Second Quantization: Creation and Annihilation Operators

Occupation number representation. Any state of a system of identical particles can be described as a linear combination of many-particle basis states: $|\Psi\rangle = \sum_j c_j |\Phi_j\rangle$. A basis state can be completely specified in terms of the occupation number n_α for each member of a complete set of orthonormal single-particle states, $\{|\alpha\rangle,\ \alpha = 1,\, 2,\, 3,\, \ldots\}$. The set of occupation numbers contains all the information necessary to construct an appropriately symmetrized or antisymmetrized basis vector, denoted

$$|\Phi\rangle = |n_1, n_2, \ldots, n_\alpha, \ldots\rangle.$$

For bosons, n_α must be a non-negative integer; for fermions, the Pauli exclusion principle restricts n_α to be either 0 or 1.

The vector space spanned by the set of all such basis states is called the *Fock space*. A feature of the Fock space is that the total number of particles is not a fixed parameter, but rather is a dynamical variable associated with a total number operator

$$N = \sum_\alpha n_\alpha.$$

There is a unique *vacuum* or no-particle state:

$$|0\rangle = |0, 0, 0, 0, \ldots\rangle.$$

The single-particle states can be represented

$$|\alpha\rangle = |0, 0, \ldots, 0, n_\alpha = 1, 0, \ldots\rangle \equiv |0_1, 0_2, \ldots, 0_{\alpha-1}, 1_\alpha, 0_{\alpha+1}, \ldots\rangle.$$

Bosonic operators. Let us define the bosonic *creation operator* $a_\alpha^\dagger$ by

$$a_\alpha^\dagger |n_1, n_2, \ldots, n_{\alpha-1}, n_\alpha, n_{\alpha+1}, \ldots\rangle = \sqrt{n_\alpha + 1}\, |n_1, n_2, \ldots, n_{\alpha-1}, n_\alpha + 1, n_{\alpha+1}, \ldots\rangle, \quad (1)$$

and the corresponding *annihilation operator* a_α by

$$a_\alpha |n_1, n_2, \ldots, n_{\alpha-1}, n_\alpha, n_{\alpha+1}, \ldots\rangle = \sqrt{n_\alpha}\, |n_1, n_2, \ldots, n_{\alpha-1}, n_\alpha - 1, n_{\alpha+1}, \ldots\rangle. \quad (2)$$

Equations (1) and (2) allow us to define the number operator $N_\alpha = a_\alpha^\dagger a_\alpha$, such that

$$N_\alpha |n_1, n_2, \ldots, n_\alpha, \ldots\rangle = n_\alpha |n_1, n_2, \ldots, n_\alpha, \ldots\rangle$$

and

$$N = \sum_\alpha N_\alpha.$$

The simplest application of the creation and annihilation operators involves the single-particle states:

$$a_\alpha^\dagger |0\rangle = |\alpha\rangle, \qquad a_\alpha |\beta\rangle = \delta_{\alpha,\beta} |0\rangle.$$

When applied to multi-particle states, the properties of the creation and annihilation operators must be consistent with the symmetry of bosonic states under pairwise interchange of particles. It is clear from Eqs. (1) and (2) that for any pair of single particle states $|\alpha\rangle$ and $|\beta\rangle$, and for any vector $|\Psi\rangle$ in the Fock space, $a_\alpha^\dagger a_\beta^\dagger|\Psi\rangle = a_\beta^\dagger a_\alpha^\dagger|\Psi\rangle$ and $a_\alpha a_\beta|\Psi\rangle = a_\beta a_\alpha|\Psi\rangle$. One also finds that $a_\alpha^\dagger a_\beta|\Psi\rangle = a_\beta a_\alpha^\dagger|\Psi\rangle$ for $\alpha \neq \beta$. However, $a_\alpha^\dagger a_\alpha|\phi\rangle = n_\alpha|\Phi\rangle$ for any basis state $|\Phi\rangle$, while $a_\alpha a_\alpha^\dagger|\Phi\rangle = (n_\alpha+1)|\Phi\rangle$. This means that for any $|\Psi\rangle$ in the Fock space

$$a_\alpha a_\alpha^\dagger|\Psi\rangle - a_\alpha^\dagger a_\alpha|\Psi\rangle = (N_\alpha+1)|\Psi\rangle - N_\alpha|\Psi\rangle = |\Psi\rangle.$$

The properties described in the preceding paragraph can be summarized in the commutation relations

$$[a_\alpha^\dagger, a_\beta^\dagger] = [a_\alpha, a_\beta] = 0, \qquad [a_\alpha, a_\beta^\dagger] = \delta_{\alpha,\beta} I. \tag{3}$$

One consequence of these commutation relations is that any multi-particle basis state can be written

$$|n_1, n_2, \ldots, n_\alpha, \ldots\rangle = \frac{\left(a_1^\dagger\right)^{n_1}}{\sqrt{n_1!}} \frac{\left(a_2^\dagger\right)^{n_2}}{\sqrt{n_2!}} \cdots \frac{\left(a_\alpha^\dagger\right)^{n_\alpha}}{\sqrt{n_\alpha!}} \cdots |0\rangle,$$

or equally well, as any permutation of the above product of operators acting on the vacuum. For example,

$$|2, 1, 0, 0, \ldots\rangle = a_1^\dagger a_1^\dagger a_2^\dagger|0\rangle = a_1^\dagger a_2^\dagger a_1^\dagger|0\rangle = a_2^\dagger a_1^\dagger a_1^\dagger|0\rangle.$$

Equations (1)–(3) define the key properties of bosonic creation and annihilation operators. Note the close formal similarity to the properties of the harmonic oscillator raising and lowering operators.

Fermionic operators. The fermionic case is a little trickier than the bosonic one because we have to enforce antisymmetry under all possible pairwise interchanges. We define the fermionic creation operator $c_\alpha^\dagger$ by

$$\begin{aligned} c_\alpha^\dagger|n_1, n_2, \ldots, n_{\alpha-1}, 0_\alpha, n_{\alpha+1}, \ldots\rangle &= (-1)^{\nu_\alpha}\,|n_1, n_2, \ldots, n_{\alpha-1}, 1_\alpha, n_{\alpha+1}, \ldots\rangle, \\ c_\alpha^\dagger|n_1, n_2, \ldots, n_{\alpha-1}, 1_\alpha, n_{\alpha+1}, \ldots\rangle &= 0, \end{aligned} \tag{4}$$

and the annihilation operator c_α by

$$\begin{aligned} c_\alpha|n_1, n_2, \ldots, n_{\alpha-1}, 1_\alpha, n_{\alpha+1}, \ldots\rangle &= (-1)^{\nu_\alpha}\,|n_1, n_2, \ldots, n_{\alpha-1}, 0_\alpha, n_{\alpha+1}, \ldots\rangle, \\ c_\alpha|n_1, n_2, \ldots, n_{\alpha-1}, 0_\alpha, n_{\alpha+1}, \ldots\rangle &= 0. \end{aligned} \tag{5}$$

In both Eqs. (4) and (5),

$$\nu_\alpha = \sum_{\beta<\alpha} N_\beta, \quad \text{where } N_\beta = c_\beta^\dagger c_\beta, \tag{6}$$

measures the total number of particles in single-particle states having an index $\beta < \alpha$. It is straightforward to check that Eqs. (4)–(6) are self-consistent, in the sense that with the phase factor $(-1)^{\nu_\alpha}$ as defined above,

$$N_\alpha|n_1, n_2, \ldots, n_\alpha, \ldots\rangle = n_\alpha|n_1, n_2, \ldots, n_\alpha, \ldots\rangle \qquad \text{for } n_\alpha = 0 \text{ or } 1.$$

From Eqs. (4)–(6) it is clear that for any $|\Psi\rangle$, $c_\alpha^\dagger c_\beta^\dagger|\Psi\rangle = -c_\beta^\dagger c_\alpha^\dagger|\Psi\rangle$ for $\alpha \neq \beta$, while $c_\alpha^\dagger c_\alpha^\dagger|\Psi\rangle = 0 = -c_\alpha^\dagger c_\alpha^\dagger|\Psi\rangle$. Similarly, $c_\alpha c_\beta|\Psi\rangle = -c_\beta c_\alpha|\Psi\rangle$ for $\alpha \neq \beta$, and $c_\alpha c_\alpha|\Psi\rangle = 0$.

We also have $c_\alpha^\dagger c_\beta|\Psi\rangle = -c_\beta c_\alpha^\dagger|\Psi\rangle$ for $\alpha \neq \beta$. However, $c_\alpha^\dagger c_\alpha|\Phi\rangle = n_\alpha|\Phi\rangle$ for any basis state $|\Phi\rangle$, whereas $c_\alpha c_\alpha^\dagger|\Phi\rangle = (1 - n_\alpha)|\Phi\rangle$. Thus,

$$(c_\alpha c_\alpha^\dagger + c_\alpha^\dagger c_\alpha)|\Psi\rangle = (1 - N_\alpha)|\Psi\rangle + N_\alpha|\Psi\rangle = |\Psi\rangle$$

for any $|\Psi\rangle$ in the Fock space.

The properties above can be summarized in the anticommutation relations

$$\{c_\alpha^\dagger, c_\beta^\dagger\} = \{c_\alpha, c_\beta\} = 0, \qquad \{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha,\beta} I, \tag{7}$$

where $\{A, B\} = AB + BA$ is the anticommutator of A and B. These anticommutation properties fundamentally distinguish the fermionic operators from their commuting bosonic counterparts. The $(-1)^{\nu_\alpha}$ phase factors entering Eqs. (4) and (5) were chosen specifically to ensure that Eqs. (7) are satisfied. Alternative phase conventions can be adopted, so long as the anticommutation relations are preserved.

Given the anticommutation relations, any multi-particle basis state can be written

$$|n_1, n_2, \ldots, n_\alpha, \ldots\rangle = \left(c_1^\dagger\right)^{n_1} \left(c_2^\dagger\right)^{n_2} \ldots \left(c_\alpha^\dagger\right)^{n_\alpha} \ldots |0\rangle,$$

or equally well, as any permutation of the above product of creation operators with a sign change for each pairwise interchange of adjacent operators. For example,

$$|1,1,1\rangle = c_1^\dagger c_2^\dagger c_3^\dagger|0\rangle = -c_2^\dagger c_1^\dagger c_3^\dagger|0\rangle = c_2^\dagger c_3^\dagger c_1^\dagger|0\rangle = -c_3^\dagger c_2^\dagger c_1^\dagger|0\rangle = c_3^\dagger c_1^\dagger c_2^\dagger|0\rangle = -c_1^\dagger c_3^\dagger c_2^\dagger|0\rangle.$$

Equations (4)–(7) define the key properties of fermionic creation and annihilation operators.

Basis transformations. The creation and annihilation operators defined above were constructed for a particular basis of single-particle states $\{|\alpha\rangle\}$. We will use the notation $b_\alpha^\dagger$ and b_α to represent these operators in situations where it is unnecessary to distinguish between the bosonic and fermionic cases.

Consider an alternative single-particle basis $\{|\tilde{\alpha}\rangle\}$, which—like $\{|\alpha\rangle\}$—is complete and orthonormal. The Fock space can be spanned by many-particle basis states of the form

$$|\tilde{\Phi}\rangle = |\tilde{n}_1, \tilde{n}_2, \ldots, \tilde{n}_{\tilde{\alpha}}, \ldots\rangle,$$

and one can define operators $\tilde{b}_{\tilde{\alpha}}^\dagger$ and $\tilde{b}_{\tilde{\alpha}}$ by analogy with those for $\{|\alpha\rangle\}$. It is important to note that the vacuum state $|0\rangle$ can (and will) be chosen to be the same in both the original and new bases.

The relations $|\alpha\rangle = b_\alpha^\dagger|0\rangle$, $|\tilde\alpha\rangle = \tilde b_{\tilde\alpha}^\dagger|0\rangle$, and $|\tilde\alpha\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|\tilde\alpha\rangle$ (completeness) are all consistent with the unitary transformation

$$\tilde b_{\tilde\alpha}^\dagger = \sum_\alpha \langle\alpha|\tilde\alpha\rangle b_\alpha^\dagger, \qquad \tilde b_{\tilde\alpha} = \sum_\alpha \langle\tilde\alpha|\alpha\rangle b_\alpha. \tag{8}$$

An important special case of a basis transformation involves single-particle basis states of well-defined position $\mathbf{r}$ and spin z component σ: $\{|\tilde\alpha\rangle\} = \{|\mathbf{r},\sigma\rangle\}$, where $\langle \mathbf{r},\sigma|\mathbf{r}',\sigma'\rangle = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}$. The corresponding operators are called the *field creation and annihilation operators*, and are given the special notation $\Psi_\sigma^\dagger(\mathbf{r})$ and $\Psi_\sigma(\mathbf{r})$. For bosons or fermions,

$$\Psi_\sigma(\mathbf{r}) = \sum_\alpha \langle \mathbf{r},\sigma|\alpha\rangle\, b_\alpha = \sum_\alpha \psi_\alpha(\mathbf{r},\sigma)\, b_\alpha,$$

where $\psi_\alpha(\mathbf{r},\sigma)$ is the wave function of the single-particle state $|\alpha\rangle$. The field operators create/annihilate a particle of spin-z σ at position $\mathbf{r}$:

$$\Psi_\sigma^\dagger(\mathbf{r})|0\rangle = |\mathbf{r},\sigma\rangle, \qquad \Psi_\sigma(\mathbf{r})|\mathbf{r}',\sigma'\rangle = \delta(\mathbf{r}-\mathbf{r}')\,\delta_{\sigma,\sigma'}\,|0\rangle.$$

The total number operator can be written

$$N = \sum_\sigma \int d\mathbf{r}\; \Psi_\sigma^\dagger(\mathbf{r})\Psi_\sigma(\mathbf{r}).$$

Dynamical variables. Now we consider how to represent dynamical variables in terms of the creation and annihilation operators introduced above.

The simplest dynamical variables are additive *one-particle operators* of the form $\Omega = \sum_{j=1}^n \Omega_j$, where Ω_j acts just on the j'th particle. Examples of one-particle quantities include the momentum $\mathbf{P} = \sum_j \mathbf{P}_j$, the kinetic energy $K = \sum_j K_j$, where $K_j = |\mathbf{P}_j|^2/2m$, and the external potential $V = \sum_j V_j$, where $V_j = v(\mathbf{r}_j)$.

If we choose a single-particle basis $\{|\tilde\alpha\rangle\}$ in which Ω_j is diagonal (e.g., momentum eigenstates in the cases of $\mathbf{P}_j$ and K_j, position eigenstates for V_j), then the total operator can be represented $\Omega = \sum_{\tilde\alpha} \omega_{\tilde\alpha} \tilde N_{\tilde\alpha}$.

In any other basis $\{|\alpha\rangle\}$, related to $\{|\tilde\alpha\rangle\}$ by Eq. (8), the most general form of an additive one-particle operator is

$$\Omega = \sum_{\alpha,\beta} \langle\alpha|\Omega_1|\beta\rangle\, b_\alpha^\dagger b_\beta.$$

We will also consider *additive two-particle operators*, most commonly encountered as a pairwise interaction potential $U = \sum_{i<j} u(\mathbf{r}_i,\mathbf{r}_j)$. In the basis of position eigenkets, $\{|\tilde\alpha\rangle\} = \{|\mathbf{r}\rangle\}$, such an operator can be represented $U = \frac{1}{2}\sum_{\tilde\alpha,\tilde\beta} u_{\tilde\alpha,\tilde\beta}\left(\tilde N_{\tilde\alpha}\tilde N_{\tilde\beta} - \delta_{\tilde\alpha,\tilde\beta}\tilde N_{\tilde\alpha}\right)$, where the second term is introduced to eliminate self-interaction. It is straightforward to show that $\tilde N_{\tilde\alpha}\tilde N_{\tilde\beta} - \delta_{\tilde\alpha,\tilde\beta}\tilde N_{\tilde\alpha} = \tilde b_{\tilde\alpha}^\dagger \tilde b_{\tilde\beta}^\dagger \tilde b_{\tilde\beta}\tilde b_{\tilde\alpha}$ for both bosons and fermions.

In an arbitrary basis $\{|\alpha\rangle\}$, the most general form of an additive two-particle operator is

$$U = \tfrac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \langle\alpha,\beta|U_{12}|\gamma,\delta\rangle\, b_\alpha^\dagger b_\beta^\dagger b_\delta b_\gamma, \tag{9}$$

where

$$\langle \alpha, \beta | U_{12} | \gamma, \delta \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \; \psi_\alpha^*(\mathbf{r}_1)\psi_\beta^*(\mathbf{r}_2) u(\mathbf{r}_1, \mathbf{r}_2) \psi_\gamma(\mathbf{r}_1)\psi_\delta(\mathbf{r}_2).$$

Note the reversal of the order of the operators b_γ and b_δ in Eq. (9), which allows the same expression to be used for bosons and fermions.

We are now in a position to consider applications of the formalism outlined above to many-boson and many-fermion systems.