1

Second Quantization

In this chapter we revisit the quantum mechanical description of one-particle systems and many-particle systems. We highlight the differences between distinguishable and indistinguishable, or identical, particles and bring to the front the mathematical complications that arise when dealing with identical particles. We then introduce the second quantization formalism and show how to overcome these complications. The main actors of the second quantization formalism are the field operators, which can be used to represent states and quantum observables in the Hilbert space of identical particles.

1.1 Quantum Mechanics of One Particle

In quantum mechanics the physical state of a particle is described in terms of a *ket* $|\Psi\rangle$. This ket belongs to a *Hilbert space*, which is nothing but a vector space endowed with an inner product. The dimension of the Hilbert space is essentially fixed by our physical intuition; it is us who decide which kets are relevant to the description of the particle. For instance, if we want to describe how a laser works we can choose those energy eigenkets that get populated and depopulated, and discard the rest. This selection of states leads to the well-known description of a laser in terms of a three-level system, four-level system, etc. A fundamental property following from the vector nature of the Hilbert space is that any linear superposition of kets is another ket in the Hilbert space. In other words, we can make a linear superposition of physical states and the result is another physical state. In quantum mechanics, however, it is only the "direction" of the ket that matters, so $|\Psi\rangle$ and $C|\Psi\rangle$ represent the same physical state for all complex numbers C. This redundancy prompts us to work with *normalized* kets. What do we mean by that? We said before that there is an inner product in the Hilbert space. Let us denote by $\langle\Phi|\Psi\rangle = \langle\Psi|\Phi\rangle^*$ the inner product between two kets $|\Psi\rangle$ and $|\Phi\rangle$ of the Hilbert space. Then every ket has a real positive inner product with itself,

$$0 < \langle\Psi|\Psi\rangle < \infty.$$

A ket is said to be normalized if the inner product with itself is 1. Throughout this book we always assume that a ket is normalized unless otherwise stated. Every ket can be normalized by choosing the complex constant $C = e^{i\alpha}/\sqrt{\langle\Psi|\Psi\rangle}$ with α an arbitrary real number. Thus, the normalization fixes the ket of a physical state only modulo a phase factor. As we see in Section 1.3, this freedom is the basis of a fundamental property about the nature

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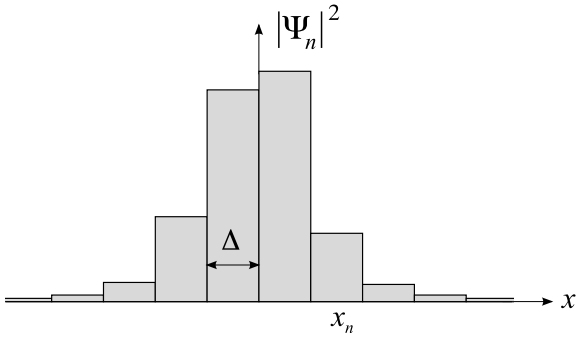

Figure 1.1 Histogram of the normalized number of clicks of the detector in $x_n = n\Delta$. The height of the bars corresponds to the probabilities $|\Psi_n|^2$.

of elementary particles. The notion of inner product also allows us to define the *dual space* as the vector space of linear operators $\langle\Phi|$, which deliver the complex number $\langle\Phi|\Psi\rangle$ when acting on the ket $|\Psi\rangle$. The elements of the dual space are called *bra*, and we can think of the inner product as the action of a bra on a ket. The formulation of quantum mechanics in terms of bras and kets is due to Dirac [1, 2] and turns out to be extremely useful.

According to the basic principles of quantum mechanics [2],

- With every physical observable is associated a Hermitian operator whose eigenvalues λ represent the outcome of an experimental measurement of the observable.
- If the particle is described by the ket $|\Psi\rangle$, then the probability of measuring λ is given by
$$P(\lambda) = |\langle\lambda|\Psi\rangle|^2,$$
where $|\lambda\rangle$ is the eigenket of the operator with eigenvalue λ.
- The experimental measurement is so invasive that just after measurement the particle *collapses* in the ket $|\lambda\rangle$.

Let us discuss the implications of these principles with an example.

Discrete formulation Suppose that we want to measure the position of a particle living in a one-dimensional world. We can construct a detector with the property that it clicks whenever the particle is no further away than, say, $\Delta/2$ from the position of the detector. We distribute these detectors on a uniform grid $x_n = n\Delta$, with n integers, so as to cover the entire one-dimensional world. The experiment consists in preparing the particle in a state $|\Psi\rangle$ and in taking note of which detector clicks. After the click, we know for sure that the particle is in the interval $x_n \pm \Delta/2$, where x_n is the position of the detector that clicked. Repeating the experiment $N \gg 1$ times, counting the number of times that a given detector clicks, and dividing the result by N, we obtain the probability that the particle is in the interval $x_n \pm \Delta/2$, see histogram in Fig. 1.1. Quantum mechanics tells us that this probability is
$$P(n) = |\langle n|\Psi\rangle|^2,$$

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where $|n\rangle$ is the ket describing the particle in the interval $x_n \pm \Delta/2$. The experimental setup does not allow us to say where exactly the particle is within this interval. In fact, it does not make sense to speak about the exact position of the particle since it cannot be measured. From the experimental output we could even argue that the one-dimensional world is discrete! What we want to say is that in our experiment the "exact position" of the particle is a mere speculative concept, like the gender, color, or happiness of the particle. These degrees of freedom may also exist, but if they cannot be measured then we should not include them in the description of the physical world. As scientists we can only assign a ket $|n\rangle$ to the state of the particle just after measurement, and we can interpret this ket as describing the particle in some discrete position. The probability of finding the particle in $|n'\rangle$ just after the nth detector has clicked is zero for all $n' \neq n$ and unity for $n' = n$, and hence,

$$\langle n'|n\rangle = \delta_{n'n}. \tag{1.1}$$

The kets $|n\rangle$ are orthonormal and it is easy to show that they form a basis of our Hilbert space. Suppose by absurdum that there exists another ket $|\chi\rangle$ orthogonal to all the $|n\rangle$. If the particle is described by this ket then the probability that the nth detector clicks is $|\langle n|\chi\rangle|^2 = 0$ for all n. This cannot be the case unless the particle is somewhere outside the one-dimensional world – that is, in a state not included in our original description.

Let us continue to elaborate on the example of the particle in a one-dimensional world. We said before, that the kets $|n\rangle$ form a basis. Therefore, any ket $|\Psi\rangle$ can be expanded as

$$|\Psi\rangle = \sum_n \Psi_n |n\rangle. \tag{1.2}$$

Since the basis is orthonormal, the coefficient Ψ_n is simply

$$\Psi_n = \langle n|\Psi\rangle, \tag{1.3}$$

and its square modulus is exactly the probability $P(n)$:

$$|\Psi_n|^2 = \begin{pmatrix} \text{probability of finding the particle in} \\ \text{volume element } \Delta \text{ around } x_n \end{pmatrix}.$$

It is important to appreciate the advantage of working with normalized kets. Since $\langle\Psi|\Psi\rangle = 1$, then

$$\sum_n |\Psi_n|^2 = 1, \tag{1.4}$$

according to which the probability of finding the particle anywhere is unity. The interpretation of the $|\Psi_n|^2$ as probabilities would not be possible if $|\Psi\rangle$ and $|n\rangle$ were not normalized.

Given an orthonormal basis, the inner product of a normalized ket $|\Psi\rangle$ with a basis ket gives the probability amplitude of having the particle in that ket.

Inserting (1.3) back into (1.2), we find the interesting relation

$$|\Psi\rangle = \sum_n \langle n|\Psi\rangle\, |n\rangle = \sum_n |n\rangle\langle n|\Psi\rangle.$$

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This relation is interesting because it is true for all $|\Psi\rangle$ and hence

$$\sum_n |n\rangle\langle n| = \hat{\mathbb{1}}, \tag{1.5}$$

with $\hat{\mathbb{1}}$ the identity operator. Equation (1.5) is known as the *completeness relation* and expresses the fact that the set $\{|n\rangle\}$ is an orthonormal basis. Vice versa, any orthonormal basis satisfies the completeness relation.

Continuum formulation We now assume that we can construct more and more precise detectors and hence reduce the range Δ. Then we can also refine the description of our particle by putting the detectors closer and closer. In the limit $\Delta \to 0$, the probability $|\Psi_n|^2$ approaches zero and it makes more sense to reason in terms of the *probability density* $|\Psi_n|^2/\Delta$ of finding the particle in x_n. Let us rewrite (1.2) as

$$|\Psi\rangle = \Delta \sum_n \frac{\Psi_n}{\sqrt{\Delta}} \frac{|n\rangle}{\sqrt{\Delta}}. \tag{1.6}$$

We now define the continuous function $\Psi(x_n)$ and the continuous ket $|x_n\rangle$ as

$$\Psi(x_n) \equiv \lim_{\Delta\to 0} \frac{\Psi_n}{\sqrt{\Delta}}, \qquad |x_n\rangle = \lim_{\Delta\to 0} \frac{|n\rangle}{\sqrt{\Delta}}.$$

In this definition the limiting function $\Psi(x_n)$ is well defined, while the limiting ket $|x_n\rangle$ makes *mathematical sense* only under an integral sign since the norm $\langle x_n|x_n\rangle = \infty$. However, we can still give to $|x_n\rangle$ a precise *physical meaning* since in quantum mechanics only the "direction" of a ket matters.[1] With these definitions (1.6) can be seen as the Riemann sum of $\Psi(x_n)|x_n\rangle$. In the limit $\Delta \to 0$ the sum becomes an integral over x, and we can write

$$|\Psi\rangle = \int dx\ \Psi(x)|x\rangle.$$

The function $\Psi(x)$ is usually called the *wavefunction* or the *probability amplitude*, and its square modulus $|\Psi(x)|^2$ is the probability density of finding the particle in x, or equivalently

$$|\Psi(x)|^2\ dx\ = \left(\begin{array}{c}\text{probability of finding the particle}\\ \text{in volume element } dx \text{ around } x\end{array}\right).$$

In the continuum formulation the orthonormality relation (1.1) becomes

$$\langle x_{n'}|x_n\rangle = \lim_{\Delta\to 0} \frac{\delta_{n'n}}{\Delta} = \delta(x_{n'} - x_n),$$

where $\delta(x)$ is the Dirac δ-function, see Appendix A. Similarly, the completeness relation becomes

$$\int dx\ |x\rangle\langle x| = \hat{\mathbb{1}}.$$

[1] The formulation of quantum mechanics using nonnormalizable states requires the extension of Hilbert spaces to *rigged Hilbert spaces*. Readers interested in the mathematical foundations of this extension can consult, for example, Ref. [3]. Here we simply note that in a rigged Hilbert space everything works as in the more familiar Hilbert space. We simply have to keep in mind that every divergent quantity comes from some continuous limit and that in all physical quantities the divergency is canceled by an infinitesimally small quantity.

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The entire discussion can easily be generalized to particles with spin in three (or any other) dimension. Let us denote by $\mathbf{x} = (\mathbf{r}\sigma)$ the collective index for the position $\mathbf{r}$ and the spin projection (say along the z axis) σ of the particle. If in every point of space we put a spin-polarized detector which clicks only if the particle has spin σ then $|\mathbf{x}\rangle$ is the state of the particle just after the spin-polarized detector in $\mathbf{r}$ has clicked. The *position–spin kets* $|\mathbf{x}\rangle$ are orthonormal

$$\langle \mathbf{x}'|\mathbf{x}\rangle = \delta_{\sigma'\sigma}\delta(\mathbf{r}' - \mathbf{r}) \equiv \delta(\mathbf{x}' - \mathbf{x}), \tag{1.7}$$

and form a basis. Hence they satisfy the completeness relation, which in this case reads

$$\boxed{\int d\mathbf{x}\ |\mathbf{x}\rangle\langle\mathbf{x}| = \hat{\mathbb{1}}} \tag{1.8}$$

Here and in the remainder of the book we use the symbol

$$\int d\mathbf{x} \equiv \sum_{\sigma} \int d\mathbf{r}$$

to signify a sum over spin and an integral over space. The expansion of a ket in this continuous Hilbert space follows directly from the completeness relation

$$|\Psi\rangle = \hat{\mathbb{1}}|\Psi\rangle = \int d\mathbf{x}\ |\mathbf{x}\rangle\langle\mathbf{x}|\Psi\rangle,$$

and the square modulus of the wavefunction $\Psi(\mathbf{x}) \equiv \langle\mathbf{x}|\Psi\rangle$ is the probability density of finding the particle in $\mathbf{x} = (\mathbf{r}\sigma)$:

$$|\Psi(\mathbf{x})|^2\, d\mathbf{r} = \begin{pmatrix} \text{probability of finding the particle with spin } \sigma \\ \text{in volume element } d\mathbf{r} \text{ around } \mathbf{r} \end{pmatrix}.$$

Operators So far we have only discussed the possible states of the particle, and the physical interpretation of the expansion coefficients. To say something about the dynamics of the particle, we must know the Hamiltonian operator $\hat{h}$. The knowledge of the Hamiltonian in quantum mechanics is analogous to knowledge of the forces in Newtonian mechanics. In Newtonian mechanics the dynamics of the particle is completely determined by the position and velocity at a certain time and by the forces. In quantum mechanics the dynamics of the wavefunction is completely determined by the wavefunction at a certain time and by $\hat{h}$. The Hamiltonian operator $\hat{h} \equiv h(\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}, \hat{\boldsymbol{\mathcal{S}}})$ does, in general, depend on the position operator $\hat{\boldsymbol{r}}$, the momentum operator $\hat{\boldsymbol{p}}$, and the spin operator $\hat{\boldsymbol{\mathcal{S}}}$. An example is the Hamiltonian for a particle of mass m, charge q, and gyromagnetic ratio g moving in an external scalar potential ϕ, vector potential $\mathbf{A}$, and whose spin is coupled to the magnetic field $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$:

$$\hat{h} = \frac{1}{2m}\left(\hat{\boldsymbol{p}} - \frac{q}{c}\mathbf{A}(\hat{\boldsymbol{r}})\right)^2 + q\phi(\hat{\boldsymbol{r}}) - g\mu_{\mathrm{B}}\mathbf{B}(\hat{\boldsymbol{r}}) \cdot \hat{\boldsymbol{\mathcal{S}}}, \tag{1.9}$$

with c the speed of light and μ_{B} the Bohr magneton.[2] Unless otherwise stated in this book we use atomic units, so $\hbar = 1$, $c \sim 137$, electron charge $e = -1$, and electron mass

[2] Other relativistic corrections like the spin–orbit interaction can be incorporated without any conceptual complication.

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$m_e = 1$. Thus, in (I.9) the Bohr magneton $\mu_{\rm B} = \frac{e\hbar}{2m_e c} \sim 3.649 \times 10^{-3}$, and charge and mass of the particles are measured in units of e and m_e, respectively. To distinguish operators from scalar or matrix quantities we always put the symbol " ˆ " (read "hat") on them. The position–spin kets are eigenstates of the position operator and of the z-component of the spin operator:

$$\hat{\boldsymbol{r}}|\mathbf{x}\rangle = \mathbf{r}|\mathbf{x}\rangle, \qquad \hat{\mathcal{S}}_z|\mathbf{x}\rangle = \sigma|\mathbf{x}\rangle,$$

with $\sigma = -S, -S+1, \ldots, S-1, S$ for spin S particles. The eigenstates of the momentum operator are instead the *momentum–spin kets* $|\mathbf{p}\sigma\rangle$:

$$\hat{\boldsymbol{p}}|\mathbf{p}\sigma\rangle = \mathbf{p}|\mathbf{p}\sigma\rangle.$$

These kets are also eigenstates of $\hat{\mathcal{S}}_z$ with eigenvalue σ. The momentum–spin kets form an orthonormal basis like the position–spin kets. The inner product between $|\mathbf{x}\rangle = |\mathbf{r}\sigma\rangle$ and $|\mathbf{p}\sigma'\rangle$ is proportional to $\delta_{\sigma\sigma'}$ times the plane wave $e^{\mathrm{i}\mathbf{p}\cdot\mathbf{r}}$. In this book we choose the constant of proportionality to be unity, so that

$$\boxed{\langle \mathbf{x}|\mathbf{p}\sigma'\rangle = \delta_{\sigma\sigma'}\langle \mathbf{r}|\mathbf{p}\rangle \qquad \text{with} \qquad \langle \mathbf{r}|\mathbf{p}\rangle = e^{\mathrm{i}\mathbf{p}\cdot\mathbf{r}}} \tag{I.10}$$

This inner product fixes uniquely the form of the completeness relation for the kets $|\mathbf{p}\sigma\rangle$. We have

$$\begin{aligned}\langle \mathbf{p}'\sigma'|\mathbf{p}\sigma\rangle &= \delta_{\sigma'\sigma}\langle \mathbf{p}'|\mathbf{p}\rangle = \delta_{\sigma'\sigma}\int d\mathbf{r}\,\langle \mathbf{p}'|\mathbf{r}\rangle\langle \mathbf{r}|\mathbf{p}\rangle = \delta_{\sigma'\sigma}\int d\mathbf{r}\,e^{\mathrm{i}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} \\ &= (2\pi)^3\delta_{\sigma'\sigma}\delta(\mathbf{p}'-\mathbf{p}),\end{aligned}$$

and therefore

$$\boxed{\sum_\sigma \int \frac{d\mathbf{p}}{(2\pi)^3}|\mathbf{p}\sigma\rangle\langle \mathbf{p}\sigma| = \hat{\mathbb{1}}} \tag{I.11}$$

as can easily be verified by acting with (I.11) on the ket $|\mathbf{p}'\sigma'\rangle$ or on the bra $\langle \mathbf{p}'\sigma'|$.

Before moving to the quantum mechanical description of many particles, let us briefly recall how to calculate the matrix elements of the Hamiltonian $\hat{h}$ in the position–spin basis. If $|\Psi\rangle$ is the ket of the particle, then

$$\langle \mathbf{x}|\hat{\boldsymbol{p}}|\Psi\rangle = -\mathrm{i}\boldsymbol{\nabla}\langle \mathbf{x}|\Psi\rangle \quad \Rightarrow \quad \langle \Psi|\hat{\boldsymbol{p}}|\mathbf{x}\rangle = \mathrm{i}\langle \Psi|\mathbf{x}\rangle\overleftarrow{\boldsymbol{\nabla}},$$

where the arrow over the gradient specifies that $\boldsymbol{\nabla}$ acts on the quantity to its left. It follows from these identities that

$$\langle \mathbf{x}|\hat{\boldsymbol{p}}|\mathbf{x}'\rangle = -\mathrm{i}\delta_{\sigma\sigma'}\boldsymbol{\nabla}\delta(\mathbf{r}-\mathbf{r}') = \mathrm{i}\delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\overleftarrow{\boldsymbol{\nabla}}', \tag{I.12}$$

where $\boldsymbol{\nabla}'$ means that the gradient acts on the primed variable. Therefore, the matrix element $\langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle$ with $\hat{h} = h(\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}, \hat{\boldsymbol{\mathcal{S}}})$ can be written as

$$\boxed{\langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle = h_{\sigma\sigma'}(\mathbf{r}, -\mathrm{i}\boldsymbol{\nabla}, \mathbf{S})\delta(\mathbf{r}-\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')h_{\sigma\sigma'}(\mathbf{r}', \mathrm{i}\overleftarrow{\boldsymbol{\nabla}}', \mathbf{S})} \tag{I.13}$$

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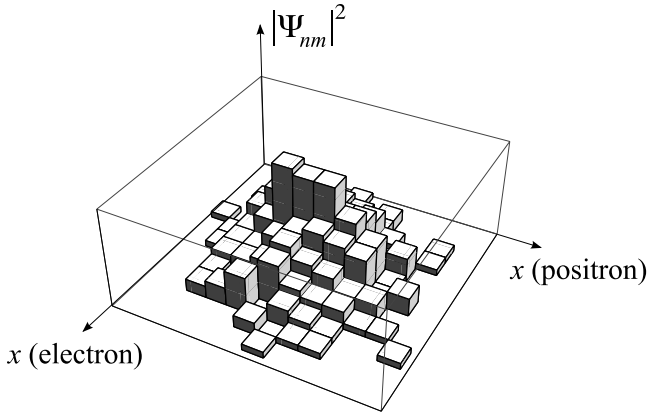

Figure 1.2 Histogram of the normalized number of simultaneous clicks of the electron and positron detectors in $x_n = n\Delta$ and $x_m = m\Delta$, respectively. The height of the parallelepipeds corresponds to the probabilities $|\Psi_{nm}|^2$.

where $\mathbf{S}$ is the matrix of the spin operator with elements $\langle\sigma|\hat{\boldsymbol{\mathcal{S}}}|\sigma'\rangle = \mathbf{S}_{\sigma\sigma'}$. For example, for the one-particle Hamiltonian in (1.9) we have

$$h_{\sigma\sigma'}(\mathbf{r}, -\mathrm{i}\boldsymbol{\nabla}, \mathbf{S}) = \frac{\delta_{\sigma\sigma'}}{2m}\left(-\mathrm{i}\boldsymbol{\nabla} - \frac{q}{c}\mathbf{A}(\mathbf{r})\right)^2 + \delta_{\sigma\sigma'} q\phi(\mathbf{r}) - g\mu_{\mathrm{B}}\mathbf{B}(\mathbf{r}) \cdot \mathbf{S}_{\sigma\sigma'}.$$

We use (1.13) over and over in the following chapters to recognize the matrix structure of several equations.

1.2 Quantum Mechanics of Many Particles

We want to generalize the concepts of the previous section to many particles. Let us first discuss the case of *distinguishable particles*. Particles are called distinguishable if one or more of their properties, such as mass, charge, spin, etc., are different. Let us consider, for instance, an electron and a positron in one dimension. These particles are distinguishable since the charge of the positron is opposite to the charge of the electron.

Discrete formulation for two particles To measure the position of the electron and the position of the positron at a certain time, we put an electron detector and a positron detector at every point $x_n = n\Delta$ of the real axis and perform a *coincidence experiment*. This means that we take note of the position of the electron detector and of the positron detector only if they click *at the same time*. The result of the experiment is the pair of points (x_n, x_m), where x_n refers to the electron and x_m refers to the positron. Performing the experiment $N \gg 1$ times, counting the number of times that the pair (x_n, x_m) is measured and dividing the result by N, we obtain the probability that the electron is in x_n and the positron in x_m, see the histogram in Fig. 1.2. According to quantum mechanics, the electron–positron pair collapses in the ket $|n\rangle|m\rangle$ just after measurement. This ket

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describes an electron in the interval $x_n \pm \Delta/2$ and a positron in the interval $x_m \pm \Delta/2$. Therefore, the probability of finding the electron–positron pair in $|n'\rangle|m'\rangle$ is zero unless $n' = n$ and $m' = m$; that is,

$$(\langle n'|\langle m'|) (|n\rangle|m\rangle) = \delta_{n'n}\delta_{m'm}.$$

The kets $|n\rangle|m\rangle$ are orthonormal and form a basis since if there was a ket $|\chi\rangle$ orthogonal to all of them then the electron–positron pair described by $|\chi\rangle$ would not be on the real axis. The orthonormality of the basis is expressed by the completeness relation

$$\sum_{nm} (|n\rangle|m\rangle) (\langle n|\langle m|) = \hat{\mathbb{1}}.$$

This relation can be used to expand any ket as

$$|\Psi\rangle = \hat{\mathbb{1}}|\Psi\rangle = \sum_{nm} (|n\rangle|m\rangle) (\langle n|\langle m|) |\Psi\rangle,$$

and if $|\Psi\rangle$ is normalized then the square modulus of the coefficients $\Psi_{nm} \equiv (\langle n|\langle m|) |\Psi\rangle$ is the probability represented in the histogram.

Continuum formulation for two particles As in the previous section, we could refine the experiment by putting the detectors closer and closer. We could also rethink the entire experiment in three (or any other) dimensions and use spin-polarized detectors. We then arrive at the position–spin kets $|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle$ for the electron–positron pair with inner product

$$(\langle \mathbf{x}_1'|\langle \mathbf{x}_2'|) (|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle) = \delta(\mathbf{x}_1' - \mathbf{x}_1)\delta(\mathbf{x}_2' - \mathbf{x}_2),$$

from which we deduce the completeness relation

$$\int d\mathbf{x}_1 d\mathbf{x}_2 (|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle) (\langle \mathbf{x}_1|\langle \mathbf{x}_2|) = \hat{\mathbb{1}}.$$

The expansion of a generic ket is

$$|\Psi\rangle = \int d\mathbf{x}_1 d\mathbf{x}_2 (|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle) (\langle \mathbf{x}_1|\langle \mathbf{x}_2|) |\Psi\rangle,$$

and if $|\Psi\rangle$ is normalized then the square modulus of the wavefunction $\Psi(\mathbf{x}_1, \mathbf{x}_2) \equiv (\langle \mathbf{x}_1|\langle \mathbf{x}_2|) |\Psi\rangle$ yields the probability density of finding the electron in $\mathbf{x}_1 = (\mathbf{r}_1\sigma_1)$ and the positron in $\mathbf{x}_2 = (\mathbf{r}_2\sigma_2)$:

$$|\Psi(\mathbf{x}_1, \mathbf{x}_2)|^2 \, d\mathbf{r}_1 d\mathbf{r}_2 = \begin{pmatrix} \text{probability of finding the electron with spin } \sigma_1 \\ \text{in volume element } d\mathbf{r}_1 \text{ around } \mathbf{r}_1 \text{ and the positron} \\ \text{with spin } \sigma_2 \text{ in volume element } d\mathbf{r}_2 \text{ around } \mathbf{r}_2 \end{pmatrix}.$$

Continuum formulation for N particles The generalization to N distinguishable particles is straightforward. The position–spin ket $|\mathbf{x}_1\rangle \ldots |\mathbf{x}_N\rangle$ describes the physical state in which the first particle is in $\mathbf{x}_1$, the second particle is in $|\mathbf{x}_2\rangle$, etc. These kets form an orthonormal basis with inner product

$$(\langle \mathbf{x}_1'| \ldots \langle \mathbf{x}_N'|) (|\mathbf{x}_1\rangle \ldots |\mathbf{x}_N\rangle) = \delta(\mathbf{x}_1' - \mathbf{x}_1) \ldots \delta(\mathbf{x}_N' - \mathbf{x}_N), \tag{1.14}$$

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and therefore the completeness relation reads

$$\int d\mathbf{x}_1 \dots d\mathbf{x}_N \; (\; |\mathbf{x}_1\rangle \dots |\mathbf{x}_N\rangle \;) \; (\; \langle \mathbf{x}_1| \dots \langle \mathbf{x}_N| \;) = \hat{\mathbb{1}}.$$

Operators Having discussed the Hilbert space for N distinguishable particles, we now consider the operators acting on the N-particle kets. We start with an example and consider again the electron–positron pair. Suppose that there is an electric field $\mathbf{E}(\mathbf{r}) = -\boldsymbol{\nabla}\phi(\mathbf{r})$ extending across all of space and that we are interested in measuring the total potential energy. This is an observable quantity and, hence, associated with it there exists an operator $\hat{\mathcal{H}}_{\text{pot}}$. By definition the eigenstates of this operator are the position–spin kets $|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle$ and the corresponding eigenvalues are $-\phi(\mathbf{r}_1) + \phi(\mathbf{r}_2)$, independent of the spin of the particles (in atomic units the charge of the electron is $q = -1$ and hence the charge of the positron is $q = +1$). The operator $\hat{\mathcal{H}}_{\text{pot}}$ is then the sum of the electrostatic potential operator acting on the first particle and doing nothing to the second particle and the electrostatic potential operator acting on the second particle and doing nothing to the first particle:

$$\hat{\mathcal{H}}_{\text{pot}} = -\phi(\hat{\boldsymbol{r}}) \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes \phi(\hat{\boldsymbol{r}}). \tag{1.15}$$

The symbol $\otimes$ denotes the *tensor product* of operators acting on different particles:

$$\hat{\mathcal{H}}_{\text{pot}}|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle = -\phi(\hat{\boldsymbol{r}})|\mathbf{x}_1\rangle\hat{\mathbb{1}}|\mathbf{x}_2\rangle + \hat{\mathbb{1}}|\mathbf{x}_1\rangle\phi(\hat{\boldsymbol{r}})|\mathbf{x}_2\rangle = \big[-\phi(\mathbf{r}_1) + \phi(\mathbf{r}_2)\big]|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle.$$

The generalization of the potential energy operator to N particles of charge $q_1, \dots, q_N$ is rather voluminous

$$\hat{\mathcal{H}}_{\text{pot}} = q_1\phi(\hat{\boldsymbol{r}}) \otimes \underbrace{\hat{\mathbb{1}} \otimes \dots \otimes \hat{\mathbb{1}}}_{N-1 \text{ times}} + q_2\hat{\mathbb{1}} \otimes \phi(\hat{\boldsymbol{r}}) \otimes \underbrace{\dots \otimes \hat{\mathbb{1}}}_{N-2 \text{ times}} + \dots + q_N \underbrace{\hat{\mathbb{1}} \otimes \hat{\mathbb{1}} \otimes \dots}_{N-1 \text{ times}} \otimes \phi(\hat{\boldsymbol{r}}), \tag{1.16}$$

and it is typically shortened to

$$\hat{\mathcal{H}}_{\text{pot}} = \sum_{j=1}^{N} q_j \phi(\hat{\boldsymbol{r}}_j),$$

where $\hat{\boldsymbol{r}}_j$ is the position operator acting on the jth particle and doing nothing to the other particles. Similarly, the noninteracting part of the Hamiltonian of N particles is typically written as

$$\hat{\mathcal{H}}_0 = \sum_{j=1}^{N} \hat{h}_j = \sum_{j=1}^{N} h(\hat{\boldsymbol{r}}_j, \hat{\boldsymbol{p}}_j, \hat{\boldsymbol{\mathcal{S}}}_j), \tag{1.17}$$

while the interaction part is written as

$$\hat{\mathcal{H}}_{\text{int}} = \frac{1}{2} \sum_{i \neq j}^{N} v(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{r}}_j), \tag{1.18}$$

with $v(\mathbf{r}_1, \mathbf{r}_2)$ the interparticle interaction. We observe that these operators depend explicitly on the number of particles and are therefore difficult to manipulate in problems where the

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number of particles can fluctuate, such as in systems at finite temperature. As we see later in this chapter, another disadvantage is that the evaluation of their action on kets describing *identical* particles is very lengthy. Fortunately, an incredible simplification occurs for identical particles and the expressions for operators and kets become much lighter and easier to manipulate. To appreciate this simplification, however, we first have to understand how the quantum-mechanical formulation changes when the particles are identical.

1.3 Quantum Mechanics of Many Identical Particles

Two particles are called *identical particles* or *indistinguishable particles* if they have the same internal properties (i.e., the same mass, charge, spin etc.). For example, two electrons are two identical particles. To understand the qualitative difference between distinguishable and identical particles, let us perform the coincidence experiment of the previous section for two electrons both with spin projection $1/2$ and again in one dimension.

Discrete formulation for two particles At every point $x_n = n\Delta$ we put a spin-polarized electron detector and since the particles are identical we need only one kind of detector. If the detectors in x_n and x_m click at the same time, then we can be sure that just after this time there is one electron around x_n and another electron around x_m. Let us denote by $|nm\rangle$ with $n \geq m$ the ket describing the physical state in which the two electrons collapse after measurement. For mathematical convenience we also define the ket $|nm\rangle$ with $n \leq m$ as the ket describing the *same physical state* as $|mn\rangle$. Notice the different notation with respect to the previous section, where we have used the ket $|n\rangle|m\rangle$ to describe the first particle around x_n and the second particle around x_m. In the case of the electron–positron pair we could make the positron-click louder than the electron-click and hence distinguish the state $|n\rangle|m\rangle$ from the state $|m\rangle|n\rangle$. However, in this case we only have electron detectors and it is impossible to distinguish which electron has made a given detector click.

In Section 1.1 we observed that the normalized ket of a physical state is uniquely defined up to a phase factor. For our mathematical description to make sense, we then must impose that

$$|nm\rangle = e^{\mathrm{i}\alpha}|mn\rangle \qquad \text{for all } n, m.$$

Using the above relation twice, we find that $e^{2\mathrm{i}\alpha} = 1$, or equivalently $e^{\mathrm{i}\alpha} = \pm 1$. Consequently, the ket

$$|nm\rangle = \pm|mn\rangle \tag{1.19}$$

is either symmetric or antisymmetric under the interchange of the electron positions. This is a fundamental property of nature: All particles can be grouped in two main classes. Particles described by a symmetric ket are called *bosons*, while those described by an antisymmetric ket are called *fermions*. The electrons of our example are fermions. Here and in the rest of the book the upper sign always refers to bosons and the lower sign to fermions. In the case of fermions (1.19) implies $|nn\rangle = -|nn\rangle$ and hence $|nn\rangle$ must be the *null ket* $|\emptyset\rangle$ – that is, it is not possible to create two fermions in the same position and with the same spin. This peculiarity of fermions is known as the *Pauli exclusion principle*.

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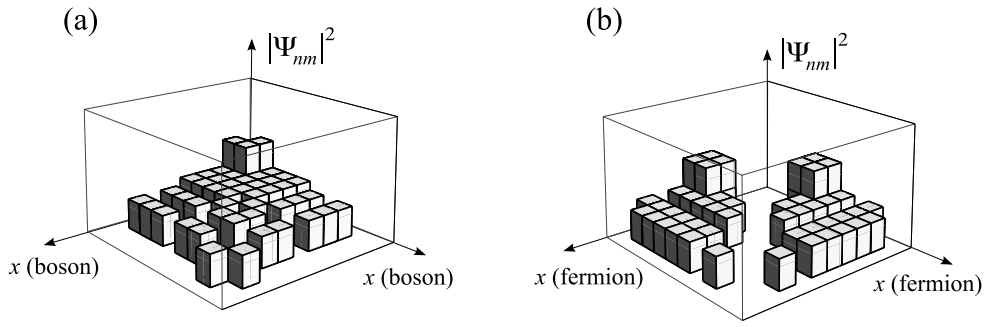

Figure 1.3 Histogram of the normalized number of simultaneous clicks of the detector in $x_n = n\Delta$ and in $x_m = m\Delta$ for (a) two bosons and (b) two fermions. The height of the parallelepipeds corresponds to the probabilities $|\Psi_{nm}|^2$.

If we now repeat the coincidence experiment $N \gg 1$ times, count the number of times that the detectors click simultaneously in x_n and x_m, and divide the result by N we can draw the histograms of Fig. 1.3 for bosons and fermions. The probability is symmetric under the interchange $n \leftrightarrow m$ due to property (1.19). The fermions are easily recognizable since the probability of finding them in the same place is zero.

In this book we learn how to deal with systems of many identical particles, such as molecules or solids, and therefore we do not always repeat that the particles are identical: by *particles* we mean *identical particles* unless otherwise stated. Unlike the case of the electron–positron pair, the probability of measuring a particle in $x_{n'}$ and the other in $x_{m'}$ just after the detectors in x_n and x_m have simultaneously clicked is zero unless $n = n'$ and $m = m'$ or $n = m'$ and $m = n'$, and hence

$$\langle n'm'|nm\rangle = c_1\delta_{n'n}\delta_{m'm} + c_2\delta_{m'n}\delta_{n'm}. \tag{1.20}$$

To fix the constants c_1 and c_2 we observe that

$$\langle n'm'|nm\rangle = \pm\langle n'm'|mn\rangle = \pm c_1\delta_{n'm}\delta_{m'n} \pm c_2\delta_{m'm}\delta_{n'n},$$

from which it follows that $c_1 = \pm c_2$. Furthermore, since the kets are normalized we must have for all $n \neq m$

$$1 = \langle nm|nm\rangle = c_1.$$

For $n = m$ the ket $|nn\rangle$ exists only for bosons, and one finds $\langle nn|nn\rangle = 2c_1$. It is therefore more convenient to work with a nonnormalized ket $|nn\rangle$ so that $c_1 = 1$ in all cases. We choose the normalization of the bosonic ket $|nn\rangle$ to be 2:

$$\langle nn|nn\rangle = 2. \tag{1.21}$$

Putting everything together we can rewrite the inner product (1.20) as

$$\langle n'm'|nm\rangle = \delta_{n'n}\delta_{m'm} \pm \delta_{m'n}\delta_{n'm}.$$

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The inner product for the fermionic ket $|nn\rangle$ is automatically zero, in agreement with the fact that $|nn\rangle = |\emptyset\rangle$.

Let us now come to the completeness relation in the Hilbert space of two particles. Since $|nm\rangle = \pm|mn\rangle$, a basis in this space is given by the set $\{|nm\rangle\}$ with $n \geq m$. In other words the basis comprises only *inequivalent* configurations, meaning configurations not related by a permutation of the coordinates. The elements of this set are orthogonal and normalized except for the bosonic ket $|nn\rangle$, whose normalization is 2. Therefore, the completeness relation reads

$$\sum_{n>m} |nm\rangle\langle nm| + \frac{1}{2}\sum_{n} |nn\rangle\langle nn| = \hat{\mathbb{1}},$$

where the second sum does not contribute in the fermionic case. We can rewrite the completeness relation as an unrestricted sum over all n and m using the (anti)symmetry property (1.19). The resulting expression is

$$\frac{1}{2}\sum_{nm} |nm\rangle\langle nm| = \hat{\mathbb{1}},$$

which is much more elegant. The completeness relation can be used to expand any other ket in the same Hilbert space:

$$|\Psi\rangle = \hat{\mathbb{1}}|\Psi\rangle = \frac{1}{2}\sum_{nm} |nm\rangle\langle nm|\Psi\rangle, \tag{1.22}$$

and if $|\Psi\rangle$ is normalized then the square moduli of the coefficients of the expansion $\Psi_{nm} \equiv \langle nm|\Psi\rangle$ have the standard probabilistic interpretation:

$$|\Psi_{nm}|^2 = \begin{pmatrix} \text{probability of finding one particle in volume} \\ \text{element } \Delta \text{ around } x_n \text{ and the other particle} \\ \text{in volume element } \Delta \text{ around } x_m \end{pmatrix}$$

for all $n \neq m$. For $n = m$ we must remember that the normalization of the ket $|nn\rangle$ is 2 and therefore $|\Psi_{nn}|^2$ gives *twice* the probability of finding two particles in the same place (since the proper normalized ket is $|nn\rangle/\sqrt{2}$). Consequently,

$$\frac{|\Psi_{nn}|^2}{2} = \begin{pmatrix} \text{probability of finding two particles in} \\ \text{volume element } \Delta \text{ around } x_n \end{pmatrix}.$$

Continuum formulation for two particles We can now refine the experiment by putting the detectors closer and closer. The continuum limit works exactly in the same manner as in the previous two sections. We rewrite the expansion (1.22) as

$$|\Psi\rangle = \frac{1}{2}\,\Delta^2 \sum_{nm} \frac{|nm\rangle}{\Delta}\frac{\Psi_{nm}}{\Delta}, \tag{1.23}$$

and define the continuous wavefunction $\Psi(x_n, x_m)$ and the continuous ket $|x_n x_m\rangle$ according to

$$\Psi(x_n, x_m) = \lim_{\Delta\to 0} \frac{\Psi_{nm}}{\Delta}, \qquad |x_n x_m\rangle = \lim_{\Delta\to 0} \frac{|nm\rangle}{\Delta}.$$

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The expansion (1.23) can then be seen as the Riemann sum of $\Psi(x_n, x_m)|x_n x_m\rangle$ and in the limit $\Delta \to 0$ the sum becomes the integral

$$|\Psi\rangle = \frac{1}{2}\int dx dx' \; \Psi(x, x')|xx'\rangle.$$

We can also derive the continuous representation of the completeness relation and the continuous representation of the inner product between two basis kets. We have

$$\lim_{\Delta\to 0} \; \frac{1}{2}\Delta^2 \sum_{nm} \frac{|nm\rangle}{\Delta}\frac{\langle nm|}{\Delta} = \frac{1}{2}\int dx dx' |xx'\rangle\langle xx'| = \hat{\mathbb{1}} \tag{1.24}$$

and

$$\begin{aligned}\lim_{\Delta\to 0} \; \frac{\langle n'm'|nm\rangle}{\Delta^2} &= \langle x_{n'} x_{m'}|x_n x_m\rangle \\ &= \delta(x_{n'} - x_n)\delta(x_{m'} - x_m) \pm \delta(x_{m'} - x_n)\delta(x_{n'} - x_m).\end{aligned} \tag{1.25}$$

The generalization to higher dimensions and to particles with different spin projections is straightforward. We define the position–spin ket $|\mathbf{x}_1\mathbf{x}_2\rangle$ as the ket of the physical state in which the particles collapse after the simultaneous clicking of a spin-polarized detector for particles of spin projection σ_1 placed in $\mathbf{r}_1$ and a spin-polarized detector for particles of spin projection σ_2 placed in $\mathbf{r}_2$. The set of inequivalent configurations $|\mathbf{x}_1\mathbf{x}_2\rangle$ forms a basis of the Hilbert space of two identical particles. In the following we refer to this space as $\mathbb{H}_2$. In analogy with (1.25) the continuous kets have inner product

$$\begin{aligned}\langle \mathbf{x}_1'\mathbf{x}_2'|\mathbf{x}_1\mathbf{x}_2\rangle &= \delta(\mathbf{x}_1' - \mathbf{x}_1)\delta(\mathbf{x}_2' - \mathbf{x}_2) \pm \delta(\mathbf{x}_1' - \mathbf{x}_2)\delta(\mathbf{x}_2' - \mathbf{x}_1) \\ &= \sum_P (\pm)^P \delta(\mathbf{x}_1' - \mathbf{x}_{P(1)})\delta(\mathbf{x}_2' - \mathbf{x}_{P(2)}),\end{aligned} \tag{1.26}$$

where the upper/lower sign refers to bosons/fermions. The second line of this equation is an equivalent way of rewriting the (anti)symmetric product of δ-functions. The sum runs over the permutations P of $(1, 2)$, which are the identity permutation $(P(1), P(2)) = (1, 2)$ and the interchange $(P(1), P(2)) = (2, 1)$. The quantity $(\pm)^P$ is equal to $+1$ if the permutation requires an even number of interchanges and ± 1 if the permutation requires an odd number of interchanges. In the fermionic case, all position–spin kets have the same norm since (1.26) implies

$$\langle \mathbf{x}_1\mathbf{x}_2|\mathbf{x}_1\mathbf{x}_2\rangle = \delta(0)^2 \qquad \text{for fermions.}$$

Due to the possibility in the bosonic case that two coordinates are identical, the norms of the position–spin kets are instead not all the same since

$$\langle \mathbf{x}_1\mathbf{x}_2|\mathbf{x}_1\mathbf{x}_2\rangle = \delta(0)^2 \times \begin{cases} 1 & \text{if } \mathbf{x}_1 \neq \mathbf{x}_2 \\ 2 & \text{if } \mathbf{x}_1 = \mathbf{x}_2 \end{cases} \qquad \text{for bosons,}$$

in agreement with (1.21).

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In complete analogy with (1.24) we can also write the completeness relation according to

$$\frac{1}{2}\int d\mathbf{x}_1 d\mathbf{x}_2 |\mathbf{x}_1\mathbf{x}_2\rangle\langle\mathbf{x}_1\mathbf{x}_2| = \hat{\mathbb{1}}. \tag{1.27}$$

Then, any ket $|\Psi\rangle \in \mathbb{H}_2$ can be expanded in the position–spin basis as

$$|\Psi\rangle = \hat{\mathbb{1}}|\Psi\rangle = \frac{1}{2}\int d\mathbf{x}_1 d\mathbf{x}_2 \, |\mathbf{x}_1\mathbf{x}_2\rangle \underbrace{\langle\mathbf{x}_1\mathbf{x}_2|\Psi\rangle}_{\Psi(\mathbf{x}_1,\mathbf{x}_2)}. \tag{1.28}$$

If $|\Psi\rangle$ is normalized, we can give a probability interpretation to the square modulus of the wavefunction $\Psi(\mathbf{x}_1, \mathbf{x}_2)$:

$$|\Psi(\mathbf{x}_1,\mathbf{x}_2)|^2 d\mathbf{r}_1 d\mathbf{r}_2 = \begin{pmatrix} \text{probability of finding one particle with spin } \sigma_1 \text{ in} \\ \text{volume element } d\mathbf{r}_1 \text{ around } \mathbf{r}_1 \text{ and the other particle with} \\ \text{spin } \sigma_2 \text{ in volume element } d\mathbf{r}_2 \text{ around a } \textit{different} \text{ point } \mathbf{r}_2 \end{pmatrix}.$$

However, in the case $\mathbf{x}_1 = \mathbf{x}_2$ the above formula needs to be replaced by

$$\frac{|\Psi(\mathbf{x}_1,\mathbf{x}_1)|^2}{2} d\mathbf{r}_1 d\mathbf{r}_2 = \begin{pmatrix} \text{probability of finding one particle with spin } \sigma_1 \text{ in} \\ \text{volume element } d\mathbf{r}_1 \text{ around } \mathbf{r}_1 \text{ and the other particle} \\ \text{with the } \textit{same} \text{ spin in volume element } d\mathbf{r}_2 \text{ around} \\ \text{the } \textit{same} \text{ point } \mathbf{r}_1 \end{pmatrix},$$

due to the different normalization of the diagonal kets. We stress again that the above probability interpretation follows from the normalization $\langle\Psi|\Psi\rangle = 1$, which in the continuum case reads [see (1.28)]

$$1 = \frac{1}{2}\int d\mathbf{x}_1 d\mathbf{x}_2 \, |\Psi(\mathbf{x}_1,\mathbf{x}_2)|^2.$$

Continuum formulation for N particles It should now be clear how to extend the above relations to the case of N identical particles. We say that if the detector for a particle of spin projection σ_1 placed in $\mathbf{r}_1$, the detector for a particle of spin projection σ_2 placed in $\mathbf{r}_2$, etc. all click at the same time then the N-particle state collapses in the position–spin ket $|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$. Due to the nature of identical particles this ket must have the symmetry property (as usual, upper/lower sign refers to bosons/fermions):

$$\boxed{|\mathbf{x}_{P(1)} \ldots \mathbf{x}_{P(N)}\rangle = (\pm)^P |\mathbf{x}_1 \ldots \mathbf{x}_N\rangle} \tag{1.29}$$

where P is a permutation of the labels $(1, \ldots, N)$, and $(\pm)^P = 1$ for even permutations and ± 1 for odd permutations (thus for bosons is always 1). A permutation is even/odd if the number of interchanges is even/odd.[3] Therefore, given the ket $|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$ with all different coordinates there are $N!$ equivalent configurations that represent the same physical state. More generally, if the ket $|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$ has m_1 coordinates equal to $\mathbf{y}_1$, m_2 coordinates equal to $\mathbf{y}_2 \neq \mathbf{y}_1$, …, m_M coordinates equal to $\mathbf{y}_M \neq \mathbf{y}_1, \ldots, \mathbf{y}_{M-1}$, with $m_1 + \ldots + m_M = N$,

[3] The reader can learn more on how to calculate the sign of a permutation in Appendix B.

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then the number of equivalent configurations is $N!/(m_1!\dots m_M!)$. In the fermionic case, if two or more coordinates are the same then the ket $|\mathbf{x}_1\dots\mathbf{x}_N\rangle$ is the null ket $|\emptyset\rangle$. The set of position–spin kets corresponding to inequivalent configurations form a basis in the Hilbert space of N identical particles; we refer to this space as $\mathbb{H}_N$.

The inner product between two position–spin kets is

$$\langle\mathbf{x}'_1\dots\mathbf{x}'_N|\mathbf{x}_1\dots\mathbf{x}_N\rangle = \sum_P c_P \prod_{j=1}^N \delta(\mathbf{x}'_j - \mathbf{x}_{P(j)}),$$

where the c_Ps are numbers depending on the permutation P. As in the two-particle case, the (anti)symmetry (1.29) of the position–spin kets requires that $c_P = c\,(\pm)^P$, and the normalization of $|\mathbf{x}_1\dots\mathbf{x}_N\rangle$ with all *different* coordinates fixes the constant $c = 1$. Hence,

$$\boxed{\langle\mathbf{x}'_1\dots\mathbf{x}'_N|\mathbf{x}_1\dots\mathbf{x}_N\rangle = \sum_P (\pm)^P \prod_{j=1}^N \delta(\mathbf{x}'_j - \mathbf{x}_{P(j)})} \tag{1.30}$$

This is the familiar expression for the permanent/determinant $|A\,|_\pm$ of a $N\times N$ matrix A (see Appendix B):

$$|A\,|_\pm \equiv \sum_P (\pm)^P A_{1P(1)}\dots A_{NP(N)}.$$

Choosing the matrix elements of A to be $A_{ij} = \delta(\mathbf{x}'_i - \mathbf{x}_j)$, we can rewrite (1.30) as

$$\langle\mathbf{x}'_1\dots\mathbf{x}'_N|\mathbf{x}_1\dots\mathbf{x}_N\rangle = \begin{vmatrix} \delta(\mathbf{x}'_1-\mathbf{x}_1) & \dots & \delta(\mathbf{x}'_1-\mathbf{x}_N) \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \delta(\mathbf{x}'_N-\mathbf{x}_1) & \dots & \delta(\mathbf{x}'_N-\mathbf{x}_N) \end{vmatrix}_\pm . \tag{1.31}$$

As in the two-particle case, these formulas are so elegant because we take the bosonic kets at equal coordinates with a slightly different normalization. Consider N bosons in M *different* coordinates of which m_1 have coordinate $\mathbf{y}_1$, …, m_M have coordinate $\mathbf{y}_M$ (hence $m_1+\ldots+m_M = N$). Then the norm is given by

$$\langle\overbrace{\mathbf{y}_1\dots\mathbf{y}_1}^{m_1}\dots\overbrace{\mathbf{y}_M\dots\mathbf{y}_M}^{m_M}|\overbrace{\mathbf{y}_1\dots\mathbf{y}_1}^{m_1}\dots\overbrace{\mathbf{y}_M\dots\mathbf{y}_M}^{m_M}\rangle = \delta(0)^N m_1!m_2!\dots m_M!\,,$$

as follows directly from (1.30).[4] In the case of fermions, instead, all position–spin kets have norm $\delta(0)^N$ since it is not possible for two or more fermions to have the same coordinate.

Given the norm of the position–spin kets, the completeness relation for N particles is a straightforward generalization of (1.27) and reads

$$\boxed{\frac{1}{N!}\int d\mathbf{x}_1\dots d\mathbf{x}_N\;|\mathbf{x}_1\dots\mathbf{x}_N\rangle\langle\mathbf{x}_1\dots\mathbf{x}_N| = \hat{\mathbb{1}}} \tag{1.32}$$

[4] According to (1.29), the order of the arguments in the inner product does not matter.

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Therefore the expansion of a ket $|\Psi\rangle \in \mathbb{H}_N$ can be written as

$$|\Psi\rangle = \hat{\mathbb{1}}|\Psi\rangle = \frac{1}{N!}\int d\mathbf{x}_1 \dots d\mathbf{x}_N |\mathbf{x}_1 \dots \mathbf{x}_N\rangle \underbrace{\langle \mathbf{x}_1 \dots \mathbf{x}_N|\Psi\rangle}_{\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N)},$$

which generalizes the expansion (1.28) to the case of N particles. The wavefunction $\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)$ is totally symmetric for bosons and totally antisymmetric for fermions due to (1.29). If $|\Psi\rangle$ is normalized then the normalization of the wavefunction reads

$$1 = \langle\Psi|\Psi\rangle = \frac{1}{N!}\int d\mathbf{x}_1 \dots d\mathbf{x}_N |\ \Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)|^2. \tag{1.33}$$

The probabilistic interpretation of the square modulus of the wavefunction can be extracted using the same line of reasoning as for the two-particle case:

$$\frac{|\Psi(\overbrace{\mathbf{y}_1 \dots \mathbf{y}_1}^{m_1} \dots \overbrace{\mathbf{y}_M \dots \mathbf{y}_M}^{m_M})|^2}{m_1! \dots m_M!} \prod_{j=1}^{M} d\mathbf{R}_j = \begin{pmatrix} \text{probability of finding} \\ m_1 \text{ particles in } d\mathbf{R}_1 \text{ around } \mathbf{y}_1 \\ \vdots \\ m_M \text{ particles in } d\mathbf{R}_M \text{ around } \mathbf{y}_M \end{pmatrix}, \tag{1.34}$$

where $d\mathbf{R}_j$ is the product of volume elements,

$$d\mathbf{R}_j \equiv \prod_{i=m_1+\dots+m_{j-1}+1}^{m_1+\dots+m_j} d\mathbf{r}_i.$$

When all coordinates are different, (1.34) tells us that the quantity $|\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)|^2 d\mathbf{r}_1 \dots d\mathbf{r}_N$ is the probability of finding one particle in volume element $d\mathbf{r}_1$ around $\mathbf{x}_1$, ..., and one particle in volume element $d\mathbf{r}_N$ around $\mathbf{x}_N$. We could have absorbed the prefactor $1/N!$ in (1.33) in the wavefunction (as is commonly done) but then we could not interpret the quantity $|\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)|^2 d\mathbf{r}_1 \dots d\mathbf{r}_N$ as the right-hand side (r.h.s.) of (1.34) since this would amount to regarding equivalent configurations as distinguishable and consequently the probability would be overestimated by a factor of $N!$.

The reader might wonder why we have been so punctilious about the possibility of having more than one boson with the same position–spin coordinate, since these configurations are of zero measure in the space of all configurations. However, such configurations are the physically most relevant in bosonic systems at low temperature. Indeed, bosons can condense in states in which certain (continuum) quantum numbers are *macroscopically* occupied and hence have a finite probability. A common example is the zero momentum state of a free boson gas in three dimensions.

First quantization We close this section by illustrating a practical way to construct the N-particle position–spin kets using the N-particle position–spin kets of distinguishable particles. The procedure simply consists in forming (anti)symmetrized products of one-particle position–spin kets. For instance, we have for the case of two particles

$$|\mathbf{x}_1\mathbf{x}_2\rangle = \frac{|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle \pm |\mathbf{x}_2\rangle|\mathbf{x}_1\rangle}{\sqrt{2}}, \tag{1.35}$$

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and more generally for N particles

$$|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = \frac{1}{\sqrt{N!}} \sum_P (\pm)^P |\mathbf{x}_{P(1)}\rangle \dots |\mathbf{x}_{P(N)}\rangle. \tag{1.36}$$

Using the inner product (1.14), one can check directly that these states have inner product (1.30). We refer to the above representation of the position–spin kets as kets in *first quantization* since it is the representation usually found in basic quantum mechanics books. Using (1.36) we could proceed to calculate matrix elements of operators such as the potential energy, total energy, spin, angular momentum, density, etc. However, this involves rather cumbersome expressions with a large number of terms differing only in the sign and the order of the coordinates. In the next section we describe a formalism, known as *second quantization*, that makes it easy to do such calculations efficiently, as the position–spin ket is represented by a *single* ket rather than by $N!$ products of one-particle kets as in (1.36). As we see, the merits of second quantization are the compactness of the expressions and an enormous simplification in the calculation of the action of operators over states in $\mathbb{H}_N$. This formalism further treats systems with different numbers of identical particles on the same footing and it is therefore well suited to study of ionization processes, transport phenomena, and finite temperature effects within the grand canonical ensemble of quantum statistical physics.

1.4 Field Operators

The advantage of the bra-and-ket notation invented by Dirac is twofold. First of all, it provides a geometric interpretation of the physical states in Hilbert space as abstract kets independent of the basis in which they are expanded. For example, it does not matter whether we expand $|\Psi\rangle$ in terms of the position–spin kets or momentum–spin kets; $|\Psi\rangle$ remains the same although the expansion coefficients in the two bases are different. The second advantage is that the abstract kets can be systematically generated by repeated applications of a *creation operator* on the empty or zero-particle state. This approach forms the basis of an elegant formalism known as *second quantization*, which we describe in detail in this section.

Fock space To deal with arbitrary many identical particles we define a collection $\mathbb{F}$ of Hilbert spaces, also known as *Fock space*, according to

$$\mathbb{F} = \{\mathbb{H}_0, \mathbb{H}_1, \dots, \mathbb{H}_N, \dots\},$$

with $\mathbb{H}_N$ the Hilbert space for N identical particles. An arbitrary element of the Fock space is a ket that can be written as

$$|\Psi\rangle = \sum_{N=0}^{\infty} c_N |\Psi_N\rangle, \tag{1.37}$$

where $|\Psi_N\rangle$ belongs to $\mathbb{H}_N$. The inner product between the ket (1.37) and another element in the Fock space,

$$|\chi\rangle = \sum_{N=0}^{\infty} d_N |\chi_N\rangle,$$

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is defined as

$$\langle\chi|\Psi\rangle \equiv \sum_{N=0}^{\infty} d_N^* c_N \langle\chi_N|\Psi_N\rangle,$$

where $\langle\chi_N|\Psi_N\rangle$ is the inner product in $\mathbb{H}_N$. This definition is dictated by common sense: The probability of having $M \neq N$ particles in an N-particle ket is zero and therefore kets with a different number of particles are orthogonal (i.e., have zero overlap).

The Hilbert space $\mathbb{H}_0$ is the space with *zero* particles. Since an empty system has no degrees of freedom, $\mathbb{H}_0$ is a one-dimensional space and we denote by $|0\rangle$ the only normalized ket in $\mathbb{H}_0$,

$$\langle 0|0\rangle = 1.$$

According to the expansion (1.37), the ket $|0\rangle$ has all $c_N = 0$ except for c_0. This state should not be confused with the null ket $|\emptyset\rangle$, which is defined as the state in Fock space with all $c_N = 0$ and, therefore, is *not* a physical state. The *empty ket* $|0\rangle$ is a physical state; indeed the normalization $\langle 0|0\rangle = 1$ means that the probability of finding nothing in an empty space is 1.

Field operators The goal of this section is to find a clever way to construct a basis for each Hilbert space $\mathbb{H}_1$, $\mathbb{H}_2, \ldots$. To accomplish this goal the central idea of the second quantization formalism is to define a *field operator* $\hat{\psi}^\dagger(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{r}\sigma)$ that generates the position–spin kets by repeated action on the empty ket:

$$\begin{aligned} |\mathbf{x}_1\rangle &= \hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\ |\mathbf{x}_1\mathbf{x}_2\rangle &= \hat{\psi}^\dagger(\mathbf{x}_2)|\mathbf{x}_1\rangle = \hat{\psi}^\dagger(\mathbf{x}_2)\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\ |\mathbf{x}_1 \ldots \mathbf{x}_N\rangle &= \hat{\psi}^\dagger(\mathbf{x}_N)|\mathbf{x}_1 \ldots \mathbf{x}_{N-1}\rangle = \hat{\psi}^\dagger(\mathbf{x}_N)\ldots\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \end{aligned} \tag{1.38}$$

Since an operator is uniquely defined from its action on a complete set of states in the Hilbert space (the Fock space in our case), the above relations *define* the field operator $\hat{\psi}^\dagger(\mathbf{x})$ for all $\mathbf{x}$. The field operator $\hat{\psi}^\dagger(\mathbf{x})$ transforms a ket of $\mathbb{H}_N$ into a ket of $\mathbb{H}_{N+1}$ for all N, see Fig. 1.4(a). We may say that the field operator $\hat{\psi}^\dagger(\mathbf{x})$ creates a particle in $\mathbf{x}$ and it is therefore called the *creation operator*. Since the position–spin kets change a plus or minus sign under interchange of any two particles, it follows that

$$\begin{aligned} \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle &= |\mathbf{x}_1 \ldots \mathbf{x}_N\, \mathbf{y}\, \mathbf{x}\rangle = \pm|\mathbf{x}_1 \ldots \mathbf{x}_N\, \mathbf{x}\, \mathbf{y}\rangle \\ &= \pm\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{x})|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle, \end{aligned}$$

where we recall that the upper sign in $\pm$ refers to bosons and the lower sign to fermions. This identity is true for all $\mathbf{x}_1, \ldots, \mathbf{x}_N$ and for all N (i.e., for all states in $\mathbb{F}$), and hence

$$\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y}) = \pm\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{x}).$$

If we define the (anti)commutator between two generic operators $\hat{A}$ and $\hat{B}$ according to

$$\left[\hat{A}, \hat{B}\right]_\mp = \hat{A}\hat{B} \mp \hat{B}\hat{A},$$

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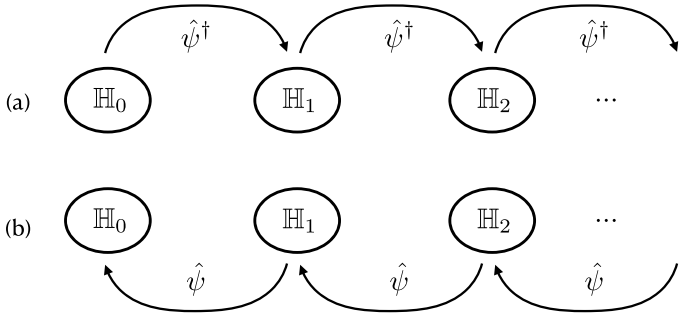

Figure 1.4 Schematic action of the creation operator $\hat{\psi}^\dagger$ in (a) and of the annihilation operator $\hat{\psi}$ in (b).

we can rewrite the above relation as

$$\boxed{\left[\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_\mp = 0} \tag{1.39}$$

Corresponding to the operator $\hat{\psi}^\dagger(\mathbf{x})$ there is the adjoint operator $\hat{\psi}(\mathbf{x})$ [or equivalently $\hat{\psi}^\dagger(\mathbf{x})$ is the adjoint of $\hat{\psi}(\mathbf{x})$]. Let us remind the reader about the definition of adjoint operators. An operator $\hat{O}^\dagger$ with the superscript "†" (read *dagger*) is the adjoint of the operator $\hat{O}$ if

$$\langle\chi|\hat{O}|\Psi\rangle = \langle\Psi|\hat{O}^\dagger|\chi\rangle^*$$

for all $|\chi\rangle$ and $|\Psi\rangle$, which implies $(\hat{O}^\dagger)^\dagger = \hat{O}$. In particular, when $\hat{O} = \hat{\psi}(\mathbf{x})$ we have

$$\langle\chi|\hat{\psi}(\mathbf{x})|\Psi\rangle = \langle\Psi|\hat{\psi}^\dagger(\mathbf{x})|\chi\rangle^*.$$

Since for any $|\Psi\rangle \in \mathbb{H}_{N+1}$ the quantity $\langle\Psi|\hat{\psi}^\dagger(\mathbf{x})|\chi\rangle$ is zero for all $|\chi\rangle$ with no components in $\mathbb{H}_N$, the above equation implies that $\hat{\psi}(\mathbf{x})|\Psi\rangle \in \mathbb{H}_N$ – that is, the operator $\hat{\psi}(\mathbf{x})$ maps the elements of $\mathbb{H}_{N+1}$ into elements of $\mathbb{H}_N$, see Fig. 1.4(b). Thus, whereas the operator $\hat{\psi}^\dagger(\mathbf{x})$ adds a particle, its adjoint operator $\hat{\psi}(\mathbf{x})$ removes a particle and, for this reason, is called the *annihilation operator*. Below we study its properties and how it acts on the position–spin kets.

By taking the adjoint of the identity (1.39), we immediately obtain the (anti)commutation relation

$$\boxed{\left[\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y})\right]_\mp = 0} \tag{1.40}$$

The action of $\hat{\psi}(\mathbf{x})$ on any state can be deduced from its definition as the adjoint of $\hat{\psi}^\dagger(\mathbf{x})$ together with the inner product (1.31) between the position–spin kets. Let us illustrate this first for the action on the empty ket $|0\rangle$. For any $|\Psi\rangle \in \mathbb{F}$,

$$\langle\Psi|\hat{\psi}(\mathbf{x})|0\rangle = \langle 0|\hat{\psi}^\dagger(\mathbf{x})|\Psi\rangle^* = 0,$$

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since $\hat{\psi}^\dagger(\mathbf{x})|\Psi\rangle$ contains at least one particle and is therefore orthogonal to $|0\rangle$. We conclude that $\hat{\psi}(\mathbf{x})|0\rangle$ is orthogonal to all $|\Psi\rangle$ in $\mathbb{F}$ and hence it must be equal to the null ket

$$\hat{\psi}(\mathbf{x})|0\rangle = |\emptyset\rangle. \tag{1.41}$$

The action of $\hat{\psi}(\mathbf{x})$ on the one-particle ket $|\mathbf{y}\rangle$ can be inferred from (1.30) and (1.38); we have

$$\delta(\mathbf{y}-\mathbf{x}) = \langle \mathbf{y}|\mathbf{x}\rangle = \langle \mathbf{y}|\hat{\psi}^\dagger(\mathbf{x})|0\rangle = \langle 0|\hat{\psi}(\mathbf{x})|\mathbf{y}\rangle^*.$$

Since $\hat{\psi}(\mathbf{x})|\mathbf{y}\rangle \in \mathbb{H}_0$, it follows that

$$\hat{\psi}(\mathbf{x})|\mathbf{y}\rangle = \delta(\mathbf{y}-\mathbf{x})|0\rangle. \tag{1.42}$$

We see from this relation that the operator $\hat{\psi}(\mathbf{x})$ removes a particle from the state $|\mathbf{y}\rangle$ when $\mathbf{x}=\mathbf{y}$ and otherwise yields zero.

The derivation of the action of $\hat{\psi}(\mathbf{x})$ on the empty ket and on the one-particle ket was rather elementary. Let us now derive the action of $\hat{\psi}(\mathbf{x})$ on the general N-particle ket $|\mathbf{y}_1 \ldots \mathbf{y}_N\rangle$. For this purpose we consider the matrix element

$$\langle \mathbf{x}_1 \ldots \mathbf{x}_{N-1}|\hat{\psi}(\mathbf{x}_N)|\mathbf{y}_1 \ldots \mathbf{y}_N\rangle = \langle \mathbf{x}_1 \ldots \mathbf{x}_N|\mathbf{y}_1 \ldots \mathbf{y}_N\rangle. \tag{1.43}$$

The overlap on the r.h.s. is given in (1.31); expanding the permanent/determinant along row N (see Appendix B), we get

$$\begin{aligned}&\langle \mathbf{x}_1 \ldots \mathbf{x}_{N-1}|\hat{\psi}(\mathbf{x}_N)|\mathbf{y}_1 \ldots \mathbf{y}_N\rangle \\ &\quad = \sum_{k=1}^{N} (\pm)^{N+k}\delta(\mathbf{x}_N-\mathbf{y}_k)\langle \mathbf{x}_1 \ldots \mathbf{x}_{N-1}|\mathbf{y}_1 \ldots \mathbf{y}_{k-1}\mathbf{y}_{k+1}\ldots \mathbf{y}_N\rangle.\end{aligned}$$

This expression is valid for any $|\mathbf{x}_1 \ldots \mathbf{x}_{N-1}\rangle$ and since $\hat{\psi}(\mathbf{x})$ maps from $\mathbb{H}_N$ only to $\mathbb{H}_{N-1}$, we conclude that

$$\boxed{\hat{\psi}(\mathbf{x})|\mathbf{y}_1 \ldots \mathbf{y}_N\rangle = \sum_{k=1}^{N} (\pm)^{N+k}\delta(\mathbf{x}-\mathbf{y}_k)\ |\mathbf{y}_1 \ldots \mathbf{y}_{k-1}\mathbf{y}_{k+1}\ldots \mathbf{y}_N\rangle} \tag{1.44}$$

We have just derived an important equation for the action of the annihilation operator on a position–spin ket. It correctly reduces to (1.42) when $N=1$ and for $N>1$ yields, for example,

$$\begin{aligned}\hat{\psi}(\mathbf{x})|\mathbf{y}_1\mathbf{y}_2\rangle &= \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\rangle \pm \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\rangle, \\ \hat{\psi}(\mathbf{x})|\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle &= \delta(\mathbf{x}-\mathbf{y}_3)|\mathbf{y}_1\mathbf{y}_2\rangle \pm \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\mathbf{y}_3\rangle + \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\mathbf{y}_3\rangle.\end{aligned}$$

So the annihilation operator removes subsequently a particle from every position–spin coordinate while keeping the final result totally symmetric or antisymmetric in all $\mathbf{y}$ variables by adjusting the signs of the prefactors.

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(Anti)commutation rule With the help of (1.44) we can derive a fundamental (anti)commutation relation between the annihilation and creation operators. Acting on both sides of (1.44) with $\hat{\psi}^\dagger(\mathbf{y})$ and denoting by $|R\rangle$ the ket on the r.h.s., we have

$$\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{x})|\mathbf{y}_1 \dots \mathbf{y}_N\rangle = \hat{\psi}^\dagger(\mathbf{y})|R\rangle. \tag{1.45}$$

Exchanging the order of the field operators in the left-hand side (l.h.s.) of the above identity and using (1.44), we find

$$\begin{aligned}\hat{\psi}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})|\mathbf{y}_1 \dots \mathbf{y}_N\rangle &= \hat{\psi}(\mathbf{x})|\mathbf{y}_1 \dots \mathbf{y}_N\mathbf{y}\rangle = \delta(\mathbf{x}-\mathbf{y})\,|\mathbf{y}_1 \dots \mathbf{y}_N\rangle \\ &\quad + \sum_{k=1}^{N}(\pm)^{N+1+k}\delta(\mathbf{x}-\mathbf{y}_k)\;|\mathbf{y}_1 \dots \mathbf{y}_{k-1}\mathbf{y}_{k+1} \dots \mathbf{y}_N\mathbf{y}\rangle \\ &= \delta(\mathbf{x}-\mathbf{y})\,|\mathbf{y}_1 \dots \mathbf{y}_N\rangle \pm \hat{\psi}^\dagger(\mathbf{y})|R\rangle. \end{aligned} \tag{1.46}$$

Subtraction and addition of (1.45) and (1.46) for bosons and fermions respectively then gives

$$\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_\mp |\mathbf{y}_1 \dots \mathbf{y}_N\rangle = \delta(\mathbf{x}-\mathbf{y})|\mathbf{y}_1 \dots \mathbf{y}_N\rangle,$$

which must be valid for all position–spin kets and for all N, and therefore

$$\boxed{\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{y})\right]_\mp = \delta(\mathbf{x}-\mathbf{y})} \tag{1.47}$$

The (anti)commutation relations (1.39), (1.40), and (1.47) are the main results of this section and form the basis of most derivations in this book. As we see in Section 1.6, all many-particle operators, such as total energy, density, current, spin, etc., consist of simple expressions in terms of the field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$, and the calculation of their averages can easily be performed with the help of the (anti)commutation relations. It is similar to the harmonic oscillator of quantum mechanics: Both the eigenstates and the operators are expressed in terms of the raising and lowering operators $\hat{a}^\dagger$ and $\hat{a}$, and to calculate all sorts of averages it is enough to know the commutation relations $[\hat{a}, \hat{a}]_- = [\hat{a}^\dagger, \hat{a}^\dagger]_- = 0$ and $[\hat{a}, \hat{a}^\dagger]_- = 1$. The difference with second quantization is that we have a "harmonic oscillator" for every $\mathbf{x}$. Using the (anti)commutation properties we can manipulate directly the kets and never have to deal with the rather cumbersome expressions of the wavefunctions; the field operators take care of the symmetry of the kets automatically. The great achievement of second quantization is comparable to that of a programming language. When we program we use a nice, friendly text editor to write code that tells the computer what operations to do, and we do not worry about whether the instructions given through the text editor are correctly executed by the machine. A bug in the code is an error in the text of the program (the way we manipulate the field operators) and not an erroneous functioning of some logic gate (the violation of the symmetry properties of the many-particle kets).

Exercise 1.1 We define the *density operator*

$$\hat{n}(\mathbf{x}) \equiv \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}).$$

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Using the identities $[\hat{A}\hat{B},\hat{C}]_- = \hat{A}[\hat{B},\hat{C}]_- + [\hat{A},\hat{C}]_-\hat{B} = \hat{A}[\hat{B},\hat{C}]_+ - [\hat{A},\hat{C}]_+\hat{B}$, prove the following relations for fermionic and bosonic field operators:

$$[\hat{n}(\mathbf{x}),\hat{\psi}(\mathbf{x}')]_- = -\delta(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x}), \tag{1.48}$$

$$[\hat{n}(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{x}')]_- = \delta(\mathbf{x}-\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x}). \tag{1.49}$$

1.5 General Basis States

In the previous section we learned how to construct states of many identical particles with a given spin and position. The position–spin is, however, just one possible choice of quantum numbers to characterize every single particle. We now show how the field operators can be used to construct states of many identical particles in which every particle is labeled by general quantum numbers, such as momentum, energy, etc.

Let us consider a normalized one-particle ket $|n\rangle$. The quantum number $n = (s\tau)$ comprises an orbital quantum number s and the spin projection τ along some quantization axis. Choosing the quantization axis of the spin to be the same as that of the position–spin ket $|\mathbf{x}\rangle = |\mathbf{r}\sigma\rangle$, the overlap between $|n\rangle$ and $|\mathbf{x}\rangle$ is

$$\langle\mathbf{x}|n\rangle \equiv \varphi_n(\mathbf{x}) = \varphi_s(\mathbf{r})\delta_{\tau\sigma}. \tag{1.50}$$

The one-particle ket $|n\rangle$ can be expanded in the position–spin kets using the completeness relation (1.8):

$$|n\rangle = \int d\mathbf{x}\,|\mathbf{x}\rangle\langle\mathbf{x}|n\rangle = \int d\mathbf{x}\,\varphi_n(\mathbf{x})|\mathbf{x}\rangle = \int d\mathbf{x}\,\varphi_n(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})|0\rangle. \tag{1.51}$$

One can easily check that the normalization $\langle n|n\rangle = 1$ is equivalent to saying that $\int d\mathbf{x}|\varphi_n(\mathbf{x})|^2 = 1$. From (1.51) we see that $|n\rangle$ is obtained by applying to the empty ket $|0\rangle$ the operator

$$\boxed{\hat{d}_n^\dagger \equiv \int d\mathbf{x}\,\varphi_n(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})} \tag{1.52}$$

that is, $\hat{d}_n^\dagger|0\rangle = |n\rangle$. We may say that $\hat{d}_n^\dagger$ creates a particle with quantum number n. Similarly, if we take the adjoint of (1.52),

$$\boxed{\hat{d}_n \equiv \int d\mathbf{x}\,\varphi_n^*(\mathbf{x})\hat{\psi}(\mathbf{x})} \tag{1.53}$$

we obtain an operator that destroys a particle with quantum number n since

$$\hat{d}_n|n\rangle = \hat{d}_n\hat{d}_n^\dagger|0\rangle = \int d\mathbf{x}d\mathbf{x}'\varphi_n^*(\mathbf{x})\varphi_n(\mathbf{x}')\underbrace{\hat{\psi}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')|0\rangle}_{\delta(\mathbf{x}-\mathbf{x}')|0\rangle} = \int d\mathbf{x}\,|\varphi_n(\mathbf{x})|^2|0\rangle = |0\rangle.$$

The operators $\hat{d}_n$ and $\hat{d}_n^\dagger$, being linear combinations of field operators at different $\mathbf{x}$, can act on states with arbitrary many particles. Below we derive some important relations for

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the $\hat{d}$-operators when the set $\{|n\rangle\}$ forms an orthonormal basis in the one-particle Hilbert space.

We can easily derive the important (anti)commutation relations using the corresponding relations for the field operators,

$$\left[\hat{d}_n, \hat{d}_m^\dagger\right]_\mp = \int d\mathbf{x} d\mathbf{x}' \, \varphi_n^*(\mathbf{x})\varphi_m(\mathbf{x}') \underbrace{\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\right]_\mp}_{\delta(\mathbf{x}-\mathbf{x}')} = \langle n|m\rangle = \delta_{nm}, \tag{1.54}$$

and the more obvious ones,

$$\left[\hat{d}_n, \hat{d}_m\right]_\mp = \left[\hat{d}_n^\dagger, \hat{d}_m^\dagger\right]_\mp = 0, \tag{1.55}$$

that follow similarly. It is worth noticing that the $\hat{d}$-operators obey the same (anti)commutation relations as the field operators, with the index n playing the role of $\mathbf{x}$. This is a very important observation since the results of the previous section rely only on the (anti)commutation relations of $\hat{\psi}$ and $\hat{\psi}^\dagger$, and hence remain valid in this more general basis. To convince the reader of this fact, we derive some of the results of the previous section directly from the (anti)commutation relations. We define the N-particle ket

$$|n_1 \dots n_N\rangle \equiv \hat{d}_{n_N}^\dagger \dots \hat{d}_{n_1}^\dagger |0\rangle = \hat{d}_{n_N}^\dagger |n_1 \dots n_{N-1}\rangle \tag{1.56}$$

which has the symmetry property

$$|n_{P(1)} \dots n_{P(N)}\rangle = (\pm)^P |n_1 \dots n_N\rangle,$$

as follows immediately from (1.55). Like the position–spin kets, the kets $|n_1 \dots n_N\rangle$ span the N-particle Hilbert space $\mathbb{H}_N$. The action of $\hat{d}_n$ on $|n_1 \dots n_N\rangle$ is similar to the action of $\hat{\psi}(\mathbf{x})$ on $|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$. Using the (anti)commutation relation (1.54), we can move the $\hat{d}_n$-operator through the string of $d^\dagger$-operators:[5]

$$\begin{aligned}
\hat{d}_n|n_1 \dots n_N\rangle &= \left(\left[\hat{d}_n, \hat{d}_{n_N}^\dagger\right]_\mp \pm \hat{d}_{n_N}^\dagger \hat{d}_n\right)|n_1 \dots n_{N-1}\rangle \\
&= \delta_{nn_N}|n_1 \dots n_{N-1}\rangle \pm \hat{d}_{n_N}^\dagger \left(\left[\hat{d}_n, \hat{d}_{n_{N-1}}^\dagger\right]_\mp \pm \hat{d}_{n_{N-1}}^\dagger \hat{d}_n\right)|n_1 \dots n_{N-2}\rangle \\
&= \delta_{nn_N}|n_1 \dots n_{N-1}\rangle \pm \delta_{nn_{N-1}}|n_1 \dots n_{N-2} n_N\rangle \\
&\quad (\pm)^2 \hat{d}_{n_N}^\dagger \hat{d}_{n_{N-1}}^\dagger \left(\left[\hat{d}_n, \hat{d}_{n_{N-2}}^\dagger\right]_\mp \pm \hat{d}_{n_{N-2}}^\dagger \hat{d}_n\right)|n_1 \dots n_{N-3}\rangle \\
&= \sum_{k=1}^{N} (\pm)^{N+k} \delta_{nn_k}|n_1 \dots n_{k-1} n_{k+1} \dots n_N\rangle.
\end{aligned} \tag{1.57}$$

This result can also be used to calculate directly the overlap between two states of the general basis. For example, for the case of two particles we have

$$\begin{aligned}
\langle n_1' n_2'|n_1 n_2\rangle &= \langle n_1'|\hat{d}_{n_2'}|n_1 n_2\rangle = \langle n_1'|\left(\delta_{n_2' n_2}|n_1\rangle \pm \delta_{n_2' n_1}|n_2\rangle\right) \\
&= \delta_{n_1' n_1}\delta_{n_2' n_2} \pm \delta_{n_1' n_2}\delta_{n_2' n_1},
\end{aligned}$$

[5] Alternatively (1.57) can be derived from (1.44) together with the definitions of the $\hat{d}$-operators.

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which is the analog of (1.26). More generally, for N particles we have

$$\langle n'_1 \dots n'_N | n_1 \dots n_N \rangle = \sum_P (\pm)^P \prod_{j=1}^{N} \delta_{n'_j \, n_{P(j)}}, \tag{1.58}$$

which should be compared with the overlap $\langle \mathbf{x}'_1 \dots \mathbf{x}'_N | \mathbf{x}_1 \dots \mathbf{x}_N \rangle$ in (1.30).

The states $|n_1 \dots n_N\rangle$ are orthonormal (with the exception of the bosonic kets with two or more equal quantum numbers) and can be used to construct a basis. In analogy with (1.32), the completeness relation is

$$\frac{1}{N!} \sum_{n_1,\dots,n_N} |n_1 \dots n_N\rangle\langle n_1 \dots n_N| = \hat{\mathbb{1}},$$

and hence the expansion of a ket $|\Psi\rangle$ belonging to $\mathbb{H}_N$ reads

$$|\Psi\rangle = \hat{\mathbb{1}}|\Psi\rangle = \frac{1}{N!} \sum_{n_1,\dots,n_N} |n_1 \dots n_N\rangle \underbrace{\langle n_1 \dots n_N | \Psi\rangle}_{\Psi(n_1,\dots,n_N)}. \tag{1.59}$$

If $|\Psi\rangle$ is normalized, then the coefficients $\Psi(n_1, \dots, n_N)$ have the following probabilistic interpretation

$$\frac{|\Psi(\overbrace{n_1 \dots n_1}^{m_1} \dots \overbrace{n_M \dots n_M}^{m_M})|^2}{m_1! \dots m_M!} = \begin{pmatrix} \text{probability of finding} \\ m_1 \text{ particles with quantum number } n_1 \\ \vdots \\ m_M \text{ particles with quantum number } n_M \end{pmatrix}.$$

We already observed that the $\hat{d}$-operators obey the same (anti)commutation relations as the field operators provided that $\{|n\rangle\}$ is an orthonormal basis in $\mathbb{H}_1$. Likewise, we can construct linear combinations of the $\hat{d}$-operators that preserve the (anti)commutation relations. It is left as an exercise for the reader to prove that the operators

$$\hat{c}_\alpha = \sum_n U_{\alpha n} \hat{d}_n, \qquad \hat{c}^\dagger_\alpha = \sum_n U^*_{\alpha n} \hat{d}^\dagger_n$$

obey

$$\left[\hat{c}_\alpha, \hat{c}^\dagger_\beta\right]_\mp = \delta_{\alpha\beta},$$

provided that

$$U_{\alpha n} \equiv \langle \alpha | n \rangle$$

is the inner product between the elements of the original orthonormal basis $\{|n\rangle\}$ and the elements of another orthonormal basis $\{|\alpha\rangle\}$. Indeed, in this case the $U_{\alpha n}$ are the matrix elements of a unitary matrix since

$$\sum_n U_{\alpha n} U^\dagger_{n\beta} = \sum_n \langle \alpha | n \rangle \langle n | \beta \rangle = \langle \alpha | \beta \rangle = \delta_{\alpha\beta},$$

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where we use the completeness relation. In particular, when $\alpha = \mathbf{x}$ we have $U_{\mathbf{x}n} = \langle \mathbf{x}|n\rangle = \varphi_n(\mathbf{x})$, and we find that $\hat{c}_{\mathbf{x}} = \hat{\psi}(\mathbf{x})$. We thus recover the field operators as

$$\hat{\psi}(\mathbf{x}) = \sum_n \varphi_n(\mathbf{x})\hat{d}_n, \qquad \hat{\psi}^\dagger(\mathbf{x}) = \sum_n \varphi_n^*(\mathbf{x})\hat{d}_n^\dagger. \tag{1.60}$$

These relations tell us that the expansion of the position–spin kets in terms of the kets $|n_1 \dots n_N\rangle$ is simply

$$\boxed{|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = \sum_{n_1 \dots n_N} \varphi_{n_1}^*(\mathbf{x}_1) \dots \varphi_{n_N}^*(\mathbf{x}_N)|n_1 \dots n_N\rangle} \tag{1.61}$$

Conversely, using (1.52) we can expand the general basis kets in terms of the position–spin kets as

$$\boxed{|n_1 \dots n_N\rangle = \int d\mathbf{x}_1 \dots d\mathbf{x}_N \, \varphi_{n_1}(\mathbf{x}_1) \dots \varphi_{n_N}(\mathbf{x}_N)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle} \tag{1.62}$$

Slater determinants If we are given a state $|\Psi\rangle$ that is expanded in a general basis and we subsequently want to calculate properties in position–spin space, such as the particle density or the current density, we need to calculate the overlap between $|n_1 \dots n_N\rangle$ and $|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$. This overlap is the wavefunction for N particles with quantum numbers $n_1, \dots, n_N$:

$$\Psi_{n_1 \dots n_N}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \langle \mathbf{x}_1 \dots \mathbf{x}_N | n_1 \dots n_N\rangle.$$

The explicit form of the wavefunction follows directly from the inner product (1.30) and from the expansion (1.62), and reads

$$\begin{aligned}\Psi_{n_1 \dots n_N}(\mathbf{x}_1, \dots, \mathbf{x}_N) &= \sum_P (\pm)^P \varphi_{n_1}(\mathbf{x}_{P(1)}) \dots \varphi_{n_N}(\mathbf{x}_{P(N)}) \\ &= \begin{vmatrix} \varphi_{n_1}(\mathbf{x}_1) & \dots & \varphi_{n_1}(\mathbf{x}_N) \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \varphi_{n_N}(\mathbf{x}_1) & \dots & \varphi_{n_N}(\mathbf{x}_N) \end{vmatrix}_{\pm}.\end{aligned} \tag{1.63}$$

Since for any matrix A we have $|A|_{\mp} = |A^T|_{\mp}$ with A^T the transpose of A, we can equivalently write

$$\Psi_{n_1 \dots n_N}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \begin{vmatrix} \varphi_{n_1}(\mathbf{x}_1) & \dots & \varphi_{n_N}(\mathbf{x}_1) \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \varphi_{n_1}(\mathbf{x}_N) & \dots & \varphi_{n_N}(\mathbf{x}_N) \end{vmatrix}_{\pm}.$$

In the case of fermions, the determinant is also known as the *Slater determinant*. For those readers already familiar with Slater determinants we note that the absence on the r.h.s. of the prefactor $1/\sqrt{N!}$ is a consequence of forcing on the square modulus of the wavefunction a probability interpretation, as discussed in detail in Section 1.3. The action of the $\hat{d}$-operators has a simple algebraic interpretation in terms of permanents or determinants.

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The action of the creation operator $\hat{d}_n^\dagger$ on $|n_1 \dots n_N\rangle$ in the position–spin representation, $\langle \mathbf{x}_1 \dots \mathbf{x}_{N+1}|\hat{d}_n^\dagger|n_1 \dots n_N\rangle$, simply amounts to adding a column with coordinate $\mathbf{x}_{N+1}$ and a row with wavefunction φ_n in (1.63). For the annihilation operator we have a similar algebraic interpretation. Taking the inner product with $\langle \mathbf{x}_1 \dots \mathbf{x}_{N-1}|$ of both sides of (1.57), we get

$$\langle \mathbf{x}_1 \dots \mathbf{x}_{N-1}|\hat{d}_n|n_1 \dots n_N\rangle = \sum_{k=1}^{N} (\pm)^{N+k}\, \delta_{nn_k} \times \begin{vmatrix} \varphi_{n_1}(\mathbf{x}_1) & \dots & \dots & \varphi_{n_1}(\mathbf{x}_{N-1}) & \varphi_{n_1}(\mathbf{x}_N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \varphi_{n_{k-1}}(\mathbf{x}_1) & \dots & \dots & \varphi_{n_{k-1}}(\mathbf{x}_{N-1}) & \varphi_{n_{k-1}}(\mathbf{x}_N) \\ \cancel{\varphi_{n_k}(\mathbf{x}_1)} & \dots & \dots & \cancel{\varphi_{n_k}(\mathbf{x}_{N-1})} & \cancel{\varphi_{n_k}(\mathbf{x}_N)} \\ \varphi_{n_{k+1}}(\mathbf{x}_1) & \dots & \dots & \varphi_{n_{k+1}}(\mathbf{x}_{N-1}) & \varphi_{n_{k+1}}(\mathbf{x}_N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \varphi_{n_N}(\mathbf{x}_1) & \dots & \dots & \varphi_{n_N}(\mathbf{x}_{N-1}) & \varphi_{n_N}(\mathbf{x}_N) \end{vmatrix}_{\pm} .$$

That is, the action of the $\hat{d}_n$-operator amounts to deleting the last column and, if present, the row with quantum number n from the permanent/determinant of (1.63), and otherwise yields zero. Already at this stage the reader can appreciate how powerful it is to work with the field operators and not to have anything to do with Slater determinants.

Exercise 1.2 Prove the inverse relations (1.60).

Exercise 1.3 Let $|n\rangle = |\mathbf{p}\tau\rangle$ be a momentum–spin ket so that $\langle \mathbf{x}|\mathbf{p}\tau\rangle = e^{i\mathbf{p}\cdot\mathbf{r}}\delta_{\sigma\tau}$, see (1.10). Show that the (anti)commutation relation in (1.54) then reads

$$\left[\hat{d}_{\mathbf{p}\tau}, \hat{d}^\dagger_{\mathbf{p}'\tau'}\right]_{\mp} = (2\pi)^3\delta(\mathbf{p}-\mathbf{p}')\delta_{\tau\tau'}, \tag{1.64}$$

and that the expansion (1.60) of the field operators in terms of the $\hat{d}$-operators is

$$\hat{\psi}(\mathbf{x}) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{r}}\hat{d}_{\mathbf{p}\sigma}, \qquad \hat{\psi}^\dagger(\mathbf{x}) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{-i\mathbf{p}\cdot\mathbf{r}}\hat{d}^\dagger_{\mathbf{p}\sigma}. \tag{1.65}$$

1.6 Hamiltonian in Second Quantization

The field operators are useful not only to construct the kets of N identical particles but also the operators acting on them. Let us consider again two identical particles and the total potential energy (1.16), with $N = 2$ and $q_1 = q_2 = q$. In first quantization the ket $|\mathbf{x}_1\mathbf{x}_2\rangle$ is represented by the (anti)symmetrized product (1.35) of one-particle kets. It is instructive

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to calculate the action of $\hat{\mathcal{H}}_{\rm pot}$ on $|\mathbf{x}_1\mathbf{x}_2\rangle$ to later appreciate the advantages of second quantization. We have

$$\begin{aligned}\hat{\mathcal{H}}_{\rm pot}&\frac{|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle\pm|\mathbf{x}_2\rangle|\mathbf{x}_1\rangle}{\sqrt{2}}\\&=q\frac{\phi(\mathbf{r}_1)|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle\pm\phi(\mathbf{r}_2)|\mathbf{x}_2\rangle|\mathbf{x}_1\rangle+\phi(\mathbf{r}_2)|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle\pm\phi(\mathbf{r}_1)|\mathbf{x}_2\rangle|\mathbf{x}_1\rangle}{\sqrt{2}}\\&=q\big[\phi(\mathbf{r}_1)+\phi(\mathbf{r}_2)\big]\frac{|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle\pm|\mathbf{x}_2\rangle|\mathbf{x}_1\rangle}{\sqrt{2}}.\end{aligned}\tag{1.66}$$

Throughout this book we use calligraphic letters for operators acting on kets written in first quantization as opposed to operators (such as the field operators) acting on kets written in second quantization (e.g., $\hat{\psi}^\dagger(\mathbf{x}_N)\dots\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle$). We refer to the former as *operators in first quantization* and to the latter as *operators in second quantization*. We now show that the very same result (1.66) can be obtained if we write the potential energy operator as

$$\hat{H}_{\rm pot}=q\int d\mathbf{x}\,\phi(\mathbf{r})\,\hat{n}(\mathbf{x}),$$

where

$$\boxed{\hat{n}(\mathbf{x})=\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})}\tag{1.67}$$

is the so-called *density operator* already introduced in Exercise 1.1. The origin of this name for the operator $\hat{n}(\mathbf{x})$ stems from the fact that $|\mathbf{x}_1\dots\mathbf{x}_N\rangle$ is an eigenket of the density operator whose eigenvalue is exactly the density of N particles in the position–spin coordinates $\mathbf{x}_1,\dots,\mathbf{x}_N$. Indeed,

$$\begin{aligned}\hat{n}(\mathbf{x})\underbrace{\hat{\psi}^\dagger(\mathbf{x}_N)\hat{\psi}^\dagger(\mathbf{x}_{N-1})\dots\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle}_{|\mathbf{x}_1\dots\mathbf{x}_N\rangle}&=\Big[\hat{n}(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{x}_N)\Big]_-\hat{\psi}^\dagger(\mathbf{x}_{N-1})\dots\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle\\&+\hat{\psi}^\dagger(\mathbf{x}_N)\Big[\hat{n}(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{x}_{N-1})\Big]_-\dots\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle\\&\;\;\vdots\\&+\hat{\psi}^\dagger(\mathbf{x}_N)\hat{\psi}^\dagger(\mathbf{x}_{N-1})\dots\Big[\hat{n}(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{x}_1)\Big]_-|0\rangle\\&=\underbrace{\left(\sum_{i=1}^{N}\delta(\mathbf{x}-\mathbf{x}_i)\right)}_{\substack{\text{density of }N\text{ particles}\\\text{in }\mathbf{x}_1,\dots,\mathbf{x}_N}}|\mathbf{x}_1\dots\mathbf{x}_N\rangle,\end{aligned}\tag{1.68}$$

where we repeatedly use (1.49). This result tells us that any ket with N particles is an eigenket of the operator

$$\boxed{\hat{N}\equiv\int d\mathbf{x}\,\hat{n}(\mathbf{x})}$$

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with eigenvalue N. For this reason $\hat{N}$ is called the *operator of the total number of particles*.

By acting with $\hat{H}_{\rm pot}$ on $|\mathbf{x}_1\mathbf{x}_2\rangle = \hat{\psi}^\dagger(\mathbf{x}_2)\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle$ and taking into account (1.68), we find

$$\hat{H}_{\rm pot}|\mathbf{x}_1\mathbf{x}_2\rangle = q\int d\mathbf{x}\,\phi(\mathbf{r})\sum_{i=1}^{2}\delta(\mathbf{x}-\mathbf{x}_i)|\mathbf{x}_1\mathbf{x}_2\rangle = q\big[\phi(\mathbf{r}_1+\phi(\mathbf{r}_2)\big]|\mathbf{x}_1\mathbf{x}_2\rangle.$$

Simple and elegant! Both the operator and the ket are easy to manipulate and their expressions are undoubtedly shorter than the corresponding expressions in first quantization. A further advantage of second quantization is that the operator $\hat{H}_{\rm pot}$ keeps the very same form independently of the number of particles; using (1.68) it is straightforward to verify that

$$\hat{H}_{\rm pot}|\mathbf{x}_1\ldots\mathbf{x}_N\rangle = q\left(\sum_{i=1}^{N}\phi(\mathbf{r}_i)\right)|\mathbf{x}_1\ldots\mathbf{x}_N\rangle.$$

To the contrary, $\hat{\mathcal{H}}_{\rm pot}$ in (1.16) acts only on kets belonging to $\mathbb{H}_N$. Thus, when working in Fock space it would be more rigorous to specify on which Hilbert space $\hat{\mathcal{H}}_{\rm pot}$ acts. Denoting by $\hat{\mathcal{H}}_{\rm pot}(N)$ the operator in (1.16), we can write down the relation between operators in first and second quantization as

$$\hat{H}_{\rm pot} = \sum_{N=0}^{\infty}\hat{\mathcal{H}}_{\rm pot}(N),$$

with the extra rule that $\hat{\mathcal{H}}_{\rm pot}(N)$ yields the null ket when acting on a state of $\mathbb{H}_{M\neq N}$. In this book, however, we are not so meticulous with the notation. The Hilbert space on which operators in first quantization act is clear from the context.

The goal of this section is to extend the above example to general operators and in particular to derive an expression for the many-particle Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_{\rm int}$. According to (1.17), the matrix element of the noninteracting Hamiltonian $\hat{H}_0$ between a position–spin ket and a generic ket $|\Psi\rangle$ is

$$\langle\mathbf{x}_1\ldots\mathbf{x}_N|\hat{H}_0|\Psi\rangle = \sum_{j=1}^{N}\sum_{\sigma'}h_{\sigma_j\sigma'}(\mathbf{r}_j,-\mathrm{i}\boldsymbol{\nabla}_j,\mathbf{S})\,\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_{j-1},\mathbf{r}_j\sigma',\mathbf{x}_{j+1},\ldots,\mathbf{x}_N). \tag{1.69}$$

It is worth observing that for $N=1$ this expression reduces to

$$\langle\mathbf{x}|\hat{H}_0|\Psi\rangle = \sum_{\sigma'}h_{\sigma\sigma'}(\mathbf{r},-\mathrm{i}\boldsymbol{\nabla},\mathbf{S})\Psi(\mathbf{r}\sigma'),$$

which agrees with (1.13) when $|\Psi\rangle = |\mathbf{x}''\rangle$ since in this case $\Psi(\mathbf{r}\sigma') = \langle\mathbf{r}\sigma'|\mathbf{r}''\sigma''\rangle = \delta(\mathbf{r}-\mathbf{r}'')\delta_{\sigma'\sigma''}$. Similarly, we see from (1.18) that the matrix element of the interaction Hamiltonian $\hat{H}_{\rm int}$ between a position–spin ket and a generic ket $|\Psi\rangle$ is

$$\langle\mathbf{x}_1\ldots\mathbf{x}_N|\hat{H}_{\rm int}|\Psi\rangle = \frac{1}{2}\sum_{i\neq j}^{N}v(\mathbf{x}_i,\mathbf{x}_j)\,\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N). \tag{1.70}$$

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In (1.70) we consider the more general case of spin-dependent interactions $v(\mathbf{x}_1, \mathbf{x}_2)$, according to which the interaction energy between a particle in $\mathbf{r}_1$ and a particle in $\mathbf{r}_2$ depends also on the spin orientation σ_1 and σ_2 of these particles. Now the question is: How do we express $\hat{H}_0$ and $\hat{H}_{\rm int}$ in terms of field operators?

Noninteracting Hamiltonian We start our discussion with the noninteracting Hamiltonian. For pedagogical purposes we derive the operator $\hat{H}_0$ in second quantization in two different ways.

Derivation I: In first quantization the noninteracting Hamiltonian $\hat{\mathcal{H}}_0$ of a system of N particles each described by $\hat{h}$ is given in (1.17). The first quantization eigenkets of $\hat{\mathcal{H}}_0$ are obtained by forming (anti)symmetrized products of one-particle eigenkets of $\hat{h}$, and look like

$$|n_1 \dots n_N\rangle = \frac{1}{\sqrt{N!}} \sum_P (\pm)^P |n_{P(1)}\rangle \dots |n_{P(N)}\rangle, \tag{1.71}$$

with

$$\hat{h}|n\rangle = \epsilon_n |n\rangle.$$

We leave it as an exercise for the reader to show that

$$\hat{\mathcal{H}}_0 |n_1 \dots n_N\rangle = (\epsilon_{n_1} + \dots + \epsilon_{n_N})\, |n_1 \dots n_N\rangle.$$

The proof of this identity involves the same kind of manipulations used to derive (1.66). To carry them out is useful to appreciate the simplicity of second quantization. We show below that in second quantization the noninteracting Hamiltonian $\hat{H}_0$ takes the compact form

$$\boxed{\hat{H}_0 = \int d\mathbf{x} d\mathbf{x}'\, \hat{\psi}^\dagger(\mathbf{x}) \langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle \hat{\psi}(\mathbf{x}')} \tag{1.72}$$

independently of the number of particles. We prove (1.72) by showing that the second quantization ket $|n_1 \dots n_N\rangle$ is an eigenket of $\hat{H}_0$ with eigenvalue $\epsilon_{n_1} + \dots + \epsilon_{n_N}$. In second quantization $|n_1 \dots n_N\rangle = \hat{d}^\dagger_{n_N} \dots \hat{d}^\dagger_{n_1} |0\rangle$, with the $\hat{d}$-operators defined in (1.52) and (1.53). It is then natural to express $\hat{H}_0$ in terms of the $\hat{d}$-operators. Inserting a completeness relation between $\hat{h}$ and $|\mathbf{x}'\rangle$, we find

$$\begin{aligned} \hat{H}_0 &= \sum_n \int d\mathbf{x} d\mathbf{x}'\, \hat{\psi}^\dagger(\mathbf{x}) \langle \mathbf{x}|\hat{h}|n\rangle \langle n|\mathbf{x}'\rangle \hat{\psi}(\mathbf{x}') \\ &= \sum_n \epsilon_n \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x}) \underbrace{\langle \mathbf{x}|n\rangle}_{\varphi_n(\mathbf{x})} \int d\mathbf{x}' \underbrace{\langle n|\mathbf{x}'\rangle}_{\varphi_n^*(\mathbf{x}')} \hat{\psi}(\mathbf{x}') = \sum_n \epsilon_n \hat{d}^\dagger_n \hat{d}_n, \end{aligned} \tag{1.73}$$

where we use $\hat{h}|n\rangle = \epsilon_n |n\rangle$. The $\hat{d}$-operators bring the Hamiltonian into a diagonal form – that is, none of the off-diagonal combinations $\hat{d}^\dagger_n d_m$ with $m \neq n$ appear in $\hat{H}_0$. The *occupation operator*

$$\hat{n}_n \equiv \hat{d}^\dagger_n \hat{d}_n \tag{1.74}$$

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is the analog of the density operator $\hat{n}(\mathbf{x})$ in the position–spin basis; it counts how many particles have quantum number n. Using the (anti)commutation relations (1.54) and (1.55), it is easy to prove that

$$\left[\hat{n}_n, \hat{d}_m^\dagger\right]_- = \delta_{nm}\hat{d}_m^\dagger, \qquad \left[\hat{n}_n, \hat{d}_m\right]_- = -\delta_{nm}\hat{d}_m, \tag{1.75}$$

which should be compared with the relations (1.48) and (1.49). The action of $\hat{H}_0$ on $|n_1 \dots n_N\rangle$ is then

$$\begin{aligned}\hat{H}_0 \underbrace{\hat{d}_{n_N}^\dagger \hat{d}_{n_{N-1}}^\dagger \dots \hat{d}_{n_1}^\dagger |0\rangle}_{|n_1 \dots n_N\rangle} = \sum_n \epsilon_n \Big(&\left[\hat{n}_n, \hat{d}_{n_N}^\dagger\right]_- \hat{d}_{n_{N-1}}^\dagger \dots \hat{d}_{n_1}^\dagger |0\rangle \\ &+ \hat{d}_{n_N}^\dagger \left[\hat{n}_n, \hat{d}_{n_{N-1}}^\dagger\right]_- \dots \hat{d}_{n_1}^\dagger |0\rangle \\ &\vdots \\ &+ \hat{d}_{n_N}^\dagger \hat{d}_{n_{N-1}}^\dagger \dots \left[\hat{n}_n, \hat{d}_{n_1}^\dagger\right]_- |0\rangle \Big) \\ = (\epsilon_{n_1} + \dots + \epsilon_{n_N})\, &\hat{d}_{n_N}^\dagger \hat{d}_{n_{N-1}}^\dagger \dots \hat{d}_{n_1}^\dagger |0\rangle. \end{aligned} \tag{1.76}$$

This is exactly the result we wanted to prove: The Hamiltonian $\hat{H}_0$ is the correct second quantized form of $\hat{\mathcal{H}}_0$. We can write $\hat{H}_0$ in different ways using the matrix elements (1.13) of $\hat{h}$. For instance,

$$\hat{H}_0 = \sum_{\sigma\sigma'} \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}\sigma) h_{\sigma\sigma'}(\mathbf{r}, -\mathrm{i}\boldsymbol{\nabla}, \mathbf{S}) \hat{\psi}(\mathbf{r}\sigma'), \tag{1.77}$$

or, equivalently,

$$\hat{H}_0 = \sum_{\sigma\sigma'} \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}\sigma) h_{\sigma\sigma'}(\mathbf{r}, \mathrm{i}\overleftarrow{\boldsymbol{\nabla}}, \mathbf{S}) \hat{\psi}(\mathbf{r}\sigma'). \tag{1.78}$$

In these expressions the action of the gradient $\boldsymbol{\nabla}$ on a field operator is a formal expression which makes sense only when we sandwich $\hat{H}_0$ with a bra and a ket. For instance,

$$\langle\chi|\hat{\psi}^\dagger(\mathbf{r}\sigma)\boldsymbol{\nabla}\hat{\psi}(\mathbf{r}\sigma')|\Psi\rangle \equiv \lim_{\mathbf{r}'\to\mathbf{r}} \boldsymbol{\nabla}' \langle\chi|\hat{\psi}^\dagger(\mathbf{r}\sigma)\hat{\psi}(\mathbf{r}'\sigma')|\Psi\rangle, \tag{1.79}$$

where $\boldsymbol{\nabla}'$ is the gradient with respect to the primed variable. It is important to observe that for any arbitrary large but finite system the physical states have no particles at infinity. Therefore, if $|\chi\rangle$ and $|\Psi\rangle$ are physical states, then (1.79) vanishes when $|\mathbf{r}| \to \infty$. More generally, the sandwich of a string of field operators $\hat{\psi}^\dagger(\mathbf{x}_1) \dots \hat{\psi}^\dagger(\mathbf{x}_N)\hat{\psi}(\mathbf{y}_1) \dots \hat{\psi}(\mathbf{y}_M)$ with two physical states vanishes when one of the coordinates of the field operators approaches infinity. The equivalence between (1.77) and (1.78) has to be understood as an equivalence between the sandwich of the corresponding r.h.s. with physical states. Consider, for example, $\hat{h} = \hat{p}^2/2m$. Equating the r.h.s. of (1.77) and (1.78) we get

$$\sum_\sigma \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}\sigma) \left[-\frac{\nabla^2}{2m}\hat{\psi}(\mathbf{r}\sigma)\right] = \sum_\sigma \int d\mathbf{r}\, \left[-\frac{\nabla^2}{2m}\hat{\psi}^\dagger(\mathbf{r}\sigma)\right] \hat{\psi}(\mathbf{r}\sigma).$$

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This is an equality only provided that the integration by parts produces a vanishing boundary term – that is, only provided that for any two physical states $|\chi\rangle$ and $|\Psi\rangle$ the quantity in (1.79) vanishes when $|\mathbf{r}| \to \infty$.

Derivation 2: The second derivation consists in showing that the matrix elements of (1.77) or (1.78) are given by (1.69). Using (1.44), we find

$$\begin{aligned}
&\langle \mathbf{x}_1 \dots \mathbf{x}_N | \hat{\psi}^\dagger(\mathbf{r}\sigma) h_{\sigma\sigma'}(\mathbf{r}, -\mathrm{i}\boldsymbol{\nabla}, \mathbf{S}) \hat{\psi}(\mathbf{r}\sigma') | \Psi \rangle \\
&\quad = \lim_{\mathbf{r}' \to \mathbf{r}} h_{\sigma\sigma'}(\mathbf{r}', -\mathrm{i}\boldsymbol{\nabla}', \mathbf{S}) \sum_{j=1}^{N} (\pm)^{N+j} \delta(\mathbf{x}_j - \mathbf{x}) \langle \mathbf{x}_1 \dots \mathbf{x}_{j-1} \mathbf{x}_{j+1} \dots \mathbf{x}_N | \hat{\psi}(\mathbf{x}') | \Psi \rangle \\
&\quad = \lim_{\mathbf{r}' \to \mathbf{r}} h_{\sigma\sigma'}(\mathbf{r}', -\mathrm{i}\boldsymbol{\nabla}', \mathbf{S}) \sum_{j=1}^{N} \delta(\mathbf{x}_j - \mathbf{x}) \Psi(\mathbf{x}_1, \dots \mathbf{x}_{j-1}, \mathbf{x}', \mathbf{x}_{j+1}, \dots, \mathbf{x}_N),
\end{aligned}$$

where we use that it requires $N - j$ interchanges to put $\mathbf{x}'$ at the position between $\mathbf{x}_{j-1}$ and $\mathbf{x}_{j+1}$. Summing over σ, σ' and integrating over $\mathbf{r}$ we get

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \hat{H}_0 | \Psi \rangle = \sum_{j=1}^{N} \sum_{\sigma'} \lim_{\mathbf{r}' \to \mathbf{r}_j} h_{\sigma_j \sigma'}(\mathbf{r}', -\mathrm{i}\boldsymbol{\nabla}', \mathbf{S}) \Psi(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}', \mathbf{x}_{j+1}, \dots, \mathbf{x}_N), \tag{1.80}$$

which coincides with the matrix element (1.69). Here and in the following we call *one-body operators* those operators in second quantization that can be written as a quadratic form of the field operators. The Hamiltonian $\hat{H}_0$ and the potential energy operator $\hat{H}_{\mathrm{pot}}$ are one-body operators.

Interacting Hamiltonian From (1.76) it is evident that one-body Hamiltonians can only describe noninteracting systems since the eigenvalues are the sum of one-particle eigenvalues, and the latter do not depend on the position of the other particles. If there is an interaction $v(\mathbf{x}_1, \mathbf{x}_2)$ between one particle in $\mathbf{x}_1$ and another particle in $\mathbf{x}_2$, the corresponding interaction energy operator $\hat{H}_{\mathrm{int}}$ cannot be a one-body operator. The energy to put a particle in a given point depends on where the other particles are located. Suppose that there is a particle in $\mathbf{x}_1$. Then if we want to put a particle in $\mathbf{x}_2$ we must pay an energy $v(\mathbf{x}_1, \mathbf{x}_2)$. The addition of another particle in $\mathbf{x}_3$ costs an energy $v(\mathbf{x}_1, \mathbf{x}_3) + v(\mathbf{x}_2, \mathbf{x}_3)$. In general, if we have N particles in $\mathbf{x}_1, \dots, \mathbf{x}_N$ the total interaction energy is $\sum_{i<j} v(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{2} \sum_{i \neq j} v(\mathbf{x}_i, \mathbf{x}_j)$. To derive the form of $\hat{H}_{\mathrm{int}}$ in second quantization we simply notice that the ket $|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$ is an eigenket of $\hat{H}_{\mathrm{int}}$ with eigenvalue $\frac{1}{2} \sum_{i \neq j} v(\mathbf{x}_i, \mathbf{x}_j)$:

$$\hat{H}_{\mathrm{int}} | \mathbf{x}_1 \dots \mathbf{x}_N \rangle = \left(\frac{1}{2} \sum_{i \neq j} v(\mathbf{x}_i, \mathbf{x}_j) \right) | \mathbf{x}_1 \dots \mathbf{x}_N \rangle. \tag{1.81}$$

Equivalently, (1.81) follows directly from the matrix element (1.70), which is valid for all $|\Psi\rangle$. Due to the presence of a double sum in (1.81) the operator $\hat{H}_{\mathrm{int}}$ must be a *quartic* form in the field operators. In (1.68) we proved that $|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$ is an eigenket of the density operator

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$\hat{n}(\mathbf{x})$ with eigenvalue $\sum_i \delta(\mathbf{x}-\mathbf{x}_i)$. This implies that $|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$ is also an eigenket of the operator $\hat{n}(\mathbf{x})\hat{n}(\mathbf{x}')$ with eigenvalue $\sum_{i,j} \delta(\mathbf{x}-\mathbf{x}_i)\delta(\mathbf{x}'-\mathbf{x}_j)$. Thus, taking into account that the double sum in (1.81) does not contain terms with $i=j$, the interaction energy operator is given by

$$\begin{aligned}\hat{H}_{\rm int} &= \frac{1}{2}\int d\mathbf{x}\, d\mathbf{x}'\, v(\mathbf{x},\mathbf{x}')\hat{n}(\mathbf{x})\hat{n}(\mathbf{x}') - \frac{1}{2}\int d\mathbf{x}\, v(\mathbf{x},\mathbf{x})\hat{n}(\mathbf{x}) \\ &= \frac{1}{2}\int d\mathbf{x}\, d\mathbf{x}'\, v(\mathbf{x},\mathbf{x}')\left(\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}') - \delta(\mathbf{x}-\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\right) \\ &= \frac{1}{2}\int d\mathbf{x}\, d\mathbf{x}'\, v(\mathbf{x},\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}). \end{aligned} \tag{1.82}$$

In the last equality we first use the (anti)commutation relation (1.47) to cancel the term proportional to $\delta(\mathbf{x}-\mathbf{x}')$, and then (1.40) to exchange the operators $\hat{\psi}(\mathbf{x})$ and $\hat{\psi}(\mathbf{x}')$. It is easy to verify that the action of $\hat{H}_{\rm int}$ on $|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$ yields (1.81). Like the one-body Hamiltonian $\hat{H}_0$, the interaction energy operator keeps the very same form independently of the number of particles. We call *two-body operators* those operators that can be written as a quartic form of the field operators and, in general, *n-body operators* those operators that contain a string of n field operators $\hat{\psi}^\dagger$ followed by a string of n field operators $\hat{\psi}$.

Total Hamiltonian The total Hamiltonian of a system of interacting identical particles is the sum of $\hat{H}_0$ and $\hat{H}_{\rm int}$ and reads

$$\boxed{\hat{H} = \int d\mathbf{x} d\mathbf{x}'\, \hat{\psi}^\dagger(\mathbf{x})\langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle\hat{\psi}(\mathbf{x}') + \frac{1}{2}\int d\mathbf{x}\, d\mathbf{x}' v(\mathbf{x},\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})} \tag{1.83}$$

Equation (1.83) is the main result of this section. To calculate the action of $\hat{H}$ on a ket $|\Psi\rangle$ we only need to know the (anti)commutation relations since $|\Psi\rangle$ can always be expanded in terms of $\hat{\psi}^\dagger(\mathbf{x}_1)\dots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle$. Equivalently, given a convenient one-body basis $\{|n\rangle\}$ we may work with the $\hat{d}$-operators. This is done by expressing $\hat{H}$ in terms of the $\hat{d}$-operators, expanding $|\Psi\rangle$ on the basis $\hat{d}^\dagger_{n_1}\dots\hat{d}^\dagger_{n_N}|0\rangle$, and then using the (anti)commutation relations (1.54) and (1.55). To express $\hat{H}$ in terms of the $\hat{d}$-operators, we simply substitute the expansion (1.60) in (1.83) and find

$$\hat{H} = \underbrace{\sum_{ij} h_{ij}\hat{d}^\dagger_i\hat{d}_j}_{\hat{H}_0} + \underbrace{\frac{1}{2}\sum_{ijmn} v_{ijmn}\hat{d}^\dagger_i\hat{d}^\dagger_j\hat{d}_m\hat{d}_n}_{\hat{H}_{\rm int}}, \tag{1.84}$$

with

$$h_{ij} = \langle i|\hat{h}|j\rangle = \sum_{\sigma\sigma'}\int d\mathbf{r}\, \varphi^*_i(\mathbf{r}\sigma)h_{\sigma\sigma'}(\mathbf{r},-\mathrm{i}\boldsymbol{\nabla},\mathbf{S})\varphi_j(\mathbf{r}\sigma') = h^*_{ji}, \tag{1.85}$$

and the so-called *Coulomb integrals*[6]

$$v_{ijmn} = \int d\mathbf{x}\, d\mathbf{x}'\, \varphi^*_i(\mathbf{x})\varphi^*_j(\mathbf{x}')v(\mathbf{x},\mathbf{x}')\varphi_m(\mathbf{x}')\varphi_n(\mathbf{x}). \tag{1.86}$$

[6] In fact, the nomenclature Coulomb integral is appropriate only if v is the Coulomb interaction.

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In the new basis the single-particle Hamiltonian in first quantization can be written in the ket–bra form

$$\hat{h} = \sum_{ij} h_{ij} \, |i\rangle\langle j|, \tag{1.87}$$

as can easily be checked by taking the matrix element $\langle i|\hat{h}|j\rangle$ and comparing with (1.85).

We recall that the quantum numbers of the general basis comprise an orbital and a spin quantum number. For later purposes it is instructive to highlight the spin structure in (1.84). We write the quantum numbers i, j, m, n as

$$i = s_1\sigma_1, \quad j = s_2\sigma_2, \quad m = s_3\sigma_3, \quad n = s_4\sigma_4.$$

Then the one-body part reads

$$\hat{H}_0 = \sum_{\substack{s_1 s_2 \\ \sigma_1\sigma_2}} h_{s_1\sigma_1 \, s_2\sigma_2} \hat{d}^\dagger_{s_1\sigma_1} \hat{d}_{s_2\sigma_2}.$$

In the absence of magnetic fields or spin–orbit coupling, h does not depend on $\mathbf{S}$ and hence its matrix elements are diagonal in spin space $h_{ij} = \delta_{\sigma_1\sigma_2} h_{s_1 s_2}$. In this case $\hat{H}_0$ takes the simpler form

$$\hat{H}_0 = \sum_{s_1 s_2} \sum_{\sigma} h_{s_1 s_2} \hat{d}^\dagger_{s_1\sigma} \hat{d}_{s_2\sigma}, \tag{1.88}$$

where $h_{s_1 s_2}$ is the spatial integral in (1.85) with the functions $\varphi_s(\mathbf{r})$ defined in (1.50). For interparticle interactions $v(\mathbf{x}_1, \mathbf{x}_2) = v(\mathbf{r}_1, \mathbf{r}_2)$ which are independent of spin the interaction Hamiltonian can be manipulated in a similar manner. From (1.86) we see that v_{ijmn} vanishes if j and m have different spin projection ($\sigma_2 \neq \sigma_3$) or if i and n have different spin projection ($\sigma_1 \neq \sigma_4$):

$$v_{ijmn} = \delta_{\sigma_2\sigma_3} \delta_{\sigma_1\sigma_4} v_{s_1 s_2 s_3 s_4}, \tag{1.89}$$

where $v_{s_1 s_2 s_3 s_4}$ is the spatial integral in (1.86) with the functions $\varphi_s(\mathbf{r})$. Inserting this form of the interaction into $\hat{H}_{\text{int}}$ we find

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{\substack{s_1 s_2 s_3 s_4 \\ \sigma\sigma'}} v_{s_1 s_2 s_3 s_4} \hat{d}^\dagger_{s_1\sigma} \hat{d}^\dagger_{s_2\sigma'} \hat{d}_{s_3\sigma'} \hat{d}_{s_4\sigma}. \tag{1.90}$$

We propose below a few simple exercises to practice with operators in second quantization. In the next chapter we illustrate physically relevant examples and use some of the identities from the exercises to acquire familiarity with the formalism of second quantization.

Exercise 1.4 Let $\hat{n}_n \equiv \hat{d}^\dagger_n \hat{d}_n$ be the occupation operator for particles with quantum number n, see (1.74). Prove that in the fermionic case

$$\hat{n}_n^2 = \hat{n}_n, \tag{1.91}$$

and hence that the eigenvalues of $\hat{n}_n$ are either 0 or 1 – that is, it is not possible to create two fermions in the same state $|n\rangle$. This is a direct consequence of the Pauli exclusion principle.

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Exercise 1.5 Prove that the total number of particle operators $\hat{N} = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$ can also be written as $\hat{N} = \sum_n \hat{d}_n^\dagger \hat{d}_n$ for any orthonormal basis $|n\rangle$. Calculate the action of $\hat{N}$ on a generic ket $|\Psi_N\rangle$ with N particles ($|\Psi_N\rangle \in \mathbb{H}_N$) and prove that

$$\hat{N}|\Psi_N\rangle = N|\Psi_N\rangle.$$

Exercise 1.6 Prove that $\hat{N}$ commutes with $\hat{H}_0$ and $\hat{H}_{\rm int}$ – that is,

$$[\hat{N}, \hat{H}_0]_- = [\hat{N}, \hat{H}_{\rm int}]_- = 0. \tag{1.92}$$

This means that the eigenkets of $\hat{H}$ can be chosen as kets with a fixed number of particles.

Exercise 1.7 Let $n = s\sigma$ and $\sigma = \uparrow, \downarrow$ be the spin projection for fermions of spin $1/2$. We consider the operators

$$\hat{S}_s^z \equiv \frac{1}{2}(\hat{n}_{s\uparrow} - \hat{n}_{s\downarrow}), \qquad \hat{S}_s^+ \equiv \hat{d}_{s\uparrow}^\dagger \hat{d}_{s\downarrow}, \qquad \hat{S}_s^- \equiv \hat{d}_{s\downarrow}^\dagger \hat{d}_{s\uparrow} = (\hat{S}_s^+)^\dagger. \tag{1.93}$$

Using the anticommutation relations, prove that the action of the above operators on the kets $|s\sigma\rangle \equiv \hat{d}_{s\sigma}^\dagger|0\rangle$ is

$$\hat{S}_s^z|s\uparrow\rangle = \frac{1}{2}|s\uparrow\rangle, \qquad \hat{S}_s^+|s\uparrow\rangle = |\emptyset\rangle, \qquad \hat{S}_s^-|s\uparrow\rangle = |s\downarrow\rangle,$$

and

$$\hat{S}_s^z|s\downarrow\rangle = -\frac{1}{2}|s\downarrow\rangle, \qquad \hat{S}_s^+|s\downarrow\rangle = |s\uparrow\rangle, \qquad \hat{S}_s^-|s\downarrow\rangle = |\emptyset\rangle.$$

To what operators do $\hat{S}_s^z$, $\hat{S}_s^+$, $\hat{S}_s^-$ correspond?

Exercise 1.8 Let us define the *spin operators* along the x and y directions as

$$\hat{S}_s^x \equiv \frac{1}{2}(\hat{S}_s^+ + \hat{S}_s^-), \qquad \hat{S}_s^y \equiv \frac{1}{2\mathrm{i}}(\hat{S}_s^+ - \hat{S}_s^-),$$

and the spin operator $\hat{S}_s^z$ along the z direction as in (1.93). Prove that these operators can also be written as

$$\hat{S}_s^j = \frac{1}{2}\sum_{\sigma\sigma'} \hat{d}_{s\sigma}^\dagger \sigma^j_{\sigma\sigma'} \hat{d}_{s\sigma'}, \qquad j = x, y, z, \tag{1.94}$$

with

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

the *Pauli matrices*. Using the anticommutation relations, verify that

$$[\hat{S}_s^i, \hat{S}_{s'}^j]_- = \mathrm{i}\delta_{ss'} \sum_{k=x,y,z} \varepsilon_{ijk} \hat{S}_s^k,$$

where ε_{ijk} is the *Levi-Civita tensor*.[7]

[7] The Levi-Civita tensor is zero if at least two indices are equal and otherwise

$$\varepsilon_{P(1)P(2)P(3)} = (-)^P,$$

where P is an arbitrary permutation of the indices $1, 2, 3$.

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