Chapter 4: Identical Particles

These our actors,
As I foretold you, were all spirits and
Are melted into air, into thin air:
And, like the baseless fabric of this vision,
The cloud-capp'd towers, the gorgeous palaces,
The solemn temples, the great globe itself,
Yea, all which it inherit, shall dissolve
And, like this insubstantial pageant faded,
Leave not a rack behind.

William Shakespeare, *The Tempest*

I. QUANTUM STATES OF IDENTICAL PARTICLES

In the previous chapter, we discussed how the principles of quantum mechanics apply to systems of multiple particles. That discussion omitted an important feature of multi-particle systems, namely the fact that particles of the same type are fundamentally indistinguishable from each other. As it turns out, indistinguishability imposes a strong constraint on the form of the multi-particle quantum states, and looking into this will ultimately lead us to a fundamental re-interpretation of what "particles" are.

A. Particle exchange symmetry

Suppose we have two particles of the same type, e.g. two electrons. It is a fact of Nature that all electrons have identical physical properties: the same mass, same charge, same total spin, etc. As a consequence, the single-particle Hilbert spaces of the two electrons must be mathematically identical. Let us denote this space by $\mathscr{H}^{(1)}$. For a two-electron system, the Hilbert space is a tensor product of two single-electron Hilbert spaces, denoted by

$$\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}. \tag{4.1}$$

Moreover, any Hamiltonian must affect the two electrons in a symmetrical way. An example of such a Hamiltonian is

$$\hat{H} = \frac{1}{2m_e}\Big(|\hat{\mathbf{p}}_1|^2 + |\hat{\mathbf{p}}_2|^2\Big) + \frac{e^2}{4\pi\varepsilon_0|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|}, \tag{4.2}$$

consisting of the non-relativistic kinetic energies and the Coulomb potential energy. Operators $\hat{\mathbf{p}}_1$ and $\hat{\mathbf{r}}_1$ act on electron 1, while $\hat{\mathbf{p}}_2$ and $\hat{\mathbf{r}}_2$ act on electron 2.

Evidently, this Hamiltonian is invariant under an interchange of the operators acting on the two electrons (i.e., $\hat{\mathbf{p}}_1 \leftrightarrow \hat{\mathbf{p}}_2$ and $\hat{\mathbf{r}}_1 \leftrightarrow \hat{\mathbf{r}}_2$). This can be regarded as a kind of symmetry, called **exchange symmetry**. As we know, symmetries of quantum systems can be represented by unitary operators that commute with the Hamiltonian. Exchange symmetry is represented by an operator $\hat{P}$, defined as follows: let $\{|\mu\rangle\}$ be a basis for the single-electron Hilbert space $\mathscr{H}^{(1)}$; then $\hat{P}$ interchanges the basis vectors for the two electrons:

$$\begin{aligned}\hat{P}\Big(\sum_{\mu\nu}\psi_{\mu\nu}|\mu\rangle|\nu\rangle\Big) &\equiv \sum_{\mu\nu}\psi_{\mu\nu}|\nu\rangle|\mu\rangle \\ &= \sum_{\mu\nu}\psi_{\nu\mu}|\nu\rangle|\mu\rangle \quad \text{(interchanging } \mu\leftrightarrow\nu \text{ in the double sum)}\end{aligned} \tag{4.3}$$

The exchange operator has the following properties:

1. $\hat{P}^2 = \hat{I}$, where $\hat{I}$ is the identity operator.
2. $\hat{P}$ is linear, unitary, and Hermitian (see Exercise 1).
3. The effect of $\hat{P}$ does not depend on the choice of basis (see Exercise 1).
4. $\hat{P}$ commutes with the above Hamiltonian $\hat{H}$; more generally, it commutes with any two-particle operator built out of symmetrical combinations of single-particle operators (see Exercise 2).

According to Noether's theorem, any symmetry implies a conservation law. In the case of exchange symmetry, $\hat{P}$ is both Hermitian *and* unitary, so we can take the conserved quantity to be the eigenvalue of $\hat{P}$ itself. We call this eigenvalue, p, the **exchange parity**. Given that $\hat{P}^2 = \hat{I}$, there are just two possibilities:

$$\hat{P}|\psi\rangle = p|\psi\rangle \quad \Rightarrow \quad p = \begin{cases} +1 & (\text{“symmetric state”}), \quad \text{or} \\ -1 & (\text{“antisymmetric state”}). \end{cases} \tag{4.4}$$

Since $\hat{P}$ commutes with $\hat{H}$, if the system starts out in an eigenstate of $\hat{P}$ with parity p, it retains the same parity for all subsequent times.

The concept of exchange parity generalizes to systems of more than two particles. Given N particles, we can define a set of exchange operators $\hat{P}_{ij}$, where $i, j \in \{1, 2, \dots, N\}$ and $i \neq j$, such that $\hat{P}_{ij}$ exchanges particle i and particle j. If the particles are identical, the Hamiltonian must commute with *all* the exchange operators, so the parities (± 1) are individually conserved.

We now invoke the following postulates:

1. A multi-particle state of identical particles is an eigenstate of every $\hat{P}_{ij}$.
2. For each $\hat{P}_{ij}$, the exchange parity p_{ij} has the same value: i.e., all $+1$ or all -1.
3. The exchange parity p_{ij} is determined solely by the type of particle involved.

Do *not* think of these as statements as being derived from more fundamental facts! Rather, they are hypotheses about the way particles behave—facts about Nature that physicists have managed to deduce through examining a wide assortment of empirical evidence. Our task, for now, shall be to explore the consequences of these hypotheses.

Particles that have symmetric states ($p_{ij} = +1$) are called **bosons**. It turns out that the elementary particles that "carry" the fundamental forces are all bosons: these are the photons (elementary particles of light, which carry the electromagnetic force), gluons (elementary particles that carry the strong nuclear force, responsible for binding protons and neutrons together), and W and Z bosons (particles that carry the weak nuclear force responsible for beta decay). Other bosons include particles that carry non-fundamental forces, such as phonons (particles of sound), as well as certain composite particles such as alpha particles (helium-4 nuclei).

Particles that have antisymmetric states ($p_{ij} = -1$) are called **fermions**. All the elementary particles of "matter" are fermions: electrons, muons, tauons, quarks, neutrinos, and their anti-particles (positrons, anti-neutrinos, etc.). Certain composite particles are also fermions, including protons and neutrons, which are each composed of three quarks.

B. Bosons

A state of N bosons must be symmetric under every possible exchange operator:

$$\hat{P}_{ij}\,|\psi\rangle = |\psi\rangle \quad \forall\, i,j \in \{1,\dots,N\},\;\; i \neq j. \tag{4.5}$$

There is a standard way to construct multi-particle states obeying this symmetry condition. First, consider a two-boson system ($N = 2$). If both bosons occupy the same single-particle state, $|\mu\rangle \in \mathscr{H}^{(1)}$, the two-boson state is simply

$$|\mu,\mu\rangle = |\mu\rangle|\mu\rangle. \tag{4.6}$$

This evidently satisfies the required symmetry condition (4.5). Next, suppose the two bosons occupy *different* single-particle states, $|\mu\rangle$ and $|\nu\rangle$, which are orthonormal vectors in $\mathscr{H}^{(1)}$. It would be wrong to write the two-boson state as $|\mu\rangle|\nu\rangle$, because the particles would not be symmetric under exchange. Instead, we construct the multi-particle state

$$|\mu,\nu\rangle = \frac{1}{\sqrt{2}}\Big(|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle\Big). \tag{4.7}$$

This has the appropriate exchange symmetry:

$$\hat{P}_{12}\,|\mu,\nu\rangle \;=\; \frac{1}{\sqrt{2}}\Big(|\nu\rangle|\mu\rangle + |\mu\rangle|\nu\rangle\Big) \;=\; |\mu,\nu\rangle. \tag{4.8}$$

The $1/\sqrt{2}$ factor in Eq. (4.7) ensures that the state is normalized (check for yourself that this is true—it requires $|\mu\rangle$ and $|\nu\rangle$ to be orthonormal to work out).

The above construction can be generalized to arbitrary numbers of bosons. Suppose we have N bosons occupying single-particle states enumerated by

$$|\phi_1\rangle,\; |\phi_2\rangle,\; |\phi_3\rangle,\; \dots,\, |\phi_N\rangle. \tag{4.9}$$

Each of the states $|\phi_j\rangle$ is drawn from an orthonormal basis set $\{|\mu\rangle\}$ for $\mathscr{H}^{(1)}$. We use the ϕ labels to indicate that the listed states can overlap. For example, we could have $|\phi_1\rangle = |\phi_2\rangle = |\mu\rangle$, meaning that the single-particle state $|\mu\rangle$ is occupied by two particles.

The N-boson state can now be written as

$$|\phi_1, \phi_2, \dots, \phi_N\rangle = \mathcal{N} \sum_p \Big(|\phi_{p(1)}\rangle |\phi_{p(2)}\rangle |\phi_{p(3)}\rangle \cdots |\phi_{p(N)}\rangle \Big). \tag{4.10}$$

The sum is taken over each of the $N!$ permutations acting on $\{1, 2, \dots, N\}$. For each permutation p, we let $p(j)$ denote the integer that j is permuted into.

The prefactor $\mathcal{N}$ is a normalization constant, and it can be shown that its appropriate value is

$$\mathcal{N} = \sqrt{\frac{1}{N! n_a! n_b! \cdots}}, \tag{4.11}$$

where n_μ denotes the number of particles in each distinct state $|\varphi_\mu\rangle$, and $N = n_\alpha + n_\beta + \cdots$ is the total number of particles. The proof of this is left as an exercise (Exercise 3).

To see that the above N-particle state is symmetric under exchange, apply an arbitrary exchange operator $\hat{P}_{ij}$:

$$\begin{aligned} \hat{P}_{ij} |\phi_1, \phi_2, \dots, \phi_N\rangle &= \mathcal{N} \sum_p \hat{P}_{ij} \Big(\cdots |\phi_{p(i)}\rangle \cdots |\phi_{p(j)}\rangle \cdots \Big) \\ &= \mathcal{N} \sum_p \Big(\cdots |\phi_{p(j)}\rangle \cdots |\phi_{p(i)}\rangle \cdots \Big). \end{aligned} \tag{4.12}$$

In each term of the sum, two states i and j are interchanged. Since the sum runs through all permutations of the states, the result is the same with or without the exchange, so we still end up with $|\phi_1, \phi_2, \dots, \phi_N\rangle$. Therefore, the multi-particle state is symmetric under every possible exchange operation.

Example—A three-boson system has two particles in a state $|\mu\rangle$, and one particle in a different state $|\nu\rangle$. To express the three-particle state, define $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle\}$ where $|\phi_1\rangle = |\phi_2\rangle = |\mu\rangle$ and $|\phi_3\rangle = |\nu\rangle$. Then

$$\begin{aligned} |\phi_1, \phi_2, \phi_3\rangle = \frac{1}{\sqrt{12}} \Big(& |\phi_1\rangle|\phi_2\rangle|\phi_3\rangle + |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle + |\phi_3\rangle|\phi_1\rangle|\phi_2\rangle \\ & + |\phi_1\rangle|\phi_3\rangle|\phi_2\rangle + |\phi_3\rangle|\phi_2\rangle|\phi_1\rangle + |\phi_2\rangle|\phi_1\rangle|\phi_3\rangle \Big) \\ = \frac{1}{\sqrt{3}} \Big(& |\mu\rangle|\mu\rangle|\nu\rangle + |\mu\rangle|\nu\rangle|\mu\rangle + |\nu\rangle|\mu\rangle|\mu\rangle \Big). \end{aligned} \tag{4.13}$$

The exchange symmetry operators have the expected effects:

$$\begin{aligned} \hat{P}_{12} |\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{3}} \Big(|\mu\rangle|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle|\mu\rangle + |\mu\rangle|\nu\rangle|\mu\rangle \Big) = |\phi_1, \phi_2, \phi_3\rangle \\ \hat{P}_{23} |\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{3}} \Big(|\mu\rangle|\nu\rangle|\mu\rangle + |\mu\rangle|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle|\mu\rangle \Big) = |\phi_1, \phi_2, \phi_3\rangle \\ \hat{P}_{13} |\phi_1, \phi_2, \phi_3\rangle &= \frac{1}{\sqrt{3}} \Big(|\nu\rangle|\mu\rangle|\mu\rangle + |\mu\rangle|\nu\rangle|\mu\rangle + |\mu\rangle|\mu\rangle|\nu\rangle \Big) = |\phi_1, \phi_2, \phi_3\rangle. \end{aligned} \tag{4.14}$$

C. Fermions

A state of N fermions must be antisymmetric under every possible exchange operator:

$$\hat{P}_{ij}\,|\psi\rangle = -|\psi\rangle \quad \forall\, i,j \in \{1,\dots,N\},\; i \neq j. \tag{4.15}$$

Similar to the bosonic case, we can explicitly construct multi-fermion states based on the occupancy of single-particle state.

First consider $N = 2$, with the fermions occupying the single-particle states $|\mu\rangle$ and $|\nu\rangle$ (which, once again, we assume to be orthonormal). The appropriate two-particle state is

$$|\mu,\nu\rangle = \frac{1}{\sqrt{2}}\Big(|\mu\rangle|\nu\rangle - |\nu\rangle|\mu\rangle\Big). \tag{4.16}$$

We can easily check that this is antisymmetric:

$$\hat{P}_{12}|\mu,\nu\rangle = \frac{1}{\sqrt{2}}\Big(|\nu\rangle|\mu\rangle - |\mu\rangle|\nu\rangle\Big) = -|\mu,\nu\rangle. \tag{4.17}$$

Note that if $|\mu\rangle$ and $|\nu\rangle$ are the same single-particle state, Eq. (4.16) doesn't work, since the two terms would cancel to give the zero vector, which is not a valid quantum state. This is a manifestation of the **Pauli exclusion principle**, which states that two fermions cannot occupy the same single-particle state. Thus, each single-particle state is either unoccupied or occupied by one fermion.

For general N, let the occupied single-particle states be $|\phi_1\rangle$, $|\phi_2\rangle$, $\dots$, $|\phi_N\rangle$, each drawn from some orthonormal basis $\{|\mu\rangle\}$ for $\mathscr{H}^{(1)}$, and each distinct. Then the appropriate N-fermion state is

$$|\phi_1,\dots,\phi_N\rangle = \frac{1}{\sqrt{N!}}\sum_p s(p)\,|\phi_{p(1)}\rangle|\phi_{p(2)}\rangle\cdots|\phi_{p(N)}\rangle. \tag{4.18}$$

It is up to you to verify that the $1/\sqrt{N!}$ prefactor is the right normalization constant. The sum is taken over every permutation p of the sequence $\{1,2,\dots,N\}$, and each term in the sum has a coefficient $s(p)$ denoting the **parity of the permutation**. The parity of any permutation p is defined as $+1$ if p is constructed from an even number of transpositions (i.e., exchanges of adjacent elements) starting from the sequence $\{1,2,\dots,N\}$, and -1 if p involves an odd number of transpositions.

Note that if $|\phi_1\rangle,\dots,|\phi_N\rangle$ are not all distinct single-particle states, Eq. (4.18) would yield the zero vector, since the terms in the sum over p cancel out pairwise (you can check this). This is once again consistent with the Pauli exclusion principle.

Let's look at a couple of concrete examples.

Example—For $N = 2$, the sequence $\{1,2\}$ has two permutations:

$$\begin{aligned} p_1 &: \{1,2\} \rightarrow \{1,2\}, \quad s(p_1) = +1 \\ p_2 &: \{1,2\} \rightarrow \{2,1\}, \quad s(p_2) = -1. \end{aligned} \tag{4.19}$$

Plugging these into Eq. (4.18) yields the previously-discussed two-fermion state (4.16).

Example—For $N = 3$, the sequence $\{1, 2, 3\}$ has $3! = 6$ permutations:

$$\begin{aligned} p_1 : \{1,2,3\} &\rightarrow \{1,2,3\}, \quad s(p_1) = +1 \\ p_2 : \{1,2,3\} &\rightarrow \{2,1,3\}, \quad s(p_2) = -1 \\ p_3 : \{1,2,3\} &\rightarrow \{2,3,1\}, \quad s(p_3) = +1 \\ p_4 : \{1,2,3\} &\rightarrow \{3,2,1\}, \quad s(p_4) = -1 \\ p_5 : \{1,2,3\} &\rightarrow \{3,1,2\}, \quad s(p_5) = +1 \\ p_6 : \{1,2,3\} &\rightarrow \{1,3,2\}, \quad s(p_6) = -1. \end{aligned} \tag{4.20}$$

The permutations can be generated by consecutive transpositions of elements. Each time we perform a transposition, the sign of $s(p)$ is reversed. Hence, the three-fermion state is

$$\begin{aligned} |\phi_1, \phi_2, \phi_3\rangle = \frac{1}{\sqrt{6}}\Big(&|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle - |\phi_2\rangle|\phi_1\rangle|\phi_3\rangle \\ &+ |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle - |\phi_3\rangle|\phi_2\rangle|\phi_1\rangle \\ &+ |\phi_2\rangle|\phi_3\rangle|\phi_1\rangle - |\phi_1\rangle|\phi_3\rangle|\phi_2\rangle\Big). \end{aligned} \tag{4.21}$$

We now see why Eq. (4.18) describes the N-fermion state. Let us apply $\hat{P}_{ij}$ to it:

$$\begin{aligned} \hat{P}_{ij}|\phi_1, \dots, \phi_N\rangle &= \frac{1}{\sqrt{N!}} \sum_p s(p)\, \hat{P}_{ij} \big[\cdots |\phi_{p(i)}\rangle \cdots |\phi_{p(j)}\rangle \cdots \big] \\ &= \frac{1}{\sqrt{N!}} \sum_p s(p)\, \big[\cdots |\phi_{p(j)}\rangle \cdots |\phi_{p(i)}\rangle \cdots \big]. \end{aligned} \tag{4.22}$$

Within each term in the above sum, the single-particle states for $p(i)$ and $p(j)$ have exchanged places. The resulting term must be an exact match for another term in the original expression for $|\phi_1, \dots, \phi_N\rangle$, since the sum runs over all possible permutations, except for one difference: the coefficient $s(p)$ must have an *opposite* sign, since the two permutations are related by an exchange. It follows that $\hat{P}_{ij}|\phi_1, \dots, \phi_N\rangle = -|\phi_1, \dots, \phi_N\rangle$ for any choice of $i \neq j$.

D. Distinguishing particles

When studying the phenomenon of entanglement in the previous chapter, we implicitly assumed that the particles are distinguishable. For example, in the EPR thought experiment, we started with the two-particle state

$$|\psi_{\text{EPR}}\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big), \tag{4.23}$$

which appears to be antisymmetric. Does this mean that we cannot prepare $|\psi_{\text{EPR}}\rangle$ using photons (which are bosons)? More disturbingly, we discussed how measuring $\hat{S}_z$ on particle

A, and obtaining the result $+\hbar/2$, causes the two-particle state to collapse into $|+z\rangle|-z\rangle$, which is neither symmetric nor antisymmetric. Is this result invalidated if the particles are identical?

The answer to each question is no. The confusion arises because the particle exchange symmetry has to involve an exchange of *all* the degrees of freedom of each particle, and Eq. (4.23) only shows the spin degree of freedom.

To unpack the above statement, let us suppose the two particles in the EPR experiment are identical bosons. We have focused on each particle's spin degree of freedom, but they must also have a position degree of freedom—that's how we can have a particle at Alpha Centauri (A) and another at Betelgeuse (B). If we explicitly account for this position degree of freedom, the single-particle Hilbert space should be

$$\mathscr{H}^{(1)} = \mathscr{H}_{\text{spin}} \otimes \mathscr{H}_{\text{position}}. \tag{4.24}$$

For simplicity, let us treat position as a twofold degree of freedom, treating $\mathscr{H}_{\text{position}}$ as a 2D space spanned by the basis $\{|A\rangle, |B\rangle\}$.

Now consider the state we previously denoted by $|+z\rangle|-z\rangle$, which refers to a spin-up particle at A and a spin-down particle at B. In our previous notation, it was implicitly assumed that A refers to the left-hand slot of the tensor product, and B refers to the right-hand slot. If we account for the position degrees of freedom, the state is written as

$$|+z, A;\, -z, B\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|A\rangle|-z\rangle|B\rangle + |-z\rangle|B\rangle|+z\rangle|A\rangle\Big), \tag{4.25}$$

where the kets are written in the following order:

$$\Big[(\text{spin 1}) \otimes (\text{position 1})\Big] \otimes \Big[(\text{spin 2}) \otimes (\text{position 2})\Big]. \tag{4.26}$$

The exchange operator $\hat{P}_{12}$ swaps the two particles' Hilbert spaces—which includes both the position *and* the spin part. Hence, Eq. (4.25) is explicitly symmetric:

$$\begin{aligned}\hat{P}_{12}\,|+z, A\,;\, -z, B\rangle &= \frac{1}{\sqrt{2}}\Big(|-z\rangle|B\rangle|+z\rangle|A\rangle + |+z\rangle|A\rangle|-z\rangle|B\rangle\Big) \\ &= |+z, A\,;\, -z, B\rangle.\end{aligned} \tag{4.27}$$

Likewise, if there is a spin-down particle at A and a spin-up particle at B, the bosonic two-particle state is

$$|-z, A\,;\, +z, B\rangle = \frac{1}{\sqrt{2}}\Big(|-z\rangle|A\rangle|+z\rangle|B\rangle + |+z\rangle|B\rangle|-z\rangle|A\rangle\Big). \tag{4.28}$$

Using Eqs. (4.25) and (4.28), we can rewrite the EPR singlet state (4.23) as

$$\begin{aligned}|\psi_{\text{EPR}}\rangle &= \frac{1}{\sqrt{2}}\Big(|+z, A\,;\, -z, B\rangle - |-z, A\,;\, +z, B\rangle\Big) \\ &= \frac{1}{2}\Big(\,|+z\rangle|A\rangle|-z\rangle|B\rangle + |-z\rangle|B\rangle|+z\rangle|A\rangle \\ &\qquad - |-z\rangle|A\rangle|+z\rangle|B\rangle - |+z\rangle|B\rangle|-z\rangle|A\rangle\Big).\end{aligned} \tag{4.29}$$

As it turns out Eq. (4.29) can be further simplified with some careful re-ordering. Instead of the ordering (4.26), order by spins and then positions:

$$\Big[(\text{spin 1}) \otimes (\text{spin 2})\Big] \otimes \Big[(\text{position 1}) \otimes (\text{position 2})\Big] \tag{4.30}$$

Then Eq. (4.29) can be rewritten as

$$|\psi_{\text{EPR}}\rangle = \frac{1}{\sqrt{2}}\Big(|+z\rangle|-z\rangle - |-z\rangle|+z\rangle\Big) \otimes \frac{1}{\sqrt{2}}\Big(|A\rangle|B\rangle - |B\rangle|A\rangle\Big). \tag{4.31}$$

Evidently, even though the spin degrees of freedom form an antisymmetric combination, as described by Eq. (4.23), the position degrees of freedom in Eq. (4.31) also have an antisymmetric form, such that the overall two-particle state is symmetric!

Now suppose we perform a measurement on $|\psi_{\text{EPR}}\rangle$, and find that the particle at position A has spin $+z$. As usual, a measurement outcome can be associated with a projection operator. Using the ordering (4.26), we can write the relevant projection operator as

$$\hat{\Pi} = \Big(|+z\rangle\langle +z| \otimes |A\rangle\langle A|\Big) \otimes \Big(\hat{I} \otimes \hat{I}\Big) + \Big(\hat{I} \otimes \hat{I}\Big) \otimes \Big(|+z\rangle\langle +z| \otimes |A\rangle\langle A|\Big). \tag{4.32}$$

This accounts for the fact that the observed phenomenon—spin $+z$ at position A—may refer to either particle. Applying $\hat{\Pi}$ to the EPR state (4.29) yields

$$|\psi'\rangle \;=\; \frac{1}{2}\Big(|+z\rangle|A\rangle|-z\rangle|B\rangle + |-z\rangle|B\rangle|+z\rangle|A\rangle\Big). \tag{4.33}$$

Apart from a change in normalization, this is precisely the fermionic state $|+z, A; -z, B\rangle$ defined in Eq. (4.25). In our earlier notation, this state was simply written as $|+z\rangle|-z\rangle$. This goes to show that particle exchange symmetry is fully compatible with the concepts of partial measurements, entanglement, etc., discussed in the previous chapter.

E. Implications of exchange symmetry

The choice of exchange symmetry eigenvalue—symmetric (bosons) or antisymmetric (fermions)—is often referred to as **particle statistics**. This is because statistical ensembles of bosons and fermions are governed by different distributions, called the Bose-Einstein and Fermi-Dirac distributions respectively. The implications for statistical mechanics are profound, but fall outside the scope of this course.

Our above formulation of bosonic and fermionic multi-particle quantum states has relied on the assignment of single-particle states to (say) the "first slot" or "second slot" in a tensor product. One might question whether this is philosophically consistent with the notion of particle indistinguishability. After all, it seems unsatisfactory that our mathematical framework allows us to write down a state like $|\mu\rangle|\nu\rangle$ where $\mu \neq \nu$, which is physically impossible since it is not symmetric or antisymmetric. Moreover, we use such states to define a "particle exchange" operation that appears to have no direct physical meaning (unlike, say, a rotation operation, which is physically meaningful).

To address these unsatisfactory features, Leinaas and Myrheim (1977) developed an interesting formulation of particle indistinguishability that avoids the concept of particle exchange, by focusing on the properties of multi-particle wavefunctions. In their view, a multi-particle wavefunction is indexed by a set of coordinates $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ which are not to be regarded as an ordinary vector, but as a mathematical object that has a built-in property that interchanging entries leaves the object invariant. Bosonic or fermionic states can be constructed by carefully analyzing the topological structure of wavefunctions defined on such configuration spaces. For more details, the interested reader is referred to the paper by Leinaas and Myrheim [3].

A startling outcome of Leinaas and Myrheim's analysis is that the distinction between fermions and bosons is not absolute. In certain special quantum systems in two spatial dimensions, there can exist identical particles known as **anyons**, which act as though they are intermediate between fermions and bosons. However, a discussion of anyons requires knowledge about magnetic vector potentials in quantum mechanics, which will be discussed in Chapter 5; after having gone through that chapter, you may refer to Appendix F, which gives a brief introduction to the theory of anyons.

II. SECOND QUANTIZATION

In the usual tensor product notation, symmetric and antisymmetric states become quite cumbersome to deal with when the number of particles is large. We will now introduce a formalism called **second quantization**, which greatly simplifies manipulations of such multi-particle states. (The reason for the name "second quantization" will not be apparent until later; it is a bad name, but one we are stuck with for historical reasons.)

We start by defining a convenient way to specify states of multiple identical particles, called the **occupation number representation**. Let us enumerate a set of single-particle states, $\{|1\rangle, |2\rangle, |3\rangle, \cdots\}$, that form a complete orthonormal basis for the single-particle Hilbert space $\mathscr{H}^{(1)}$. Then, we build multi-particle states by specifying how many particles are in state $|1\rangle$, denoted n_1; how many are in state $|2\rangle$, denoted n_2; and so on. Thus,

$$|n_1, n_2, n_3, \ldots\rangle$$

is *defined* as the appropriate symmetric or antisymmetric multi-particle state, constructed using Eq. (4.10) if we're dealing with bosons (Section I B), or using Eq. (4.18) if we're dealing with fermions (Section I C).

Let us run through a couple of examples:

Example—The two-particle state $|0, 2, 0, 0, \ldots\rangle$ has both particles in the single-particle state $|2\rangle$. This is only possible if the particles are bosons, since fermions cannot share the same state. Written out in tensor product form, the symmetric state is

$$|0, 2, 0, 0, \ldots\rangle \equiv |2\rangle|2\rangle. \tag{4.34}$$

Example—The three-particle state $|1,1,1,0,0,\dots\rangle$ has one particle each occupying $|1\rangle$, $|2\rangle$, and $|3\rangle$. If the particles are bosons, this corresponds to the symmetric state

$$\begin{aligned}|1,1,1,0,0,\dots\rangle \equiv \frac{1}{\sqrt{6}}\Big(&|1\rangle|2\rangle|3\rangle + |3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle \\ &+ |1\rangle|3\rangle|2\rangle + |2\rangle|1\rangle|3\rangle + |3\rangle|2\rangle|1\rangle\Big).\end{aligned} \tag{4.35}$$

And if the particles are fermions, the appropriate antisymmetric state is

$$\begin{aligned}|1,1,1,0,0,\dots\rangle \equiv \frac{1}{\sqrt{6}}\Big(&|1\rangle|2\rangle|3\rangle + |3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle \\ &- |1\rangle|3\rangle|2\rangle - |2\rangle|1\rangle|3\rangle - |3\rangle|2\rangle|1\rangle\Big).\end{aligned} \tag{4.36}$$

A. Fock space

There is a subtle point that we have glossed over: what Hilbert space do these state vectors reside in? The state $|0,2,0,0,\dots\rangle$ is a bosonic two-particle state, which is a vector in the two-particle Hilbert space $\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}$. However, $\mathscr{H}^{(2)}$ also contains two-particle states that are not symmetric under exchange, which is not allowed for bosons. Thus, it would be more rigorous for us to narrow the Hilbert space to the space of state vectors that are symmetric under exchange. We denote this reduced space by $\mathscr{H}^{(2)}_S$.

Likewise, $|1,1,1,0,\dots\rangle$ is a three-particle state lying in $\mathscr{H}^{(3)}$. If the particles are bosons, we can narrow the space to $\mathscr{H}^{(3)}_S$. If the particles are fermions, we can narrow it to the space of three-particle states that are antisymmetric under exchange, denoted by $\mathscr{H}^{(3)}_A$. Thus, $|1,1,1,0,\dots\rangle \in \mathscr{H}^{(3)}_{S/A}$, where the subscript S/A depends on whether we are dealing with symmetric states (S) or antisymmetric states (A).

We can make the occupation number representation more convenient to work with by defining an "extended" Hilbert space, called the **Fock space**, that is the space of bosonic/fermionic states *for arbitrary numbers of particles.* In the formal language of linear algebra, the Fock space can be written as

$$\mathscr{H}^F_{S/A} = \mathscr{H}^{(0)} \oplus \mathscr{H}^{(1)} \oplus \mathscr{H}^{(2)}_{S/A} \oplus \mathscr{H}^{(3)}_{S/A} \oplus \mathscr{H}^{(4)}_{S/A} \oplus \cdots \tag{4.37}$$

Here, $\oplus$ represents the **direct sum** operation, which combines vector spaces by directly grouping their basis vectors into a larger basis set; if $\mathscr{H}_1$ has dimension d_1 and $\mathscr{H}_2$ has dimension d_2, then $\mathscr{H}_1 \oplus \mathscr{H}_2$ has dimension $d_1 + d_2$. (By contrast, the space $\mathscr{H}_1 \otimes \mathscr{H}_2$, defined via the tensor product, has dimension $d_1 d_2$.) Once again, the subscript S/A depends on whether we are dealing with bosons (S) or fermions (A).

The upshot is that any multi-particle state that we can write down in the occupation number representation, $|n_1, n_2, n_3, \dots\rangle$, is guaranteed to lie in the Fock space $\mathscr{H}^F_{S/A}$. Moreover, these states form a complete basis for $\mathscr{H}^F_{S/A}$.

In Eq. (4.37), the first term of the direct sum is $\mathscr{H}^{(0)}$, the "Hilbert space of 0 particles". This Hilbert space contains only one distinct state vector, denoted by

$$|\varnothing\rangle \equiv |0,0,0,0,\dots\rangle. \tag{4.38}$$

This refers to the **vacuum state**, a quantum state in which there are literally no particles. Note that $|\varnothing\rangle$ is *not* the same thing as a zero vector; it has the standard normalization $\langle\varnothing|\varnothing\rangle = 1$. The concept of a "state of no particles" may seem silly, but we will see that there are very good reasons to include it in the formalism.

Another subtle consequence of introducing the Fock space concept is that it is now legitimate to write down quantum states that lack definite particle numbers. For example,

$$\frac{1}{\sqrt{2}}\Big(|1,0,0,0,0,\dots\rangle + |1,1,1,0,0,\dots\rangle\Big)$$

is a valid state vector describing the superposition of a one-particle state and a three-particle state. We will revisit the phenomenon of quantum states with indeterminate particle numbers in Section II D, and in the next chapter.

B. Second quantization for bosons

After this lengthy prelude, we are ready to introduce the formalism of second quantization. Let us concentrate on bosons first.

We define an operator called the **boson creation operator**, denoted by $\hat{a}_\mu^\dagger$ and acting in the following way:

$$\hat{a}_\mu^\dagger\big|n_1,n_2,\dots,n_\mu,\dots\big\rangle = \sqrt{n_\mu+1}\,\big|n_1,n_2,\dots,n_\mu+1,\dots\big\rangle. \tag{4.39}$$

In this definition, there is one particle creation operator for each state in the single-particle basis $\{|\varphi_1\rangle, |\varphi_2\rangle, \dots\}$. Each creation operator is defined as an operator acting on state vectors in the Fock space $\mathscr{H}_S^F$, and has the effect of incrementing the occupation number of its single-particle state by one. The prefactor of $\sqrt{n_\mu+1}$ is defined for later convenience.

Applying a creation operator to the vacuum state yields a single-particle state:

$$\hat{a}_\mu^\dagger|\varnothing\rangle = |0,\dots,0,\underset{\hookleftarrow\,\mu}{1},0,0,\dots\rangle. \tag{4.40}$$

The creation operator's Hermitian conjugate, $\hat{a}_\mu$, is the **boson annihilation operator**. To characterize it, first take the Hermitian conjugate of Eq. (4.39):

$$\big\langle n_1,n_2,\dots\big|\hat{a}_\mu = \sqrt{n_\mu+1}\,\big\langle n_1,n_2,\dots,n_\mu+1,\dots\big|. \tag{4.41}$$

Right-multiplying by another occupation number state $|n_1',n_2',\dots\rangle$ results in

$$\begin{aligned}\big\langle n_1,n_2,\dots\big|\hat{a}_\mu\big|n_1',n_2',\dots\big\rangle &= \sqrt{n_\mu+1}\,\big\langle \dots,n_\mu+1,\dots\big|\dots,n_\mu',\dots\big\rangle \\ &= \sqrt{n_\mu+1}\;\delta_{n_1'}^{n_1}\;\delta_{n_2'}^{n_2}\cdots\delta_{n_\mu'}^{n_\mu+1}\cdots \\ &= \sqrt{n_\mu'}\;\delta_{n_1'}^{n_1}\;\delta_{n_2'}^{n_2}\cdots\delta_{n_\mu'}^{n_\mu+1}\cdots\end{aligned} \tag{4.42}$$

From this, we can deduce that

$$\hat{a}_\mu \big| n_1', n_2', \dots, n_\mu', \dots \big\rangle = \begin{cases} \sqrt{n_\mu'}\, \big| n_1', n_2', \dots, n_\mu' - 1, \dots \big\rangle, & \text{if } n_\mu' > 0 \\ 0, & \text{if } n_\mu' = 0. \end{cases} \tag{4.43}$$

In other words, the annihilation operator decrements the occupation number of a specific single-particle state by one (hence its name). As a special exception, if the given single-particle state is unoccupied ($n_\mu = 0$), applying $\hat{a}_\mu$ results in a zero vector (note that this is *not* the same thing as the vacuum state $|\varnothing\rangle$).

The boson creation/annihilation operators obey the following commutation relations:

$$[\hat{a}_\mu, \hat{a}_\nu] = [\hat{a}_\mu^\dagger, \hat{a}_\nu^\dagger] = 0, \qquad [\hat{a}_\mu, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}. \tag{4.44}$$

These can be derived by taking the matrix elements with respect to the occupation number basis. We will go through the derivation of the last commutation relation; the others are left as an exercise (Exercise 5).

To prove that $[\hat{a}_\mu, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}$, first consider the case where the creation/annihilation operators act on the same single-particle state:

$$\begin{aligned} \big\langle n_1, n_2, \dots \big| \hat{a}_\mu \hat{a}_\mu^\dagger \big| n_1', n_2' \dots \big\rangle &= \sqrt{(n_\mu + 1)(n_\mu' + 1)}\, \big\langle \dots, n_\mu + 1, \dots \big| \dots, n_\mu' + 1, \dots \big\rangle \\ &= \sqrt{(n_\mu + 1)(n_\mu' + 1)}\delta^{n_1}_{n_1'}\, \delta^{n_2}_{n_2'} \cdots \delta^{n_\mu+1}_{n_\mu'+1} \cdots \\ &= (n_\mu + 1)\delta^{n_1}_{n_1'}\, \delta^{n_2}_{n_2'} \cdots \delta^{n_\mu}_{n_\mu'} \cdots \\ \big\langle n_1, n_2, \dots \big| \hat{a}_\mu^\dagger \hat{a}_\mu \big| n_1', n_2' \dots \big\rangle &= \sqrt{n_\mu n_\mu'}\, \big\langle \dots, n_\mu - 1, \dots \big| \dots, n_\mu' - 1, \dots \big\rangle \\ &= \sqrt{n_\mu n_\mu'}\delta^{n_1}_{n_1'}\, \delta^{n_2}_{n_2'} \cdots \delta^{n_\mu - 1}_{n_\mu' - 1} \cdots \\ &= n_\mu \delta^{n_1}_{n_1'}\, \delta^{n_2}_{n_2'} \cdots \delta^{n_\mu}_{n_\mu'} \cdots \end{aligned} \tag{4.45}$$

In the second equation, we were a bit sloppy in handling the $n_\mu = 0$ and $n_\mu' = 0$ cases, but you can check for yourself that the result on the last line remains correct. Upon taking the difference of the two equations, we get

$$\big\langle n_1, n_2, \dots \big| \left(\hat{a}_\mu \hat{a}_\mu^\dagger - \hat{a}_\mu^\dagger \hat{a}_\mu\right) \big| n_1', n_2' \dots \big\rangle = \delta^{n_1}_{n_1'}\, \delta^{n_2}_{n_2'} \cdots \delta^{n_\mu}_{n_\mu'} \cdots = \big\langle n_1, n_2, \dots \big| n_1', n_2' \dots \big\rangle. \tag{4.46}$$

Since the occupation number states form a basis for $\mathscr{H}_S^F$, we conclude that

$$\hat{a}_\mu \hat{a}_\mu^\dagger - \hat{a}_\mu^\dagger \hat{a}_\mu = \hat{I}. \tag{4.47}$$

Next, consider the case where $\mu \neq \nu$:

$$\begin{aligned}
\big\langle n_1, \dots \big| \hat{a}_\mu \hat{a}_\nu^\dagger \big| n_1', \dots \big\rangle &= \sqrt{(n_\mu + 1)(n_\nu' + 1)}\, \langle \dots, n_\mu + 1, \dots, n_\nu, \dots | \dots, n_\mu', \dots, n_\nu' + 1, \dots \rangle \\
&= \sqrt{n_\mu' n_\nu}\;\; \delta^{n_1}_{n_1'} \;\cdots \delta^{n_\mu+1}_{n_\mu'} \cdots \delta^{n_\nu}_{n_\nu'+1} \cdots \\
\big\langle n_1, \dots \big| \hat{a}_\nu^\dagger \hat{a}_\mu \big| n_1', \dots \big\rangle &= \sqrt{n_\mu' n_\nu}\, \langle \dots, n_\mu, \dots, n_\nu - 1, \dots | \dots, n_\mu' - 1, \dots, n_\nu' \dots \rangle \\
&= \sqrt{n_\mu' n_\nu}\;\; \delta^{n_1}_{n_1'} \;\cdots \delta^{n_\mu}_{n_\mu'-1} \cdots \delta^{n_\nu-1}_{n_\nu'} \cdots \\
&= \sqrt{n_\mu' n_\nu}\;\; \delta^{n_1}_{n_1'} \;\cdots \delta^{n_\mu+1}_{n_\mu'} \cdots \delta^{n_\nu}_{n_\nu'+1} \cdots
\end{aligned}$$

Hence,

$$\hat{a}_\mu \hat{a}_\nu^\dagger - \hat{a}_\nu^\dagger \hat{a}_\mu = 0 \quad \text{for} \;\; \mu \neq \nu. \tag{4.48}$$

Combining these two results gives the desired commutation relation, $[\hat{a}_\mu, \hat{a}_\nu^\dagger] = \delta_{\mu\nu}$.

Another useful result which emerges from the first part of this proof is that

$$\big\langle n_1, n_2, \dots \big| \hat{a}_\mu^\dagger \hat{a}_\mu \big| n_1', n_2' \dots \big\rangle = n_\mu \big\langle n_1, n_2, \dots \big| n_1', n_2' \dots \big\rangle. \tag{4.49}$$

Hence, we can define the Hermitian operator

$$\hat{n}_\mu \equiv \hat{a}_\mu^\dagger \hat{a}_\mu, \tag{4.50}$$

whose eigenvalue is the occupation number of single-particle state μ.

If you are familiar with the method of creation/annihilation operators for solving the quantum harmonic oscillator, you will have noticed the striking similarity with the particle creation/annihilation operators for bosons. This is no mere coincidence. We will examine the relationship between harmonic oscillators and bosons in the next chapter.

C. Second quantization for fermions

For fermions, the multi-particle states are antisymmetric. The fermion creation operator can be defined as follows:

$$\begin{aligned}
\hat{c}_\mu^\dagger |n_1, n_2, \dots, n_\mu, \dots\rangle &= \begin{cases} (-1)^{n_1+n_2+\cdots+n_{\mu-1}} |n_1, n_2, \dots, n_{\mu-1}, 1, \dots\rangle & \text{if } n_\mu = 0 \\ 0 & \text{if } n_\mu = 1. \end{cases} \\
&= (-1)^{n_1+n_2+\cdots+n_{\mu-1}}\; \delta_0^{n_\mu}\; \big|n_1, n_2, \dots, n_{\mu-1}, 1, \dots\big\rangle.
\end{aligned} \tag{4.51}$$

In other words, if state μ is unoccupied, then $\hat{c}_\mu^\dagger$ increments the occupation number to 1, and multiplies the state by an overall factor of $(-1)^{n_1+n_2+\cdots+n_{\mu-1}}$ (i.e, $+1$ if there is an even number of occupied states preceding μ, and -1 if there is an odd number). The role of this factor will be apparent later. Note that this definition requires the single-particle states to be ordered in some way; otherwise, it would not make sense to speak of the states "preceding" μ. It does not matter which ordering we choose, so long as we make *some* choice, and stick to it consistently.

If μ is occupied, applying $\hat{c}_\mu^\dagger$ gives the zero vector. The occupation numbers are therefore forbidden from being larger than 1, consistent with the Pauli exclusion principle.

The conjugate operator, $\hat{c}_\mu$, is the fermion annihilation operator. To see what it does, take the Hermitian conjugate of the definition of the creation operator:

$$\langle n_1, n_2, \dots, n_\mu, \dots | \hat{c}_\mu = (-1)^{n_1+n_2+\cdots+n_{\mu-1}} \; \delta_0^{n_\mu} \, \big\langle n_1, n_2, \dots, n_{\mu-1}, 1, \dots \big|. \tag{4.52}$$

Right-multiplying this by $|n_1', n_2', \dots\rangle$ gives

$$\langle n_1, n_2, \dots, n_\mu, \dots | \hat{c}_\mu | n_1', n_2', \dots \rangle = (-1)^{n_1+\cdots+n_{\mu-1}} \; \delta_{n_1'}^{n_1} \cdots \; \delta_{n_{\mu-1}'}^{n_{\mu-1}} \left(\delta_0^{n_\mu} \delta_{n_\mu'}^1\right) \delta_{n_{\mu+1}'}^{n_{\mu+1}} \cdots \tag{4.53}$$

Hence, we deduce that

$$\begin{aligned} \hat{c}_\mu | n_1', \dots, n_\mu', \dots \rangle &= \begin{cases} 0 & \text{if } n_\mu' = 0 \\ (-1)^{n_1'+\cdots+n_{\mu-1}'} | n_1', \dots, n_{\mu-1}', 0, \dots \rangle & \text{if } n_\mu' = 1. \end{cases} \\ &= (-1)^{n_1'+\cdots+n_{\mu-1}'} \; \delta_{n_\mu'}^1 \, \big| n_1', \dots, n_{\mu-1}', 0, \dots \big\rangle. \end{aligned} \tag{4.54}$$

In other words, if state μ is unoccupied, then applying $\hat{c}_\mu$ gives the zero vector; if state μ is occupied, applying $\hat{c}_\mu$ decrements the occupation number to 0, and multiplies the state by the aforementioned factor of ± 1.

With these definitions, the fermion creation/annihilation operators can be shown to obey the following *anticommutation* relations:

$$\big\{\hat{c}_\mu, \hat{c}_\nu\big\} = \big\{\hat{c}_\mu^\dagger, \hat{c}_\nu^\dagger\big\} = 0, \qquad \big\{\hat{c}_\mu, \hat{c}_\nu^\dagger\big\} = \delta_{\mu\nu}. \tag{4.55}$$

Here, $\{\cdot,\cdot\}$ denotes an anticommutator, which is defined by

$$\big\{\hat{A}, \hat{B}\big\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{4.56}$$

Similar to the bosonic commutation relations (4.44), the anticommutation relations (4.55) can be derived by taking matrix elements with occupation number states. We will only go over the last one, $\big\{\hat{c}_\mu, \hat{c}_\nu^\dagger\big\} = \delta_{\mu\nu}$; the others are left for the reader to verify.

First, consider creation/annihilation operators acting on the same single-particle state μ:

$$\begin{aligned} \big\langle \dots, n_\mu, \dots \big| \hat{c}_\mu \hat{c}_\mu^\dagger \big| \dots, n_\mu', \dots \big\rangle &= (-1)^{n_1+\cdots+n_{\mu-1}} (-1)^{n_1'+\cdots+n_{\mu-1}'} \; \delta_0^{n_\mu} \delta_{n_\mu'}^0 \\ &\qquad \times \big\langle n_1, \dots, n_{\mu-1}, 1, \dots \big| n_1', \dots, n_{\mu-1}', 1, \dots \big\rangle \\ &= \delta_{n_\mu'}^0 \;\cdot\; \delta_{n_1'}^{n_1} \delta_{n_2'}^{n_2} \cdots \delta_{n_\mu'}^{n_\mu} \cdots \end{aligned} \tag{4.57}$$

By a similar calculation,

$$\big\langle \dots, n_\mu, \dots \big| \hat{c}_\mu^\dagger \hat{c}_\mu \big| \dots, n_\mu', \dots \big\rangle = \delta_{n_\mu'}^1 \;\cdot\; \delta_{n_1'}^{n_1} \delta_{n_2'}^{n_2} \cdots \delta_{n_\mu'}^{n_\mu} \cdots \tag{4.58}$$

By adding these two equations, and using the fact that $\delta_{n_\mu'}^0 + \delta_{n_\mu'}^1 = 1$, we get

$$\big\langle \dots, n_\mu, \dots \big| \, \big\{\hat{c}_\mu, \hat{c}_\mu^\dagger\big\} \, \big| \dots, n_\mu', \dots \big\rangle = \big\langle \dots, n_\mu, \dots \big| \dots, n_\mu', \dots \big\rangle \tag{4.59}$$

And hence,

$$\left\{\hat{c}_\mu, \hat{c}_\mu^\dagger\right\} = \hat{I}. \tag{4.60}$$

Next, we must prove that $\left\{\hat{c}_\mu, \hat{c}_\nu^\dagger\right\} = 0$ for $\mu \neq \nu$. We will show this for $\mu < \nu$ (the $\mu > \nu$ case follows by Hermitian conjugation). This is, once again, by taking matrix elements:

$$\begin{aligned}
\big\langle \dots, n_\mu, \dots, n_\nu, \dots \big| \hat{c}_\mu \hat{c}_\nu^\dagger \big| \dots, n'_\mu, \dots, n'_\nu, \dots \big\rangle &= (-1)^{n_1+\cdots+n_{\mu-1}} (-1)^{n'_1+\cdots+n'_{\nu-1}} \, \delta_0^{n_\mu} \delta_{n'_\nu}^0 \\
&\qquad \times \big\langle \dots, 1, \dots, n_\nu, \dots \big| \dots, n'_\mu, \dots, 1, \dots \big\rangle \\
&= (-1)^{n'_\mu+\cdots+n'_{\nu-1}} \, \delta_{n'_1}^{n_1} \delta_{n'_2}^{n_2} \cdots \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1\right) \cdots \left(\delta_1^{n_\nu} \delta_{n'_\nu}^0\right) \cdots \\
&= (-1)^{1+n_{\mu+1}+\cdots+n_{\nu-1}} \, \delta_{n'_1}^{n_1} \delta_{n'_2}^{n_2} \cdots \left(\delta_{n_\mu}^0 \delta_{n'_\mu}^1\right) \cdots \left(\delta_{n'_\nu}^0 \delta_{n_\nu}^1\right) \cdots \\
\big\langle \dots, n_\mu, \dots, n_\nu, \dots \big| \hat{c}_\nu^\dagger \hat{c}_\mu \big| \dots, n'_\mu, \dots, n'_\nu, \dots \big\rangle &= (-1)^{n_1+\cdots+n_{\nu-1}} (-1)^{n'_1+\cdots+n'_{\mu-1}} \, \delta_1^{n_\nu} \delta_{n'_\mu}^1 \\
&\qquad \times \big\langle \dots, n_\mu, \dots, 0, \dots \big| \dots, 0, \dots, n'_\nu, \dots \big\rangle \\
&= (-1)^{n_\mu+\cdots+n_{\nu-1}} \, \delta_{n'_1}^{n_1} \delta_{n'_2}^{n_2} \cdots \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1\right) \cdots \left(\delta_1^{n_\nu} \delta_{n'_\nu}^0\right) \cdots \\
&= (-1)^{0+n_{\mu+1}+\cdots+n_{\nu-1}} \, \delta_{n'_1}^{n_1} \delta_{n'_2}^{n_2} \cdots \left(\delta_0^{n_\mu} \delta_{n'_\mu}^1\right) \cdots \left(\delta_1^{n_\nu} \delta_{n'_\nu}^0\right) \cdots
\end{aligned}$$

The two equations differ by a factor of -1, so adding them gives zero. Putting everything together, we conclude that $\left\{c_\mu, c_\nu^\dagger\right\} = \delta_{\mu\nu}$, as stated in (4.55).

As you can see, the derivation of the fermionic anticommutation relations is quite hairy, in large part due to the $(-1)^{(\cdots)}$ factors in the definitions of the creation and annihilation operators. But once these relations have been derived, we can deal entirely with the creation and annihilation operators, without worrying about the underlying occupation number representation and its $(-1)^{(\cdots)}$ factors. By the way, if we had chosen to omit the $(-1)^{(\cdots)}$ factors in the definitions, the creation and annihilation operators would still satisfy the *anticommutation* relation $\{\hat{c}_\mu, \hat{c}_\nu^\dagger\} = \delta_{\mu\nu}$, but two creation operators or two annihilation operators would *commute* rather than *anticommute*. During subsequent calculations, the "algebra" of creation and annihilation operators ends up being much harder to deal with.

D. Second-quantized operators

One of the key benefits of second quantization is that it allows us to express multi-particle quantum operators clearly and succinctly, using the creation and annihilation operators defined in Sections II B–II C as "building blocks".

1. *Non-interacting particles*

Consider a system of *non-interacting* particles. When there is just one particle ($N = 1$), let the single-particle Hamiltonian be $\hat{H}^{(1)}$, which is a Hermitian operator acting on the single-particle Hilbert space $\mathscr{H}^{(1)}$. For general N, the multi-particle Hamiltonian $\hat{H}$ is a Hermitian operator acting on the Fock space $\mathscr{H}^F$. How is $\hat{H}$ related to $\hat{H}^{(1)}$?

Let us take the bosonic case. Then the multi-particle Hamiltonian should be

$$\hat{H} = \sum_{\mu\nu} \hat{a}_\mu^\dagger H_{\mu\nu} \hat{a}_\nu, \quad \text{where} \quad H_{\mu\nu} = \langle \mu | \hat{H}^{(1)} | \nu \rangle, \tag{4.61}$$

where $\hat{a}_\mu$ and $\hat{a}_\mu^\dagger$ are the boson creation and annihilation operators, and $|\mu\rangle$, $|\nu\rangle$ refer to single-particle state vectors drawn from some orthonormal basis for $\mathscr{H}^{(1)}$.

To understand why Eq. (4.61) is right, consider its matrix elements with respect to various states. First, for the vacuum state $|\varnothing\rangle$,

$$\langle \varnothing | \hat{H} | \varnothing \rangle = 0. \tag{4.62}$$

This makes sense. Second, consider the matrix elements between single-particle states:

$$\begin{aligned} \langle n_\mu = 1 | \hat{H} | n_\nu = 1 \rangle &= \langle \varnothing | a_\mu \Big(\sum_{\mu'\nu'} \hat{a}_{\mu'}^\dagger H_{\mu'\nu'} \hat{a}_{\nu'} \Big) a_\nu^\dagger | \varnothing \rangle \\ &= \sum_{\mu'\nu'} H_{\mu'\nu'} \, \langle \varnothing | a_\mu \hat{a}_{\mu'}^\dagger \hat{a}_{\nu'} a_\nu^\dagger | \varnothing \rangle \\ &= \sum_{\mu'\nu'} H_{\mu'\nu'} \, \delta_{\mu'}^{\mu} \delta_{\nu'}^{\nu} \\ &= H_{\mu\nu}. \end{aligned} \tag{4.63}$$

This exactly matches the matrix element defined in Eq. (4.61).

Finally, consider the case where $\{|\mu\rangle\}$ forms an eigenbasis of $\hat{H}_1$. Then

$$\hat{H}^{(1)} |\mu\rangle = E_\mu |\mu\rangle \quad \Rightarrow \quad H_{\mu\nu} = E_\mu \, \delta_{\mu\nu} \quad \Rightarrow \quad \hat{H} = \sum_\mu E_\mu \, \hat{n}_\mu. \tag{4.64}$$

As previously noted, $\hat{n}_\mu = \hat{a}_\mu^\dagger \hat{a}_\mu$ is the number operator, an observable corresponding to the occupation number of single-particle state μ. Thus, the total energy is the sum of the single-particle energies, as expected for a system of non-interacting particles.

We can also think of the Hamiltonian $\hat{H}$ as the generator of time evolution. Eq. (4.61) describes an infinitesimal time step that consists of a superposition of alternative evolution processes. Each term in the superposition, $\hat{a}_\mu^\dagger H_{\mu\nu} \hat{a}_\nu$, describes a particle being annihilated in state ν, and immediately re-created in state μ, which is equivalent to "transferring" a particle from ν to μ. The quantum amplitude for this process is described by the matrix element $H_{\mu\nu}$. This description of time evolution is applicable not just to single-particle states, but also to multi-particle states containing any number of particles.

Note also that the number of particles does not change during time evolution. Whenever a particle is annihilated in a state ν, it is immediately re-created in some state μ. This implies that the Hamiltonian commutes with the total particle number operator:

$$[\hat{H}, \hat{N}] = 0, \quad \text{where} \quad \hat{N} \equiv \sum_\mu \hat{a}_\mu^\dagger a_\mu. \tag{4.65}$$

The formal proof for this is left as an exercise (see Exercise 6). It follows directly from the creation and annihilation operators' commutation relations (for bosons) or anticommuattion relations (for fermions).

Apart from the total energy, other kinds of observables—the total momentum, total angular momentum, etc.—can be expressed in a similar way. Let $\hat{A}^{(1)}$ be a single-particle observable. For a multi-particle system, the operator corresponding to the "total A" is

$$\hat{A} = \sum_{\mu\nu} \hat{a}^\dagger_\mu A_{\mu\nu} \hat{a}_\nu, \quad \text{where} \;\; A_{\mu\nu} = \langle \mu | \hat{A}^{(1)} | \nu \rangle. \tag{4.66}$$

For fermions, everything from Eq. (4.61)–(4.66) also holds, but with the a operators replaced by fermionic c operators.

2. Change of basis

A given set of creation and annihilation operators is defined using a basis of single-particle states $\{|\mu\rangle\}$, but such a choice is obviously not unique. Suppose we have a different single-particle basis $\{|\alpha\rangle\}$, such that

$$|\alpha\rangle = \sum_\mu U_{\alpha\mu} |\mu\rangle, \tag{4.67}$$

where $U_{\alpha\mu}$ are the elements of a unitary matrix. Let $\hat{a}^\dagger_\alpha$ and $\hat{a}^\dagger_\mu$ denote the creation operators defined using the two different basis (once again, we will use the notation for bosons, but the equations in this section are valid for fermions too). Writing Eq. (4.67) in terms of the creation operators,

$$\hat{a}^\dagger_\alpha |\varnothing\rangle = \sum_\mu U_{\alpha\mu} \hat{a}^\dagger_\mu |\varnothing\rangle, \tag{4.68}$$

We therefore deduce that

$$\hat{a}^\dagger_\alpha = \sum_\mu U_{\alpha\mu} \hat{a}^\dagger_\mu, \quad \hat{a}_\alpha = \sum_\mu U^*_{\alpha\mu} \hat{a}_\mu. \tag{4.69}$$

Using the unitarity of $U_{\alpha\mu}$, we can verify that $\hat{a}_\alpha$ and $\hat{a}^\dagger_\alpha$ satisfy bosonic commutation relations if and only if $\hat{a}_\mu$ and $\hat{a}^\dagger_\mu$ do so. For fermions, we put c operators in place of a operators in Eq. (4.69), and use anticommutation rather than commutation relations.

To illustrate how a basis change affects a second quantized Hamiltonian, consider a system of non-interacting particles whose single-particle Hamiltonian is diagonal in the α basis. The multi-particle Hamiltonian is

$$\hat{H} = \sum_\alpha E_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha, \tag{4.70}$$

consistent with Eq. (4.65). Applying Eq. (4.69),

$$\hat{H} = \sum_{\mu\nu} \hat{a}^\dagger_\mu \left(\sum_\alpha E_\alpha U_{\alpha\mu} U^*_{\alpha\nu} \right) \hat{a}_\nu \tag{4.71}$$

Compare this to single-particle bra-ket

$$\begin{aligned} H_{\mu\nu} \equiv \langle\mu|\hat{H}^{(1)}|\nu\rangle &= \sum_{\alpha\beta}\langle\alpha|U_{\alpha\mu}\hat{H}^{(1)}U^*_{\beta\nu}|\beta\rangle && (4.72)\\ &= \sum_{\alpha\beta} U_{\alpha\mu}U^*_{\beta\nu}\,E_\beta\,\delta_{\alpha\beta} && (4.73)\\ &= \sum_{\alpha} E_\alpha\,U_{\alpha\mu}U^*_{\alpha\nu}. && (4.74)\end{aligned}$$

This precisely matches the term in parentheses in Eq. (4.71). This is consistent with the general form of $\hat{H}$ for non-interacting particles, Eq. (4.61).

3. *Particle interactions*

Hermitian operators can also be constructed out of other kinds of groupings of creation and annihilation operators. For example, a pairwise (two-particle) potential can be described with a superposition of creation and annihilation operator pairs, of the form

$$\hat{V} = \frac{1}{2}\sum_{\mu\nu\lambda\sigma} \hat{a}^\dagger_\mu \hat{a}^\dagger_\nu\, V_{\mu\nu\lambda\sigma}\,\hat{a}_\sigma\hat{a}_\lambda. \tag{4.75}$$

The prefactor of 1/2 is conventional. In terms of time evolution, $\hat{V}$ "transfers" (annihilates and then re-creates) a *pair* of particles during each infinitesimal time step. Since the number of annihilated particles is always equal to the number of created particles, the interaction conserves the total particle number. We can ensure that $\hat{V}$ is Hermitian by imposing a constraint on the coefficents:

$$\hat{V}^\dagger = \frac{1}{2}\sum_{\mu\nu\lambda\sigma} \hat{a}^\dagger_\lambda \hat{a}^\dagger_\sigma\, V^*_{\mu\nu\lambda\sigma}\,\hat{a}_\nu\hat{a}_\mu = \hat{V} \quad \Leftarrow \quad V^*_{\lambda\sigma\mu\nu} = V_{\mu\nu\lambda\sigma}. \tag{4.76}$$

Suppose we are given the two-particle potential as an operator $\hat{V}^{(2)}$ acting on the two-particle Hilbert space $\mathscr{H}^{(2)}$. We should be able to express the second-quantized operator $\hat{V}$ in terms of $\hat{V}^{(2)}$, by comparing their matrix elements. For example, consider the two-boson states

$$\begin{aligned} |n_\mu = 1, n_\nu = 1\rangle &= \frac{1}{\sqrt{2}}\Big(|\mu\rangle|\nu\rangle + |\nu\rangle|\mu\rangle\Big),\\ |n_\lambda = 1, n_\sigma = 1\rangle &= \frac{1}{\sqrt{2}}\Big(|\lambda\rangle|\sigma\rangle + |\sigma\rangle|\lambda\rangle\Big),\end{aligned} \tag{4.77}$$

where $\mu \neq \nu$ and $\lambda \neq \sigma$. The matrix elements of $\hat{V}^{(2)}$ are

$$\begin{aligned} &\langle n_\mu = 1, n_\nu = 1|\hat{V}^{(2)}|n_\lambda = 1, n_\sigma = 1\rangle \\ &\quad = \frac{1}{2}\Big(\langle\mu|\langle\nu|\hat{V}^{(2)}|\lambda\rangle\sigma\rangle + \langle\nu|\langle\mu|\hat{V}^{(2)}|\lambda\rangle\sigma\rangle + \langle\mu|\langle\nu|\hat{V}^{(2)}|\sigma\rangle\lambda\rangle + \langle\nu|\langle\mu|\hat{V}^{(2)}|\sigma\rangle\lambda\rangle\Big). \end{aligned} \tag{4.78}$$

On the other hand, the matrix elements of the second-quantized operator $\hat{V}$ are

$$\langle n_\mu = 1, n_\nu = 1|\hat{V}|n_\lambda = 1, n_\sigma = 1\rangle = \sum_{\mu'\nu'\lambda'\sigma'} V_{\mu'\nu'\lambda'\sigma'} \langle\varnothing|\hat{a}_\nu\hat{a}_\mu\hat{a}^\dagger_{\mu'}\hat{a}^\dagger_{\nu'}\hat{a}_{\sigma'}\hat{a}_{\lambda'}\hat{a}^\dagger_\lambda\hat{a}^\dagger_\sigma|\varnothing\rangle \tag{4.79}$$

$$= \frac{1}{2}\left(V_{\mu\nu\lambda\sigma} + V_{\mu\nu\sigma\lambda} + V_{\nu\mu\lambda\sigma} + V_{\nu\mu\sigma\lambda}\right). \tag{4.80}$$

In going from Eq. (4.79) to (4.80), we use the bosonic commutation relations repeatedly to "pushing" the annihilation operators to the right (so that they can act upon $|\varnothing\rangle$) and the creation operators to the left (so that they can act upon $\langle\varnothing|$). Comparing Eq. (4.78) to Eq. (4.80), we see that the matrix elements match if we take

$$V_{\mu\nu\lambda\sigma} = \langle\mu|\langle\nu|\hat{V}^{(2)}|\lambda\rangle|\sigma\rangle. \tag{4.81}$$

For instance, if the bosons have a position representation, we would have something like

$$V_{\mu\nu\lambda\sigma} = \int d^dr_1 \int d^dr_2\; \varphi^*_\mu(r_1)\,\varphi^*_\nu(r_2)\,V(r_1,r_2)\,\varphi_\lambda(r_1)\,\varphi_\sigma(r_2). \tag{4.82}$$

The appropriate coefficients for $\mu = \nu$ and/or $\lambda = \sigma$, as well as for the fermionic case, are left for the reader to work out.

4. Other observables?

Another way to build a Hermitian operator from creation and annihilation operators is

$$\hat{A} = \sum_\mu \left(\alpha_\mu \hat{a}^\dagger_\mu + \alpha^*_\mu \hat{a}_\mu\right). \tag{4.83}$$

If such a term is added to a Hamiltonian, it breaks the conservation of total particle number. Each infinitesimal time step will include processes that decrement the particle number (due to $\hat{a}_\mu$), as well as processes that increment the particle number (due to $\hat{a}^\dagger_\mu$). Even if the system starts out with a fixed number of particles, such as the vacuum state $|\varnothing\rangle$, it subsequently evolves into a superposition of states with different particle numbers. In the theory of quantum electrodynamics, this type of operator is used to describe the emission and absorption of photons caused by moving charges.

Incidentally, the name "second quantization" comes from this process of using creation and annihilation operators to define Hamiltonians. The idea is that single-particle quantum mechanics is derived by "quantizing" classical Hamiltonians via the imposition of commutation relations like $[x, p] = i\hbar$. Then, we extend the theory to multi-particle systems by using the single-particle states to define creation/annihilation operators obeying commutation or anticommutation relations. This can be viewed as a "second" quantization step.

III. QUANTUM FIELD THEORY

A. Field operators

So far, we have been agnostic about the nature of the single-particle states $\{|\varphi_1\rangle, |\varphi_2\rangle, \dots\}$ used to construct the creation and annihilation operators. Let us now consider the special case where these quantum states are representable by wavefunctions. Let $|\mathbf{r}\rangle$ denote a position eigenstate for a d-dimensional space. A single-particle state $|\varphi_\mu\rangle$ has a wavefunction

$$\varphi_\mu(\mathbf{r}) = \langle \mathbf{r}|\varphi_\mu\rangle. \tag{4.84}$$

Due to the completeness and orthonormality of the basis, these wavefunctions satisfy

$$\begin{aligned} \int d^d r\; \varphi_\mu^*(\mathbf{r})\,\varphi_\nu(\mathbf{r}) &= \langle \varphi_\mu| \left(\int d^d r\, |\mathbf{r}\rangle\langle\mathbf{r}|\right) |\varphi_\nu\rangle \;= \delta_{\mu\nu}, \\ \sum_\mu \varphi_\mu^*(\mathbf{r})\varphi_\mu(\mathbf{r}') &= \langle \mathbf{r}'| \left(\sum_\mu |\varphi_\mu\rangle\langle\varphi_\mu|\right) |\mathbf{r}\rangle \;\; = \delta^d(\mathbf{r}-\mathbf{r}'). \end{aligned} \tag{4.85}$$

We can use the wavefunctions and the creation/annihilation operators to construct a new and interesting set of operators. For simplicity, suppose the particles are bosons, and let

$$\hat{\psi}(\mathbf{r}) = \sum_\mu \varphi_\mu(\mathbf{r})\,\hat{a}_\mu, \qquad \hat{\psi}^\dagger(\mathbf{r}) = \sum_\mu \varphi_\mu^*(\mathbf{r})\,\hat{a}_\mu^\dagger. \tag{4.86}$$

Using the aforementioned wavefunction properties, we can derive the inverse relations

$$\hat{a}_\mu = \int d^d r\; \varphi_\mu^*(\mathbf{r})\,\hat{\psi}(\mathbf{r}), \qquad \hat{a}_\mu^\dagger = \int d^d r\; \varphi_\mu(\mathbf{r})\,\hat{\psi}^\dagger(\mathbf{r}). \tag{4.87}$$

From the commutation relations for the bosonic a_μ and $a_\mu^\dagger$ operators, we can show that

$$\Big[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')\Big] = \Big[\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\Big] = 0, \quad \Big[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\Big] = \delta^d(\mathbf{r}-\mathbf{r}'). \tag{4.88}$$

In the original commutation relations, the operators for different single-particle states commute; now, the operators for different *positions* commute. A straightforward interpretion for the operators $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$ is that they respectively create and annihilate one particle at a point $\mathbf{r}$ (rather than one particle in a given eigenstate).

It is important to note that $\mathbf{r}$ here does not play the role of an observable. It is an *index*, in the sense that each $\mathbf{r}$ is associated with distinct $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ operators. These $\mathbf{r}$-dependent operators serve to generalize the classical concept of a **field**. In a classical field theory, each point $\mathbf{r}$ is assigned a set of numbers corresponding to physical quantities, such as the electric field components $E_x(\mathbf{r})$, $E_y(\mathbf{r})$, and $E_z(\mathbf{r})$. In the present case, each $\mathbf{r}$ is assigned a set of quantum operators. This kind of quantum theory is called a **quantum field theory**.

We can use the $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ operators to write second quantized observables in a way that is independent of the choice of single-particle basis wavefunctions. As discussed in the previous section, given a Hermitian single-particle operator $\hat{A}_1$ we can define a multi-particle observable $\hat{A} = \sum_{\mu\nu} \hat{a}_\mu^\dagger A_{\mu\nu} \hat{a}_\nu$, where $A_{\mu\nu} = \langle\varphi_\mu|\hat{A}_1|\varphi_\nu\rangle$. This multi-particle observable can be re-written as

$$\hat{A} = \int d^d r\, d^d r'\; \hat{\psi}^\dagger(\mathbf{r})\; \langle \mathbf{r}|\hat{A}_1|\mathbf{r}'\rangle\; \hat{\psi}(\mathbf{r}'), \tag{4.89}$$

which makes no explicit reference to the single-particle basis states.

For example, consider the familiar single-particle Hamiltonian describing a particle in a potential $V(\mathbf{r})$:

$$\hat{H}_1 = \hat{T}_1 + \hat{V}_1, \quad \hat{T}_1 = \frac{|\hat{\mathbf{p}}|^2}{2m}, \quad \hat{V}_1 = V(\hat{\mathbf{r}}), \tag{4.90}$$

where $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are position and momentum operators (single-particle observables). The corresponding second quantized operators for the kinetic energy and potential energy are

$$\begin{aligned}\hat{T} &= \frac{\hbar^2}{2m} \int d^d r \, d^d r' \, \hat{\psi}^\dagger(\mathbf{r}) \left(\int \frac{d^d k}{(2\pi)^d} \, |\mathbf{k}|^2 \, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \right) \hat{\psi}(\mathbf{r}') \\ &= \frac{\hbar^2}{2m} \int d^d r \, \nabla \hat{\psi}^\dagger(\mathbf{r}) \cdot \nabla \hat{\psi}(\mathbf{r}) \\ \hat{V} &= \int d^d r \, \hat{\psi}^\dagger(\mathbf{r}) \, V(\mathbf{r}) \, \hat{\psi}(\mathbf{r}).\end{aligned} \tag{4.91}$$

(In going from the first to the second line, we performed integrations by parts.) This result is strongly reminiscent of the expression for the expected kinetic and potential energies in single-particle quantum mechanics:

$$\langle T \rangle = \frac{\hbar^2}{2m} \int d^d r \, |\nabla \psi(\mathbf{r})|^2 \,, \quad \langle V \rangle = \int d^d r \; V(\mathbf{r}) \, |\psi(\mathbf{r})|^2, \tag{4.92}$$

where $\psi(\mathbf{r})$ is the single-particle wavefunction.

How are the particle creation and annihilation operators related to the classical notion of "the value of a field at point $\mathbf{r}$", like an electric field $\mathbf{E}(\mathbf{r})$ or magnetic field $\mathbf{B}(\mathbf{r})$? Field variables are measurable quantities, and should be described by Hermitian operators. As we have just seen, Hermitian operators corresponding to the kinetic and potential energy can be constructed via *products* of $\hat{\psi}^\dagger(\mathbf{r})$ with $\hat{\psi}(\mathbf{r})$. But there is another type of Hermitian operator that we can construct by taking *linear combinations* of of $\hat{\psi}^\dagger(\mathbf{r})$ with $\hat{\psi}(\mathbf{r})$. One example is

$$\psi(\mathbf{r}) + \psi(\mathbf{r})^\dagger.$$

Other possible Hermitian operators have the form

$$F(\mathbf{r}) = \int d^d r' \Big(f(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}) + f^*(\mathbf{r}, \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}') \Big), \tag{4.93}$$

where $f(\mathbf{r}, \mathbf{r}')$ is some complex function. As we shall see, it is this type of Hermitian operator that corresponds to the classical notion of a field variable like an electric or magnetic field.

In the next two sections, we will try to get a better understanding of the relationship between classical fields and *bosonic* quantum fields. (For fermionic quantum fields, the situation is more complicated; they cannot be related to classical fields of the sort we are familiar with, for reasons that lie outside the scope of this course.)

B. Revisiting the harmonic oscillator

Before delving into the links between classical fields and bosonic quantum fields, it is first necessary to revisit the harmonic oscillator, to see how the concept of a **mode of oscillation** carries over from classical to quantum mechanics.

A classical harmonic oscillator is described by the Hamiltonian

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{4.94}$$

where x is the "position" of the oscillator, which we call the **oscillator variable**; p is the corresponding momentum variable; m is the mass; and ω is the natural frequency of oscillation. We know that the classical equation of motion has the general form

$$x(t) = \mathcal{A}\, e^{-i\omega t} + \mathcal{A}^*\, e^{i\omega t}. \tag{4.95}$$

This describes an oscillation of frequency ω. It is parameterized by the **mode amplitude** $\mathcal{A}$, a complex number that determines the magnitude and phase of the oscillation.

For the quantum harmonic oscillator, x and p are replaced by the Hermitian operators $\hat{x}$ and $\hat{p}$. From these, the operators $\hat{a}$ and $\hat{a}^\dagger$ can be defined:

$$\begin{cases} \hat{a} = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\hat{x} + \dfrac{i\hat{p}}{m\omega}\right), \\ \hat{a}^\dagger = \sqrt{\dfrac{m\omega}{2\hbar}}\left(\hat{x} - \dfrac{i\hat{p}}{m\omega}\right). \end{cases} \Leftrightarrow \begin{cases} \hat{x} = \sqrt{\dfrac{\hbar}{2m\omega}}\,\left(\hat{a} + \hat{a}^\dagger\right) \\ \hat{p} = -i\sqrt{\dfrac{m\omega\hbar}{2}}\,\left(\hat{a} - \hat{a}^\dagger\right). \end{cases} \tag{4.96}$$

We can then show that

$$\left[\,\hat{a}\,,\,\hat{a}^\dagger\,\right] = 1, \quad \hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{4.97}$$

and from these the energy spectrum of the quantum harmonic oscillator can be derived. These facts should have been covered in an earlier course.

Here, we are interested in how the creation and annihilation operators relate to the *dynamics* of the quantum harmonic oscillator. In the Heisenberg picture, with $t = 0$ as the reference time, we define the time-dependent operator

$$\hat{x}(t) = \hat{U}^\dagger(t)\,\hat{x}\,\hat{U}(t), \quad \hat{U}(t) \equiv \exp\left(-\frac{i}{\hbar}\hat{H}t\right). \tag{4.98}$$

We will adopt the convention that all operators written with an explicit time dependence are Heisenberg picture operators, while operators without an explicit time dependence are Schrödinger picture operators; hence, $\hat{x} \equiv \hat{x}(0)$. The Heisenberg picture creation and annihilation operators, $\hat{a}^\dagger(t)$ and $\hat{a}(t)$, are related to $\hat{x}(t)$ by

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}}\Big(\hat{a}(t) + \hat{a}^\dagger(t)\Big). \tag{4.99}$$

The Heisenberg equation for the annihilation operator is

$$\begin{aligned} \frac{d\hat{a}(t)}{dt} &= \frac{i}{\hbar}\left[\hat{H}, \hat{a}(t)\right] \\ &= \frac{i}{\hbar}\,\hat{U}^\dagger(t)\left[\hat{H}, \hat{a}\right]\hat{U}(t) \\ &= \frac{i}{\hbar}\,\hat{U}^\dagger(t)\Big(-\hbar\omega\hat{a}\Big)\hat{U}(t) \\ &= -i\omega\hat{a}(t). \end{aligned} \tag{4.100}$$

Hence, the solution for this differential equation is

$$\hat{a}(t) = \hat{a}\, e^{-i\omega t}, \tag{4.101}$$

and Eq. (4.99) becomes

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}} \Big(\hat{a}\, e^{-i\omega t} + \hat{a}^\dagger\, e^{i\omega t}\Big). \tag{4.102}$$

This has exactly the same form as the classical oscillatory solution (4.95)! Comparing the two, we see that $\hat{a}$ times the scale factor $\sqrt{\hbar/2m\omega}$ plays the role of the mode amplitude $\mathcal{A}$.

Now, suppose we come at things from the opposite end. Let's say we start with creation and annihilation operators satisfying Eq. (4.97), from which Eqs. (4.100)–(4.101) follow. Using the creation and annihilation operators, we would like to construct an observable that corresponds to a classical oscillator variable. A natural Hermitian ansatz is

$$\hat{x}(t) = \mathcal{C} \left(\hat{a}\, e^{-i\omega t} + \hat{a}^\dagger\, e^{i\omega t}\right), \tag{4.103}$$

where $\mathcal{C}$ is a constant that is conventionally taken to be real.

How might $\mathcal{C}$ be chosen? A convenient way is to study the behavior of the oscillator variable *in the classical limit*. The classical limit of a quantum harmonic oscillator is described by a **coherent state**. The details of how this state is defined need not concern us for now (see Appendix E). The most important things to know are that (i) it can be denoted by $|\alpha\rangle$ where $\alpha \in \mathbb{C}$, (ii) it is an eigenstate of the annihilation operator:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle. \tag{4.104}$$

And (iii) its energy expectation value is

$$\langle E\rangle = \langle\alpha|\hat{H}|\alpha\rangle = \hbar\omega\left(|\alpha|^2 + \frac{1}{2}\right) \overset{|\alpha|^2\rightarrow\infty}{\longrightarrow} \hbar\omega|\alpha|^2. \tag{4.105}$$

When the system is in a coherent state, we can effectively substitute the $\hat{a}$ and $\hat{a}^\dagger$ operators in Eq. (4.103) with the complex numbers α and α^*, which gives a classical trajectory

$$x_{\mathrm{classical}}(t) = \mathcal{C}\left(\alpha\, e^{-i\omega t} + \alpha^*\, e^{i\omega t}\right). \tag{4.106}$$

This trajectory has amplitude $2\mathcal{C}|\alpha|$. At maximum displacement, the classical momentum is zero, so the total energy of the classical oscillator must be

$$E_{\mathrm{classical}} = \frac{1}{2} m\omega^2 \Big(2\mathcal{C}|\alpha|\Big)^2 = 2m\omega^2\mathcal{C}^2|\alpha|^2. \tag{4.107}$$

Equating the classical energy (4.107) to the coherent state energy (4.105) gives

$$\mathcal{C} = \sqrt{\frac{\hbar}{2m\omega}}, \tag{4.108}$$

which is precisely the scale factor found in Eq. (4.102).

C. A scalar boson field

We now have the tools available to understand the connection between a very simple classical field and its quantum counterpart. Consider a classical scalar field variable $f(x,t)$, defined in one spatial dimension, whose classical equation of motion is the wave equation:

$$\frac{\partial^2 f(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 f(x,t)}{\partial t^2}. \tag{4.109}$$

The constant c is a wave speed. This sort of classical field arises in many physical contexts, including the propagation of sound through air, in which case c is the speed of sound.

For simplicity, let us first assume that the field is defined within a finite interval of length L, with periodic boundary conditions: $f(x,t) \equiv f(x+L,t)$. Solutions to the wave equation can be described by the following ansatz:

$$f(x,t) = \sum_n \left(\mathcal{A}_n\,\varphi_n(x)\,e^{-i\omega_n t} + \mathcal{A}_n^*\,\varphi_n^*(x)\,e^{i\omega_n t}\right). \tag{4.110}$$

This ansatz describes a superposition of **normal modes**. Each normal mode (labelled n) varies harmonically in time with a mode frequency ω_n, and varies in space according to a complex mode profile $\varphi_n(x)$; its overall magnitude and phase is specified by the mode amplitude $\mathcal{A}_n$. The mode profiles are normalized according to some fixed convention, e.g.

$$\int_0^L dx\,|\varphi_n(x)|^2 = 1. \tag{4.111}$$

Substituting Eq. (4.110) into Eq. (4.109), and using the periodic boundary conditions, gives

$$\varphi_n(x) = \frac{1}{\sqrt{L}}\exp\left(ik_n x\right), \quad \omega_n = ck_n = \frac{2\pi cn}{L}, \quad n \in \mathbb{Z}. \tag{4.112}$$

These mode profiles are orthonormal:

$$\int_0^L dx\,\varphi_m^*(x)\,\varphi_n(x) = \delta_{mn}. \tag{4.113}$$

Each normal mode carries energy. By analogy with the classical harmonic oscillator—see Eqs. (4.106)–(4.107)—we assume that the energy density (i.e., energy per unit length) is proportional to the square of the field variable. Let it have the form

$$U(x) = 2\rho\sum_n |\mathcal{A}_n|^2\,|\varphi_n(x)|^2, \tag{4.114}$$

where ρ is some parameter that has to be derived from the underlying physical context. For example, for acoustic modes, ρ is the mass density of the underlying acoustic medium; in the next chapter, we will see a concrete example involving the energy density of an electromagnetic mode. From Eq. (4.114), the total energy is

$$E = \int_0^L dx\,U(x) = 2\rho\sum_n |\mathcal{A}_n|^2. \tag{4.115}$$

To quantize the classical field, we treat each normal mode as an independent oscillator, with creation and annihilation operators $\hat{a}_n^\dagger$ and $\hat{a}_n$ satisfying

$$\left[\,\hat{a}_m\,,\,\hat{a}_n^\dagger\right] = \delta_{mn}, \quad \left[\,\hat{a}_m\,,\,\hat{a}_n\right] = \left[\,\hat{a}_m^\dagger\,,\,\hat{a}_n^\dagger\right] = 0. \tag{4.116}$$

We then take the Hamiltonian to be that of a set of independent harmonic oscillators:

$$\hat{H} = \sum_n \hbar\omega_n \hat{a}_n^\dagger \hat{a}_n + E_0, \tag{4.117}$$

where E_0 is the ground-state energy. Just like in the previous section, we can define a Heisenberg-picture annihilation operator, and solving its Heisenberg equation yields

$$\hat{a}_n(t) = \hat{a}_n e^{-i\omega_n t}. \tag{4.118}$$

We then define a Schrödinger picture Hermitian operator of the form

$$\hat{f}(x) = \sum_n \mathcal{C}_n \Big(\hat{a}_n \varphi_n(x) + \hat{a}_n^\dagger \varphi_n^*(x)\Big), \tag{4.119}$$

where $\mathcal{C}_n$ is a real constant (one for each normal mode). The corresponding Heisenberg picture operator is

$$\hat{f}(x,t) = \sum_n \mathcal{C}_n \Big(\hat{a}_n \varphi_n(x)\, e^{-i\omega_n t} + \hat{a}_n^\dagger \varphi_n^*(x)\, e^{i\omega_n t}\Big), \tag{4.120}$$

which is the quantum version of the classical solution (4.110).

To determine the $\mathcal{C}_n$ scale factors, we consider the classical limit. The procedure is a straightfoward generalization of the harmonic oscillator case discussed in Section III B. We introduce a state $|\alpha\rangle$ that is a coherent state for all the normal modes; i.e., for any given n,

$$\hat{a}_n|\alpha\rangle = \alpha_n|\alpha\rangle \tag{4.121}$$

for some $\alpha_n \in \mathbb{C}$. The energy expectation value is

$$\langle E\rangle = \sum_n \hbar\omega_n |\alpha_n|^2. \tag{4.122}$$

In the coherent state, the $\hat{a}_n$ and $\hat{a}_n^\dagger$ operators in Eq. (4.120) can be replaced with α_n and α_n^* respectively. Hence, we identify $\mathcal{C}_n\alpha_n$ as the classical mode amplitude $\mathcal{A}_n$ in Eq. (4.110). In order for the classical energy (4.115) to match the coherent state energy (4.122), we need

$$2\rho|\mathcal{A}_n|^2 = 2\rho|\mathcal{C}_n\alpha_n|^2 = \hbar\omega_n|\alpha_n|^2 \quad \Rightarrow \quad \mathcal{C}_n = \sqrt{\frac{\hbar\omega_n}{2\rho}}. \tag{4.123}$$

Hence, the appropriate field operator is

$$\hat{f}(x,t) = \sum_n \sqrt{\frac{\hbar\omega_n}{2\rho}} \Big(\hat{a}_n \varphi_n(x)\, e^{-i\omega_n t} + \hat{a}_n^\dagger \varphi_n^*(x)\, e^{i\omega_n t}\Big). \tag{4.124}$$

Returning to the Schrödinger picture, and using the explicit mode profiles from Eq. (4.112), we get

$$\hat{f}(x) = \sum_n \sqrt{\frac{\hbar\omega_n}{2\rho L}} \Big(\hat{a}_n e^{ik_n x} + \hat{a}_n^\dagger e^{-ik_n x}\Big). \tag{4.125}$$

Finally, if we are interested in the infinite-L limit, we can convert the sum over n into an integral. The result is

$$\hat{f}(x) = \int dk \, \sqrt{\frac{\hbar\omega(k)}{4\pi\rho}} \Big(\hat{a}(k)\, e^{ikx} + \hat{a}^\dagger(k)\, e^{-ikx}\Big), \tag{4.126}$$

where $\hat{a}(k)$ denotes a rescaled annihilation operator defined by $\hat{a}_n \rightarrow \sqrt{2\pi/L}\;\hat{a}(k)$, satisfying

$$\Big[\hat{a}(k)\,,\,\hat{a}^\dagger(k')\Big] = \delta(k-k'). \tag{4.127}$$

D. Looking ahead

In the next chapter, we will use these ideas to formulate a quantum theory of electromagnetism. This is a bosonic quantum field theory in which the creation and annihilation operators act upon particles called **photons**—the elementary particles of light. Linear combinations of these photon operators can be used to define Hermitian field operators that correspond to the classical electromagnetic field variables. In the classical limit, the quantum field theory reduces to Maxwell's theory of the electromagnetic field.

It is hard to overstate the importance of quantum field theories in physics. At a fundamental level, all elementary particles currently known to humanity can be described using a quantum field theory called the Standard Model. These particles are roughly divided into two categories. The first consists of "force-carrying" particles: photons (which carry the electromagnetic force), gluons (which carry the strong nuclear force), and the W/Z bosons (which carry the weak nuclear force); these particles are excitations of bosonic quantum fields, similar to the one described in the previous section. The second category consists of "particles of matter", such as electrons, quarks, and neutrinos; these are excitations of *fermionic* quantum fields, whose creation and annihilation operators obey anticommutation relations.

As Wilczek [4] has pointed out, the modern picture of fundamental physics bears a striking resemblence to the old idea of "luminiferous ether": a medium filling all of space and time, whose vibrations are physically-observable light waves. The key difference, as we now understand, is that the ether is not a classical medium, but one obeying the rules of quantum mechanics. (Another difference, which we have not discussed so far, is that modern field theories can be made compatible with relativity.)

It is quite compelling to think of fields, not individual particles, as the fundamental objects in the universe. This point of view "explains", in a sense, why all particles of the same type have the same properties (e.g., why all electrons in the universe have exactly the same mass). The particles themselves are not fundamental; they are excitations of deeper, more fundamental entities—quantum fields!

Exercises

1. Consider a system of two identical particles. Each single-particle Hilbert space $\mathscr{H}^{(1)}$ is spanned by a basis $\{|\mu_i\}$. The exchange operator is defined on $\mathscr{H}^{(2)} = \mathscr{H}^{(1)} \otimes \mathscr{H}^{(1)}$ by
$$P\Big(\sum_{ij} \psi_{ij}|\mu_i\rangle|\mu_j\rangle\Big) \;\equiv\; \sum_{ij} \psi_{ij}|\mu_j\rangle|\mu_i\rangle. \tag{4.128}$$
Prove that $\hat{P}$ is linear, unitary, and Hermitian. Moreover, prove that the operation is basis-independent: i.e., given any other basis $\{\nu_j\}$ that spans $\mathscr{H}^{(1)}$,
$$P\Big(\sum_{ij} \varphi_{ij}|\nu_i\rangle|\nu_j\rangle\Big) \;=\; \sum_{ij} \varphi_{ij}|\nu_j\rangle|\nu_i\rangle. \tag{4.129}$$

2. Prove that the exchange operator commutes with the Hamiltonian
$$\hat{H} = -\frac{\hbar^2}{2m_e}\Big(\nabla_1^2 + \nabla_2^2\Big) + \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{4.130}$$

3. An N-boson state can be written as
$$|\phi_1, \phi_2, \dots, \phi_N\rangle = \mathcal{N}\sum_p \Big(|\phi_{p(1)}\rangle|\phi_{p(2)}\rangle|\phi_{p(3)}\rangle\cdots|\phi_{p(N)}\rangle\Big). \tag{4.131}$$
Prove that the normalization constant is
$$\mathcal{N} = \sqrt{\frac{1}{N!\prod_\mu n_\mu!}}, \tag{4.132}$$
where n_μ denotes the number of particles occupying the single-particle state μ.

4. $\mathscr{H}_S^{(N)}$ and $\mathscr{H}_A^{(N)}$ denote the Hilbert spaces of N-particle states that are totally symmetric and totally antisymmetric under exchange, respectively. Prove that
$$\dim\Big(\mathscr{H}_S^{(N)}\Big) = \frac{(d+N-1)!}{N!(d-1)!}, \tag{4.133}$$
$$\dim\Big(\mathscr{H}_A^{(N)}\Big) = \frac{d!}{N!(d-N)!}. \tag{4.134}$$

5. Prove that for boson creation and annihilation operators, $[\hat{a}_\mu, \hat{a}_\nu] = [\hat{a}_\mu^\dagger, \hat{a}_\nu^\dagger] = 0$.

6. Let $\hat{A}_1$ be an observable (Hermitian operator) for single-particle states. Given a single-particle basis $\{|\varphi_1\rangle, |\varphi_2\rangle, \dots\}$, define the bosonic multi-particle observable
$$\hat{A} = \sum_{\mu\nu} a_\mu^\dagger\, \langle\varphi_\mu|\hat{A}_1|\varphi_\nu\rangle\, a_\nu, \tag{4.135}$$

where $a_\mu^\dagger$ and a_μ are creation and annihilation operators satisfying the usual bosonic commutation relations, $[a_\mu, a_\nu] = 0$ and $[a_\mu, a_\nu^\dagger] = \delta_{\mu\nu}$. Prove that $\hat{A}$ commutes with the total number operator:

$$\left[\hat{A}, \sum_\mu a_\mu^\dagger a_\mu\right] = 0. \tag{4.136}$$

Next, repeat the proof for a fermionic multi-particle observable

$$\hat{A} = \sum_{\mu\nu} c_\mu^\dagger \, \langle\varphi_\mu|\hat{A}_1|\varphi_\nu\rangle \, c_\nu, \tag{4.137}$$

where $c_\mu^\dagger$ and c_μ are creation and annihilation operators satisfying the fermionic anti-commutation relations, $\{c_\mu, c_\nu\} = 0$ and $\{c_\mu, c_\nu^\dagger\} = \delta_{\mu\nu}$. In this case, prove that

$$\left[\hat{A}, \sum_\mu c_\mu^\dagger c_\mu\right] = 0. \tag{4.138}$$

Further Reading

[1] Bransden & Joachain, §10.1–10.5

[2] Sakurai, §6

[3] J. M. Leinaas and J. Myrheim, *On the Theory of Identical Particles*, Nuovo Cimento B **37**, 1 (1977).

[4] F. Wilczek, *The Persistence of Ether*, Physics Today **52**, 11 (1999). [link]