Introduction to Second Quantization

Christophe Mora

Contents

Part of the complexity in the many-body problem - systems involving many particles - comes from the indistinguishability of identical particles, fermions or bosons. Calculations in first quantization thus involve the cumbersome (anti-)symmetrization of wavefunctions.

Second quantization is an efficient technical tool that describes many-body systems in a compact and intuitive way.

1 Preliminaries

Before entering the details of second quantization, it is worth drawing a clear distinction between the single-particle and the many-particle Hilbert spaces.

1.1 Single-particle Hilbert space

Consider a single particle described by the hamiltonian $\hat{h}$ acting on the Hilbert space $\mathcal{H}_1$. $\mathcal{H}_1$ is generated by the complete set of eigenfunctions $|\lambda\rangle$ ($\lambda = \mathbf{k}, \sigma, \nu, \dots$)

$$\hat{h}|\lambda\rangle = \varepsilon_\lambda |\lambda\rangle,$$

with the eigenvalues ε_λ. The identity operator in $\mathcal{H}_1$ is given by the completeness relation $\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$.

Examples:

1. single particle in free space, $\hat{h} = -\hbar^2 \nabla^2/(2m)$. The eigenfunctions are labeled by the wavevectors $\mathbf{k}$ with $\psi_k(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}}$ and the energies $\varepsilon_k = \hbar^2 k^2/2m$.

2. spin $1/2$ in a magnetic field, $\hat{h} = -BS^z$. The Hilbert space has dimension 2, generated by the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ of the spin operator S^z.

The basis of two-particle states, given by the set of (anti-)symmetrized functions, $+$ for bosons and $-$ for fermions,

$$\psi_{\lambda,\nu}(1,2) = \frac{1}{\sqrt{2}} \left[\varphi_\lambda(1)\, \varphi_\nu(2) \pm \varphi_\lambda(2)\, \varphi_\nu(1) \right],$$

is built out of the single-particle states $\varphi_\lambda(1) = \langle 1|\lambda\rangle$. The corresponding Hilbert space[1] is denoted $\mathcal{F}_2$.

1.2   Many-particle Hilbert space

We first discuss fermions. Following the two-particle case, the set of antisymmetrized Slater determinants

$$\psi_{\lambda_1,\ldots,\lambda_N}(1,\ldots,N) = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P \varphi_{\lambda_1}(P_1) \ldots \varphi_{\lambda_N}(P_N), \tag{1}$$

where the summation runs over all permutations of $\{1,\ldots,N\}$, forms the basis[2] of the Hilbert space $\mathcal{F}_N$. In the bosonic case, the basis is obtained from symmetrized states, *i.e.* Eq. (1) where $(-1)^P$ is replaced by 1.

The hamiltonian may describe independent particles in which case

$$\hat{H} = \sum_{i=1}^N \hat{h}^{(i)},$$

where each piece $\hat{h}^{(i)}$ acts only on the particle i.

Examples:

1. for particles in free space, $\hat{H} = \sum_i \mathbf{p}_i^2/(2m)$.

2. for an assembly of N distinguishable spins in a magnetic field, $\hat{H} = -B \sum_{i=1}^N S_i^z$. The Hilbert space has dimension 2^N and symmetrization is not required.

Interactions between particles can be added, $\hat{H} = \sum_i \hat{h}^{(i)} + \hat{V}$, where $\hat{V}$ includes all multi-particle interactions. For example, Coulomb interactions read

$$\hat{V}_{\text{Coulomb}} = \sum_{i=1}^N \sum_{j>i}^N \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{2}$$

2   Basics of second quantization

So far, we have introduced and discussed the many-body problem in the language of first quantization. Second quantization corresponds to a different labelling of the basis of states Eq. (1) together with the introduction of creation and annihilation operators that connect spaces with different numbers of particles.

---

[1]Restricted to (anti-)symmetrized wavefunctions, $\mathcal{F}_2$ is a subset of the larger space $\mathcal{H}_1 \otimes \mathcal{H}_1$.

[2]A different choice for the set of single-particle states $|\lambda\rangle$ gives, using Eq. (1), a different many-particle basis that nevertheless spans the same Hilbert space $\mathcal{F}_N$.

2.1   Occupation number representation

Since identical particles are indistinguishable, it is not possible, for a state of the form Eq. (1), to ascribe a definite single-particle state to a given particle. Therefore, instead of focusing on the wavefunction of each particle individually, one can reverse the perspective and characterize the states of Eq. (1) by the set of single-particle states $\{\lambda_1, \ldots, \lambda_N\}$ that are occupied by particles, all other single-particle states being empty.

In terms of notations, $|\{n_\lambda\}\rangle$ represents $|\psi_{\lambda_1,\ldots,\lambda_N}\rangle^3$ with, for fermions, $n_\lambda = 1$ for $\lambda = \lambda_i$, $i = 1 \ldots N$, and $n_\lambda = 0$ otherwise. The state can be written schematically as

$$|\{n_\lambda\}\rangle = |0 \ldots \overset{\lambda_1}{1} \ldots 0 \ldots \overset{\lambda_2}{1} \ldots 0 \ldots (\ldots) \overset{\lambda_N}{1} \rangle, \tag{3}$$

where it is explicitly specified on the right-hand-side which states are occupied and which state are empty.

Bosonic states have similar expressions although the occupation numbers n_λ can take values larger than 1, for example

$$|\{n_\lambda\}\rangle = |0 \ldots \overset{\lambda_1}{5} \ldots 0 \ldots \overset{\lambda_2}{1} \ldots 0 \ldots (\ldots) \overset{\lambda_N}{7} \rangle, \tag{4}$$

for $n_{\lambda_1} = 5$, $n_{\lambda_2} = 1$, …, $n_{\lambda_N} = 7$.

2.2   Creation and annihilation operators

The constraint on the number of particles, $\sum_\lambda n_\lambda = N$, can be released by working in the extended Hilbert space

$$\mathcal{F} = \bigoplus_{N=0}^{+\infty} \mathcal{F}_N,$$

called the Fock space. Here, $\mathcal{F}_1 = \mathcal{H}_1$ is the single-particle Hilbert space, $\mathcal{F}_0$ contains a unique vacuum state, often noted $|0\rangle$, in which no particle is present.

In the Fock space, creation operators are introduced that raise the number of particles in a given single-particle state by 1. For fermions, it reads

$$c_{\lambda_1}^\dagger |0 \ldots \overset{\lambda_1}{0} \ldots 0 \ldots \overset{\lambda_2}{1} \ldots 0 \ldots (\ldots) \overset{\lambda_N}{1} \rangle = |0 \ldots \overset{\lambda_1}{1} \ldots 0 \ldots \overset{\lambda_2}{1} \ldots 0 \ldots (\ldots) \overset{\lambda_N}{1} \rangle,$$

while particle creation in a single-particle state that is already occupied gives zero,

$$c_{\lambda_2}^\dagger |0 \ldots \overset{\lambda_1}{1} \ldots 0 \ldots \overset{\lambda_2}{1} \ldots 0 \ldots (\ldots) \overset{\lambda_N}{1} \rangle = 0.$$

The annihilation operator c_λ, lowering the number by 1, is the hermitian conjugate of $c_\lambda^\dagger$. The full basis of the Fock space $\mathcal{F}$ is in fact generated by creation operators applied on the vacuum state, namely $|n_{\lambda_1} = 1, \ldots, n_{\lambda_N} = 1\rangle = c_{\lambda_1}^\dagger \ldots c_{\lambda_N}^\dagger |0 >$.

The antisymmetric properties of the basis states (Slater determinants) $|n_{\lambda_1} \ldots n_{\lambda_N}\rangle$ are ensured by the anticommutation relations

$$\{c_\alpha, c_\beta\} = c_\alpha c_\beta + c_\beta c_\alpha = 0, \qquad \{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha,\beta}. \tag{5}$$

The product $\hat{n}_\lambda = c_\lambda^\dagger c_\lambda$ gives the number of fermions occupying the state $|\lambda\rangle$,

$$c_\lambda^\dagger c_\lambda |\{n_\alpha\}\rangle = n_\lambda |\{n_\alpha\}\rangle$$

where $n_\lambda = 0$ or 1.

$^3\psi_{\lambda_1,\ldots,\lambda_N}(1, \ldots, N) = \langle 1, \ldots, N | \psi_{\lambda_1,\ldots,\lambda_N}\rangle.$

2.3 Bosons

There are only slight differences in the way second quantization works for fermions and for bosons. In the case of bosons, the basis states are symmetrized functions and the number of bosons in a given single-particle state is not restricted. These properties are ensured by the commutation relations

$$[b_\alpha, b_\beta] = b_\alpha b_\beta - b_\beta b_\alpha = 0, \qquad [b_\alpha, b_\beta^\dagger] = \delta_{\alpha,\beta}, \tag{6}$$

with the (annihilation) creation operators (b_α) $b_\alpha^\dagger$. From Eq. (6), one can prove[4] that

$$b_\lambda^\dagger |n_\lambda\rangle = \sqrt{n_\lambda + 1}|n_\lambda + 1\rangle$$
$$b_\lambda |n_\lambda\rangle = \sqrt{n_\lambda}|n_\lambda - 1\rangle \tag{7}$$

such that $\hat{n}_\lambda = b_\lambda^\dagger b_\lambda$ is indeed the number operator, $\hat{n}_\lambda |n_\lambda\rangle = n_\lambda |n_\lambda\rangle$.

3 Representation of operators

The complexity associated with wavefunction (anti)symmetrization has been reduced, in the formalism of second quantization, to the surprisingly simple commutation relations, Eq. (5) for fermions and Eq. (6) for bosons. Had the usual operators of the theory complicated expressions in terms of creation/annihilation operators, this would not be very useful. However, as we shall see below, the hamiltonian as well as standard operators do have simple expressions in second quantization.

3.1 Change of basis and the field operator

Starting with the expression $|\lambda\rangle = c_\lambda^\dagger |0\rangle$, one can insert the closure relation $\mathbb{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$ to derive the transformation law for the creation/annihilation operators

$$c_\alpha^\dagger = \sum_\lambda \langle\lambda|\alpha\rangle\, c_\lambda^\dagger, \qquad c_\alpha = \sum_\lambda \langle\alpha|\lambda\rangle\, c_\lambda, \tag{8}$$

from one basis to another. Hence, the change of basis only requires the calculation of matrix elements $\langle\alpha|\lambda\rangle$ involving single-particle states.

By convention, the field operator $\Psi(\mathbf{r})$ in a continuous problem is associated to the basis of position states $|\mathbf{r}\rangle$,

$$\Psi(\mathbf{r}) = \sum_\lambda \langle\mathbf{r}|\lambda\rangle\, c_\lambda. \tag{9}$$

Using Eq. (5) and Eq. (6), one finds the commutation relation

$$\{\Psi(\mathbf{r}), \Psi(\mathbf{r}')\} = 0, \qquad \{\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}'), \qquad \text{fermions,}$$
$$[\Psi(\mathbf{r}), \Psi(\mathbf{r}')] = 0, \qquad [\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), \qquad \text{bosons.} \tag{10}$$

The total number of particles (fermions or bosons) is then given by

$$\hat{N} = \sum_\lambda c_\lambda^\dagger c_\lambda = \int d^d r\, \hat{\rho}(\mathbf{r}) \tag{11}$$

---

[4]The states $|n_\lambda\rangle$ are chosen to be normalized to 1.

where the local density operator $\hat{\rho}(\mathbf{r}) = \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})$ has been introduced.

Example: The transformation to the Fourier momentum representation reads

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\, c_{\mathbf{k}}, \tag{12}$$

where $c_{\mathbf{k}}$ destroys a particle with momentum $\mathbf{k}$. The total number of particle is given by $\hat{N} = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$.

3.2 Representation of one-body and two-body operators

Single-particle or one-body operators have the form $\hat{O}^{(1)} = \sum_{i=1}^{N} \hat{o}^{(1)}[i]$ in first quantization, where $\hat{o}^{(1)}[i]$ is a single-particle operator acting on the ith particle. In the language of second quantization, they take the form

$$\hat{O}^{(1)} = \sum_{\alpha,\beta} \langle\alpha|\hat{o}^{(1)}|\beta\rangle\, c_\alpha^\dagger c_\beta, \tag{13}$$

with the matrix elements $\langle\alpha|\hat{o}^{(1)}|\beta\rangle = \int d1\, d2\, \varphi_\alpha^*(1)\langle 1|\hat{o}^{(1)}|2\rangle\varphi_\beta(2)$.

Examples:

1. The kinetic energy operator $\hat{T} = \sum_i \mathbf{p}_i^2/(2m)$, describing independent particles, reads in second quantization

$$\hat{T} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m}\, c_{\mathbf{k}}^\dagger c_{\mathbf{k}}, \tag{14}$$

   i.e. it is diagonal in the momentum basis. An alternative expression involving the field operator is

$$\hat{T} = \int d^d r\, \Psi^\dagger(\mathbf{r}) \frac{(\hbar\nabla/i)^2}{2m} \Psi(\mathbf{r}) = \int d^d r\, \frac{\hbar^2}{2m} \nabla\Psi^\dagger(\mathbf{r}) \cdot \nabla\Psi(\mathbf{r}). \tag{15}$$

2. Tight-binding models are simplified band models for electrons in solids where only neighboring sites hybridize. A particularly simple example is given by the hamiltonian

$$\hat{H} = -t \sum_{\langle i,j\rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right), \tag{16}$$

   where $c_i^\dagger$ creates an electron on site i and $\langle i, j\rangle$ denotes neighboring sites. The product $c_i^\dagger c_j$ describes intuitively the hopping of an electron from site j to site i: one electron is annihilated on site j while a novel electron appears on site i. The hamiltonian Eq. (16) is diagonalized by going to the Fourier space $c_{\mathbf{k}} = \frac{1}{\sqrt{N_s}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_i$ (N_s is the number of sites of the lattice), with the result $\hat{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$. In one dimension, $\varepsilon_k = -2t\cos(ka)$, a being the lattice spacing.

We now consider a two-body operator such as the Coulomb interaction of Eq. (2). In first quantization, it has the form

$$\hat{O}^{(2)} = \frac{1}{2} \sum_{i\neq j} \hat{o}^{(2)}[i,j], \tag{17}$$

where $\hat{o}^{(2)}[i,j]$ accounts for pair interactions. In second quantization, it reads[5]

$$\hat{O}^{(2)} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\,\beta | \hat{o}^{(2)} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma, \tag{18}$$

with the matrix elements

$$\langle \alpha\,\beta | \hat{o}^{(2)} | \gamma\delta \rangle = \int d1\,d2\,\varphi_\alpha^*(1)\varphi_\beta^*(2)\hat{o}^{(2)}[1,2]\varphi_\gamma(1)\varphi_\delta(2). \tag{19}$$

Example: Electron-electron Coulomb interaction is given in second quantization by

$$\hat{V}_{\text{Coulomb}} = \frac{1}{2} \sum_{\sigma_1,\sigma_2} \int d\mathbf{r}_1\,d\mathbf{r}_2\,\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1 - \mathbf{r}_2|}\,\Psi_{\sigma_1}^\dagger(\mathbf{r}_1)\Psi_{\sigma_2}^\dagger(\mathbf{r}_2)\Psi_{\sigma_2}(\mathbf{r}_2)\Psi_{\sigma_1}(\mathbf{r}_1), \tag{20}$$

in terms of the field operator $\Psi_\sigma(\mathbf{r})$. Here the spin σ of electrons has been included. After going to the Fourier momentum representation of Eq. (12), one obtains the alternative expression

$$\hat{V}_{\text{Coulomb}} = \frac{1}{2V} \sum_{\sigma_1,\sigma_2} \sum_{\mathbf{q},\mathbf{k}_1,\mathbf{k}_2} v(q)\, c_{\mathbf{k}_1+\mathbf{q},\sigma_1}^\dagger c_{\mathbf{k}_2-\mathbf{q},\sigma_2}^\dagger c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1}$$

with the Fourier transform of the Coulomb pair potential $v(q) = e^2/(\varepsilon_0\,q^2)$.

References

[1] H. Bruus and K. Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics* (Oxford University Press, Oxford, 2004).

[2] A. Altland and B. Simons, *Condensed Matter Field Theory* (Cambridge University Press, Cambridge, 2010).

---

[5]Note the ordering of indices which, in the product of annihilation operators, is reversed with respect to the ordering in the matrix element.