, ..., n_j, ...\rangle \propto |n_1, n_2, ..., n_j + 1, ...\rangle \tag{18}$$

$$\hat{a}_j |n_1, n_2, ..., n_j, ...\rangle \propto |n_1, n_2, ..., n_j - 1, ...\rangle \tag{19}$$

If you replay it backwards in time, the effect of the creation operator, $a_j^\dagger$, is to remove particle from the state. This implies that $a_j^\dagger$ is the Hermitian adjoint of a_j, hence they deserve the $\dagger$ symbol. As a_j keeps lowering the number of particles, it should not come as a surprise that it has a null vector:

$$\hat{a}_j|n_1, n_2, \dots, n_j = 0, \dots\rangle = 0 \tag{20}$$

The vacuum state is defined as the state that has 0 as the eigenvalue of the annihilation operators: $\hat{a}_j|\emptyset\rangle = 0$ for any j.

We now derive the commutation relations for the creation and annihilation operators. Assume that we start from a given state and apply $\hat{a}_i^\dagger\hat{a}_j^\dagger$ we will get a new state with n_i+1 particles in state i and n_j+1 particles in state j. Instead, if we apply $\hat{a}_j^\dagger\hat{a}_i^\dagger$, we will still get a state with n_i+1 particles in state i and n_j+1 particles in state j. This should be physically equivalent to the first case, hence we should have:

$$\hat{a}_i^\dagger\hat{a}_j^\dagger|\Psi\rangle = \hat{a}_i^\dagger\hat{a}_j^\dagger|\Psi\rangle = \lambda\hat{a}_j^\dagger\hat{a}_i^\dagger|\Psi\rangle, \tag{21}$$

where λ is some complex number. Since $|\Psi\rangle$ is an arbitrary state, we need to operator to satisfy:

$$\hat{a}_i^\dagger\hat{a}_j^\dagger - \lambda\hat{a}_j^\dagger\hat{a}_i^\dagger = 0. \tag{22}$$

Note that i and j are just dummy variables, and we can swap them, $i \leftrightarrow j$, to get:

$$\hat{a}_j^\dagger\hat{a}_i^\dagger - \lambda\hat{a}_i^\dagger\hat{a}_j^\dagger = 0. \tag{23}$$

Now insert Eq. (22) into Eq. (23) to eliminate $\hat{a}_i^\dagger\hat{a}_j^\dagger$. This leads to

$$(1-\lambda^2)\hat{a}_j^\dagger\hat{a}_i^\dagger = 0. \tag{24}$$

For this relation to hold for any i and j, we must have

$$\lambda = \pm 1. \tag{25}$$

We have two distinct cases:

Case 1: Commutation relation when $\lambda = +1$:

$$\hat{a}_i^\dagger\hat{a}_j^\dagger - \hat{a}_j^\dagger\hat{a}_i^\dagger = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \tag{26}$$

Case 2: Anti-commutation relation when $\lambda = -1$:

$$\hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \tag{27}$$

We can now approach the $\hat{a}_i$ and $\hat{a}_j^\dagger$ cases. Consider the operators $\hat{a}_j$ and $\hat{a}_i^\dagger$ with $j \neq i$.

$$\hat{a}_j \hat{a}_i^\dagger |\Psi\rangle = \mu \hat{a}_i^\dagger \hat{a}_j |\Psi\rangle. \tag{28}$$

The argument above identically applies if $i \neq j$ implying $\mu = \pm 1$. For different j and k we therefore find

$$[\hat{a}_j, \hat{a}_i^\dagger] = 0 \quad \text{or} \quad \{\hat{a}_j, \hat{a}_i^\dagger\} = 0 \tag{29}$$

For $i = j$, let's take$|\Psi\rangle = |\emptyset\rangle$:

$$(\hat{a}_i \hat{a}_i^\dagger - \mu \hat{a}_i^\dagger \hat{a}_i)|\emptyset\rangle = |\emptyset\rangle, \tag{30}$$

we find for the two possible values of μ

$$\hat{a}_i \hat{a}_i^\dagger - \hat{a}_i^\dagger \hat{a}_i = 1 \quad \text{or} \quad \hat{a}_i \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i = 1 \tag{31}$$

which is equivalent to

$$[\hat{a}_i, \hat{a}_i^\dagger] = 1 \quad \text{or} \quad \{\hat{a}_i, \hat{a}_i^\dagger\} = 1. \tag{32}$$

The full commutation relations can be summarized as:

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0 \quad \text{and} \quad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}. \tag{33}$$

We are now in a position to define the normalizations of the creation and annihilation operators. Note that in Eq. (30) we implicitly assumed a normalization:

$$\hat{a}_i \hat{a}_i^\dagger |\emptyset\rangle = 1|\emptyset\rangle, \tag{34}$$

We want to define the overall normalization consistent with Eq. (34), and furthermore, we want have as particle number operator $N = \sum_i \hat{a}_i^\dagger \hat{a}_i$.

For this we can define the operators with the proper normalization of the creation operator as:

$$a_i^\dagger|\cdots, n_i, \cdots\rangle = \sqrt{n_i + 1}\,|\cdots, n_i + 1, \cdots\rangle \tag{35}$$

Taking the adjoint of this equation and relabeling $n_i \to n_i'$, we have

$$\langle\cdots, n_i', \cdots|a_i = \sqrt{n_i' + 1}\,\langle\cdots, n_i' + 1, \cdots| \tag{36}$$

Multiplying this equation by $|\cdots, n_i, \cdots\rangle$ yields:

$$\langle\cdots, n_i', \cdots|a_i|\cdots, n_i, \cdots\rangle = \sqrt{n_i}\,\delta_{n_i'+1, n_i} \tag{37}$$

Eq. (35) uniquely determines the normalization of the adjoint operator:

$$a_i|\cdots, n_i, \cdots\rangle = \sqrt{n_i}\,|\cdots, n_i - 1, \cdots\rangle \quad \text{for } n_i \geq 1. \tag{38}$$

We can see this by resolving the identity operator in the space of N-particle states:

$$a_i|\cdots, n_i, \cdots\rangle = \sum_{n_i'=0}^{\infty} |\cdots, n_i', \cdots\rangle\langle\cdots, n_i', \cdots|a_i|\cdots, n_i, \cdots\rangle \tag{39}$$

$$= \sum_{n_i'=0}^{\infty} |\cdots, n_i', \cdots\rangle\sqrt{n_i}\delta_{n_i'+1, n_i} \tag{40}$$

$$= \begin{cases} \sqrt{n_i}|\cdots, n_i - 1, \cdots\rangle & \text{for } n_i \geq 1 \\ 0 & \text{for } n_i = 0 \end{cases} \tag{41}$$

Also note that the normalization is consistent with the commutation relations:

$$[a_i, a_j] = 0 \tag{42}$$

$$[a_i^\dagger, a_j^\dagger] = 0 \tag{43}$$

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{44}$$

It is clear that Eq. (42) holds for $i = j$, since a_i commutes with itself. For $i \neq j$, it follows from Eq. (38) that:

$$a_i a_j|\cdots, n_i, \cdots, n_j, \cdots\rangle = \sqrt{n_i}\sqrt{n_j}|\cdots, n_i - 1, \cdots, n_j - 1, \cdots\rangle = a_j a_i|\cdots, n_i, \cdots, n_j, \cdots\rangle \tag{45}$$

which proves Eq. (42), and by taking the hermitian conjugate, also Eq. (43).

For $j \neq i$ we have:

$$a_i a_j^\dagger|\cdots, n_i, \cdots, n_j, \cdots\rangle = \sqrt{n_i}\sqrt{n_j + 1}|\cdots, n_i - 1, \cdots, n_j + 1, \cdots\rangle = a_j^\dagger a_i|\cdots, n_i, \cdots, n_j, \cdots\rangle \tag{46}$$

and

$$(a_i a_i^\dagger - a_i^\dagger a_i)|\cdots, n_i, \cdots, n_j, \cdots\rangle = \left(\sqrt{n_i + 1}\sqrt{n_i + 1} - \sqrt{n_i}\sqrt{n_i}\right)|\cdots, n_i, \cdots, n_j, \cdots\rangle \tag{47}$$

hence also proving Eq. (44).

[1] F. Schwabl, *Advanced quantum mechanics*, 4th ed. Springer, 2008.

[2] P. Kok, "Creation and annihilation operators," in *Advanced quantum mechanics*, LibreTexts, 2022 [Online]. Available: https://phys.libretexts.org/Bookshelves/Quantum_Mechanics/Advanced_Quantum_Mechanics_(Kok)/08%3A_Identical_Particles/8.02%3A_Creation_and_Annihilation_Operators. [Accessed: 07-Apr-2025]