Chapter 3

Second Quantization

The formulation of quantum many-body systems introduced so far dealt first with distinguishable particles and necessitated then to perform afterwards a(n) (anti-)symmetrization of wave functions in order to describe indistinguishable particles in form of bosons (fermions). Usually this procedure turns out to be quite cumbersome due the huge number of particles involved in a quantum many-body system. Therefore, one has worked out second quantization as an alternative formulation for describing quantum many-body systems, which has the advantage that it automatically takes into account the (anti-)symmetrization of wave functions. It is based on the ladder formalism, which allows an algebraic treatment of the first quantized harmonic oscillator and is therefore initially reviewed. Afterwards, we heuristically formulate second quantization, which represents the technical basis for non-relativistic quantum many-body theory. Due to the introduction of creation and annihilation operators for identical particles we are able to describe interacting bosonic and fermionic systems involving an arbitrary number of particles. This is relevant for concrete applications in the realm of solid-state physics like the description of Bose-Einstein condensation and superfluidity as well as the Bardeen-Cooper-Schrieffer theory of superconductivity, which is not the content of this lecture. But, a similar second quantization formalism is later on used to quantize relativistic fields like the Maxwell and the Dirac field and, thus, represents the very basis for quantum electrodynamics.

3.1 Harmonic Oscillator

The harmonic oscillator represents a standard quantum mechanical model with which it is possible to describe quite successfully, for instance, collective oscillations in molecules or in solids. The Hamilton operator of a one-dimensional harmonic oscillator with mass M and frequency ω reads

$$\hat{H} = \frac{\hat{p}^2}{2M} + \frac{M}{2}\,\omega^2 \hat{x}^2 \,, \tag{3.1}$$

where one demands non-trivial commutation relations between the coordinate operator $\hat{q}$ and the momentum operator $\hat{p}$ analogous to (2.12):

$$\left[\hat{x},\hat{x}\right]_- = \left[\hat{p},\hat{p}\right]_- = 0\,, \qquad \left[\hat{p},\hat{x}\right]_- = \frac{\hbar}{i}\,. \tag{3.2}$$

The problem is now to solve the eigenvalue problem of the Hamilton operator

$$\hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle\,, \tag{3.3}$$

i.e. to determine how the energy eigenvalues E_α and the energy eigenfunctions $|\alpha\rangle$ depend on the quantum number α. Usually this representation-free eigenvalue problem (3.3) is transformed into the coordinate representation, so it amounts to solve the corresponding Schrödinger equation by taking into account the appropriate Dirichlet boundary condition. In the following, however, we proceed differently by solving the representation-free eigenvalue problem (3.3) directly by taking into account the cummator relations (3.2).

At first, the two hermitian operators $\hat{x}$ and $\hat{p}$ are transformed into two new operators $\hat{a}^\dagger$ and $\hat{a}$, which are adjoint with respect to each other:

$$\hat{a}^\dagger = \sqrt{\frac{M\omega}{2\hbar}}\left(\hat{x} - \frac{i}{M\omega}\,\hat{p}\right)\,, \qquad \hat{a} = \sqrt{\frac{M\omega}{2\hbar}}\left(\hat{x} + \frac{i}{M\omega}\,\hat{p}\right)\,. \tag{3.4}$$

The inverse transformation reads correspondingly

$$\hat{x} = \sqrt{\frac{\hbar}{2M\omega}}\left(\hat{a}^\dagger + \hat{a}\right)\,, \qquad \hat{p} = \sqrt{\frac{\hbar M\omega}{2}}\,i\left(\hat{a}^\dagger - \hat{a}\right)\,. \tag{3.5}$$

Here the physical dimension of the coordinate operator $\hat{x}$ is provided by the oscillator length $\sqrt{\hbar/(2M\omega)}$, whereas the corresponding one $\sqrt{\hbar M\omega/2}$ of the momentum operator $\hat{p}$ is related to the oscillator length via the Heisenberg uncertainty relation. Inserting (3.5) into (3.1), the Hamilton operator of the harmonic oscillator can be expressed in terms of the new operators $\hat{a}^\dagger$ and $\hat{a}$, yielding

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right)\,. \tag{3.6}$$

Furthermore, the transformation (3.4) allows to deduce from (3.2) the commutation relations between the new operators $\hat{a}^\dagger$ and $\hat{a}$:

$$\left[\hat{a},\hat{a}\right]_- = \left[\hat{a}^\dagger,\hat{a}^\dagger\right]_- = 0\,, \qquad \left[\hat{a},\hat{a}^\dagger\right]_- = 1\,. \tag{3.7}$$

Using (3.7) the Hamilton operator of the harmonic oscillator (3.6) reduces to

$$\hat{H} = \hbar\omega\left(\hat{n} + \frac{1}{2}\right)\,, \tag{3.8}$$

where the zero-point energy $\hbar\omega/2$ and the operator

$$\hat{n} = \hat{a}^\dagger\hat{a} \tag{3.9}$$

appear. In order to calculate commutators the following identity turns out to be quite useful

$$\left[\hat{A}\hat{B},\hat{C}\right]_- = \hat{A}\left[\hat{B},\hat{C}\right]_- + \left[\hat{A},\hat{C}\right]_- \hat{B}\,, \tag{3.10}$$

which follows immediately from the definition of the commutator (2.13). Indeed, applying (3.10) we obtain the commutation relations for the operator (3.9):

$$\left[\hat{n},\hat{a}^\dagger\right]_- = \hat{a}^\dagger\,, \tag{3.11}$$

$$\left[\hat{n},\hat{a}\right]_- = -\hat{a}\,. \tag{3.12}$$

Let us now consider the eigenvalue problem of the operator (3.9):

$$\hat{n}|\lambda\rangle = \lambda|\lambda\rangle \tag{3.13}$$

As the operator (3.9) is hermitian, its eigenvalues λ must be real. Furthermore, the commutation relations (3.11) and (3.12) allow to investigate which consequences occur once the operators $\hat{a}^\dagger$ and $\hat{a}$ are applied to the eigenfunctions $|\lambda\rangle$. On the one hand we read off from (3.11) and (3.13)

$$\hat{n}\hat{a}^\dagger|\lambda\rangle = \left(\hat{a}^\dagger\hat{n} + \hat{a}^\dagger\right)|\lambda\rangle = (\lambda+1)\hat{a}^\dagger|\lambda\rangle \qquad \Longrightarrow \qquad \hat{a}^\dagger|\lambda\rangle \sim |\lambda+1\rangle\,, \tag{3.14}$$

on the other hand we conclude from (3.12) and (3.13)

$$\hat{n}\hat{a}|\lambda\rangle = \left(\hat{a}\hat{n} - \hat{a}\right) = (\lambda-1)\hat{a}|\lambda\rangle \qquad \Longrightarrow \qquad \hat{a}|\lambda\rangle \sim |\lambda-1\rangle\,. \tag{3.15}$$

Thus, the operators $\hat{a}^\dagger$ and $\hat{a}$ can be considered as ladder operators, which allow to climb up or down the ladder of eigenfunctions $|\lambda\rangle$. Applying the raising (lowering) ladder operator $\hat{a}^\dagger$ ($\hat{a}$) to $|\lambda\rangle$ yields an eigenfunction corresponding to an eigenvalue which is increased (decreased) by one, see Fig. 3.1

Furthermore, one can show that the eigenvalues λ of the operator $\hat{N}$ are always positive by taking into account (3.9) and (3.13) and by assuming without loss of generality that the eigenfunctions $|\lambda\rangle$ are normalized:

$$0 \leq \langle\hat{a}\lambda|\hat{a}\lambda\rangle = \langle\lambda|\hat{a}^\dagger\hat{a}|\lambda\rangle = \langle\lambda|\hat{n}|\lambda\rangle = \lambda\langle\lambda|\lambda\rangle = \lambda\,. \tag{3.16}$$

From (3.15) and (3.16) we conclude that the eigenvalues λ are given by positive integer number including zero:

$$\lambda = n = 0,1,2,\ldots\,. \tag{3.17}$$

If there were a positive, non-integer eigenvalue λ, one could apply iteratively the lowering ladder operator $\hat{a}$ and reduce in this way the eigenvalue due to (3.15) until it would become negative. But this would then contradict the inequality (3.16). Thus, due to this contradiction proof, there must be a ground state $|0\rangle$ with the property

$$\hat{a}|0\rangle = 0 \qquad \Longleftrightarrow \qquad \langle 0|\hat{a}^\dagger = 0\,. \tag{3.18}$$

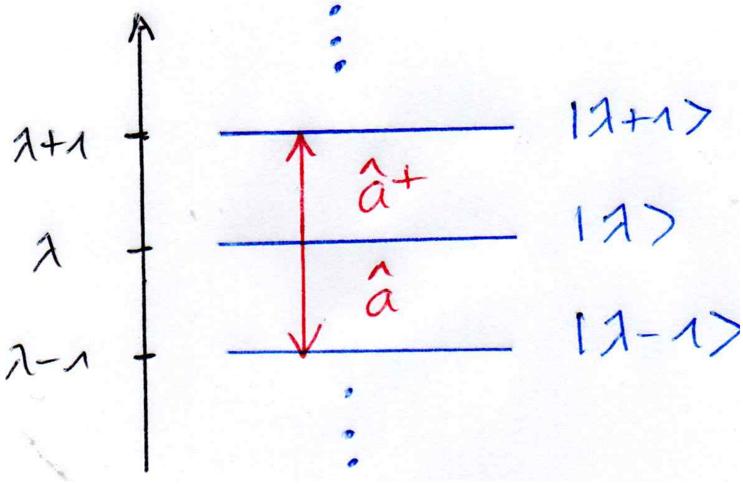

Figure 3.1: Raising (lowering) operator $\hat{a}^\dagger$ ($\hat{a}$) increases (decreases) the quantum number λ of the harmonic oscillator by one.

Normalized eigenfunctions $|n\rangle$ can then be constructed as follows. At first, we deduce from (3.7), (3.9), (3.13), and (3.17):

$$\langle \hat{a}^\dagger n|\hat{a}^\dagger n\rangle = \langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|\big(\hat{a}^\dagger\hat{a}+1\big)|n\rangle = \langle n|\big(\hat{n}+1\big)|n\rangle = n+1\,. \tag{3.19}$$

From (3.14), (3.17), and (3.19) follows a rule how applying the raising ladder operator $\hat{a}^\dagger$ upon the normalized eigenfunction $|n\rangle$ yields the next normalized eigenfunction $|n+1\rangle$:

$$\hat{a}^\dagger|n\rangle = C_n|n+1\rangle \quad\Longrightarrow\quad C_n^2\langle n+1|n+1\rangle = (n+1) \quad\Longrightarrow\quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{3.20}$$

And then iterating (3.20) yields a prescription how the eigenfunctions $|n\rangle$ can be constructed from the ground state $|0\rangle$ defined by (3.18):

$$|n\rangle = \frac{1}{\sqrt{n}}\,\hat{a}^\dagger|n-1\rangle = \frac{1}{\sqrt{n(n-1)}}\,\big(\hat{a}^2\big)^2|n-2\rangle = \dots \quad\Longrightarrow\quad |n\rangle = \frac{1}{\sqrt{n!}}\,\big(\hat{a}^\dagger\big)^n|0\rangle\,. \tag{3.21}$$

For the sake of completeness we also determine the action of the lowering ladder operator $\hat{a}$ upon the eigenfunction $|n\rangle$. At first we obtain from (2.68), (3.13), and (3.17)

$$\langle \hat{a}n|\hat{a}n\rangle = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n|\hat{n}|n\rangle = n\,. \tag{3.22}$$

Thus, we conclude from (3.15) and (3.22)

$$\hat{a}|n\rangle = D_n|n-1\rangle \quad\Longrightarrow\quad D_n^2\langle n-1|n-1\rangle = n \quad\Longrightarrow\quad \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle\,. \tag{3.23}$$

Furthermore, we read off from (3.8), (3.9), (3.13), and (3.17) the energy eigenvalues of the harmonic oscillator

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right)\,. \tag{3.24}$$

3.2 Creation and Annihilation Operators for Bosons

This ladder formalism for the algebraic treatment of the first quantized harmonic oscillator is now used in the realm of second quantization for describing indistinguishable identical bosons. We outline heuristically this basic idea by working out the analogy step by step:

- Whereas n describes the quantum number of the 1-particle system, we denote from now on with $n_{\mathbf{x}}$ the number of bosons at space point $\mathbf{x}$.

- The ladder operators $\hat{a}^\dagger$ and $\hat{a}$, which are defined by the commutator relations (3.7), allow to increase and decrease the quantum number n of the harmonic oscillator. Correspondingly we introduce operators $\hat{a}_{\mathbf{x}}^\dagger$ and $\hat{a}_{\mathbf{x}}$ via the commutator relations

$$\left[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}\right]_- = \left[\hat{a}_{\mathbf{x}}^\dagger, \hat{a}_{\mathbf{x}'}^\dagger\right]_- = 0\,, \qquad \left[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}^\dagger\right]_- = \delta(\mathbf{x}-\mathbf{x}')\,. \tag{3.25}$$

  With these commutator relations at hand, we can now proceed and deduce similar conclusions for the second quantized description of many bosons as we have just obtained for the first quantized harmonic oscillator. In particular, this allows to determine a concrete physical interpretation for the operators $\hat{a}_{\mathbf{x}}^\dagger$ and $\hat{a}_{\mathbf{x}}$.

- The operator $\hat{n} = \hat{a}^\dagger\hat{a}$ has turned out to have the eigenvalues n, which follows ultimately from the commutator relations (3.11) and (3.12). Analogously we define the particle number operator

$$\hat{N} = \int d^3x'\, \hat{a}_{\mathbf{x}'}^\dagger \hat{a}_{\mathbf{x}'} \tag{3.26}$$

  which obeys due to (3.10), (3.25), and (3.26) the commutator relations

$$\left[\hat{N}, \hat{a}_{\mathbf{x}}^\dagger\right]_- = \hat{a}_{\mathbf{x}}^\dagger\,, \tag{3.27}$$

$$\left[\hat{N}, \hat{a}_{\mathbf{x}}\right]_- = -\hat{a}_{\mathbf{x}}\,. \tag{3.28}$$

  Note that we have deliberately introduced in the commutator relations (3.25) a delta function in order to obtain for the particle number operator (3.26) commutator relations (3.27), (3.28) in analogy to (3.11) and (3.12). This has the consequence that the operators $\hat{a}_{\mathbf{x}}^\dagger$ and $\hat{a}_{\mathbf{x}}$ can be interpreted as a creation and annihilator operator as they create and annihilate a boson at space point $\mathbf{x}$, respectively.

- The first quantized harmonic oscillator has a ground state $|0\rangle$, which is introduced according to (3.18). In a similar way we define in second quantization a vacuum state $|0\rangle$ via

$$\hat{a}_{\mathbf{x}}|0\rangle = 0 \qquad \Longleftrightarrow \qquad \langle 0|\hat{a}_{\mathbf{x}}^\dagger = 0\,. \tag{3.29}$$

- Similar to (3.21) an iterative application of creation operators to the vacuum state yields the basis states of the underlying Hilbert space for describing bosons

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^{+1} = \hat{a}^\dagger_{\mathbf{x}_1} \cdots \hat{a}^\dagger_{\mathbf{x}_n} |0\rangle \,, \tag{3.30}$$

where we assume that the space coordinates differ pairwise, i.e. $\mathbf{x}_i \neq \mathbf{x}_j$ for all $i \neq j$. For the sake of illustration we exemplary verify the identity of (2.73) and (3.30) for $n = 1$ and $n = 2$ bosons in the coordinate representation. From (2.72), (3.25), (3.29), and (3.30) we obtain at first

$$\begin{aligned} {}^{+1}\langle \mathbf{x}_1 | \mathbf{x}_1' \rangle^{+1} &= \langle \hat{a}^\dagger_{\mathbf{x}_1} 0 | \hat{a}^\dagger_{\mathbf{x}_1'} 0 \rangle = \langle 0 | \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}_1'} | 0 \rangle \\ &= \langle 0 | \hat{a}^\dagger_{\mathbf{x}_1'} \hat{a}_{\mathbf{x}_1} + \delta(\mathbf{x}_1 - \mathbf{x}_1') | 0 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}_1') = \delta^{+1}(\mathbf{x}_1; \mathbf{x}_1') \,. \end{aligned} \tag{3.31}$$

Correspondingly, we get then

$$\begin{aligned} &{}^{+1}\langle \mathbf{x}_1, \mathbf{x}_2 | \mathbf{x}_1', \mathbf{x}_2' \rangle^{+1} = \langle \hat{a}^\dagger_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}_2} 0 | \hat{a}^\dagger_{\mathbf{x}_1'} \hat{a}^\dagger_{\mathbf{x}_2'} 0 \rangle = \langle 0 | \hat{a}_{\mathbf{x}_2} \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}_1'} \hat{a}^\dagger_{\mathbf{x}_2'} | 0 \rangle \\ &= \langle 0 | \hat{a}_{\mathbf{x}_2} \left[\hat{a}^\dagger_{\mathbf{x}_1'} \hat{a}_{\mathbf{x}_1} + \delta(\mathbf{x}_1 - \mathbf{x}_1') \right] \hat{a}^\dagger_{\mathbf{x}_2'} | 0 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}_1') \langle 0 | \hat{a}^\dagger_{\mathbf{x}_2'} \hat{a}_{\mathbf{x}_2} + \delta(\mathbf{x}_2 - \mathbf{x}_2') | 0 \rangle \\ &+ \langle 0 | \left[\hat{a}^\dagger_{\mathbf{x}_1'} \hat{a}_{\mathbf{x}_2} + \delta(\mathbf{x}_1' - \mathbf{x}_2) \right] \left[\hat{a}^\dagger_{\mathbf{x}_2'} \hat{a}_{\mathbf{x}_1} + \delta(\mathbf{x}_1 - \mathbf{x}_2') \right] | 0 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}_1') \delta(\mathbf{x}_2 - \mathbf{x}_2') \\ &+ \delta(\mathbf{x}_1 - \mathbf{x}_2') \delta(\mathbf{x}_2 - \mathbf{x}_1') = \delta^{+1}(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_1', \mathbf{x}_2') \,. \end{aligned} \tag{3.32}$$

3.3 Schrödinger Equation for Interacting Bosons

Introducing local creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}$ has not only the advantage of constructing many-particle states, which automatically have the correct symmetry. In addition one obtains a universal form of the time-dependent Schrödinger equation, which turns out to be independent of the particle number n. In its representation-independent form it reads

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \,. \tag{3.33}$$

Here $|\psi(t)\rangle$ denotes some many-particle state in the second-quantized Hilbert space, which is spanned by the basis states (3.30). The second-quantized Hamilton operator $\hat{H}$ consists of two terms:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 \,. \tag{3.34}$$

The local Hamilton operator $\hat{H}_1$ is determined the 1-particle Hamilton operator of non-interacting bosons

$$-\frac{\hbar^2}{2M} \Delta + V_1(\mathbf{x}) \,. \tag{3.35}$$

Due to the sandwich principle the first-quantized Hamilton operator (3.35) is multiplied with the local creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}$ to the left and to the right, respectively, so a subsequent integration over the coordinate $\mathbf{x}$ yields the corresponding second-quantized 1-particle Hamilton operator:

$$\hat{H}_1 = \int d^3x \, \hat{a}^\dagger_{\mathbf{x}} \left\{ -\frac{\hbar^2}{2M} \, \Delta + V_1(\mathbf{x}) \right\} \hat{a}_{\mathbf{x}} \, . \tag{3.36}$$

Correspondingly the bi-local Hamilton operator $\hat{H}_2$ is constructed with the help of the 2-particle interaction $V_2(\mathbf{x} - \mathbf{x}')$:

$$\hat{H}_2 = \frac{1}{2} \int d^3x \int d^3x' \, \hat{a}^\dagger_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}'} \, V_2(\mathbf{x} - \mathbf{x}') \hat{a}_{\mathbf{x}'} \, \hat{a}_{\mathbf{x}} \, . \tag{3.37}$$

Note that in both terms (3.36) and (3.37) the creation and annihilation operators appear at the left and at the right, respectively. This particular ordering of second-quantized operators is called normal ordering. It has the consequence that the vacuum energy of the Hamilton operator defined by (3.34), (3.36), and (3.37) vanishes due to the definition of the vacuum state in (3.29):

$$\hat{H}|0\rangle = 0 \qquad \Longleftrightarrow \qquad \langle 0|\hat{H} = 0 \, . \tag{3.38}$$

In the following we demonstrate that the operator character of $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}$ is essential for the fact that the Schrödinger equation (3.33) describes a many-body problem. To this end we multiply (3.33) from the left with the adjoint of the basis state (3.30)

$$^{+1}\langle \mathbf{x}_1, \ldots, \mathbf{x}_n| = \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} \, . \tag{3.39}$$

With this we get at first

$$i\hbar \, \frac{\partial}{\partial t} \, \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}|\psi(t)\rangle = \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1} \hat{H}|\psi(t)\rangle \, . \tag{3.40}$$

Due to (3.38) we can express the right-hand side of (3.40) in terms of a commutator

$$i\hbar \, \frac{\partial}{\partial t} \, \langle 0|\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}|\psi(t)\rangle = \langle 0| \left[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{H}\right]_- |\psi(t)\rangle \, . \tag{3.41}$$

Taking into account both contributions (3.36) and (3.37) of the Hamilton operator this leads to the expression

$$\int d^3y \int d^3z \, \delta(\mathbf{y} - \mathbf{z}) \left\{ -\frac{\hbar^2}{2M} \, \Delta_{\mathbf{z}} + V_1(\mathbf{z}) \right\} \langle 0| \left[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}} \hat{a}_{\mathbf{z}}\right]_- |\psi(t)\rangle + \frac{1}{2} \int d^3y_1 \int d^3y_2$$
$$\cdot \int d^3z_1 \int d^3z_2 \, \delta(\mathbf{y}_1 - \mathbf{z}_1)\delta(\mathbf{y}_2 - \mathbf{z}_2) \, V_2(\mathbf{z}_1 - \mathbf{z}_2)\langle 0| \left[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}_1} \hat{a}^\dagger_{\mathbf{y}_2} \hat{a}_{\mathbf{z}_2} \hat{a}_{\mathbf{z}_1}\right]_- |\psi(t)\rangle \, . \tag{3.42}$$

In order to evaluate the first commutator in (3.42) we use an identity similar to (3.10)

$$\left[\hat{A}, \hat{B}\hat{C}\right]_- = \left[\hat{A}, \hat{B}\right]_- \hat{C} + \hat{B}\left[\hat{A}, \hat{C}\right]_- \, , \tag{3.43}$$

which yields

$$\left[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}} \hat{a}_{\mathbf{z}}\right]_- = \left[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{y}}\right]_- \hat{a}_{\mathbf{z}} + \hat{a}^\dagger_{\mathbf{y}} \left[\hat{a}_{\mathbf{x}_n} \cdots \hat{a}_{\mathbf{x}_1}, \hat{a}_{\mathbf{z}}\right]_- \, . \tag{3.44}$$

Note that here the second term vanishes as the annihilation operators commute with respect to each other due to (3.25). Applying now recursively the identity (3.10), we get

$$\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}}\right]_- = \sum_{\nu=1}^{n}\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\left[\hat{a}_{\mathbf{x}_\nu},\hat{a}^{\dagger}_{\mathbf{y}}\right]_-\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}\,, \tag{3.45}$$

where the remaining commutators yield a delta function $\delta(\mathbf{x}_\nu-\mathbf{y})$ due to (3.25):

$$\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}}\right]_- = \sum_{\nu=1}^{n}\delta(\mathbf{y}-\mathbf{x}_\nu)\,\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}\,. \tag{3.46}$$

Thus, the first expectation value in (3.42) yields

$$\langle 0|\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}}\hat{a}_{\mathbf{z}}\right]_-|\psi(t)\rangle = \sum_{\nu=1}^{n}\delta(\mathbf{x}_\nu-\mathbf{y})\langle 0|\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{z}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}|\psi(t)\rangle\,. \tag{3.47}$$

In a similar manner we proceed also for the second commutator in (3.42) by applying the identity (3.43) twice, yielding

$$\begin{aligned}\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\left(\hat{a}^{\dagger}_{\mathbf{y}_1}\hat{a}^{\dagger}_{\mathbf{y}_2}\right)\left(\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\right)\right]_- &= \left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_1}\hat{a}^{\dagger}_{\mathbf{y}_2}\right]_-\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\\ = \left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_1}\right]_-\hat{a}^{\dagger}_{\mathbf{y}_2}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1} &+ \hat{a}^{\dagger}_{\mathbf{y}_1}\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_2}\right]_-\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\end{aligned} \tag{3.48}$$

Thus, taking into account (3.46) reduces (3.48) to

$$\begin{aligned}\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_1}\hat{a}^{\dagger}_{\mathbf{y}_2}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\right]_- &= \sum_{\nu=1}^{n}\delta(\mathbf{x}_\nu-\mathbf{y}_1)\,\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}\hat{a}^{\dagger}_{\mathbf{y}_2}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\\ +\sum_{\nu=1}^{n}\delta(\mathbf{x}_\nu-\mathbf{y}_2)\,\hat{a}^{\dagger}_{\mathbf{y}_1}\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\,.\end{aligned} \tag{3.49}$$

Now we determine the second expectation value in (3.42) from (3.49). Due to (3.29) we observe that the second term in (3.49) then vanishes and the first term can be rewritten as a commutator:

$$\begin{aligned}&\langle 0|\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_1}\hat{a}^{\dagger}_{\mathbf{y}_2}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\right]_-|\psi(t)\rangle\\ &= \sum_{\nu=1}^{n}\delta(\mathbf{x}_\nu-\mathbf{y}_1)\,\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_2}\right]_-\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}|\psi(t)\rangle\,.\end{aligned} \tag{3.50}$$

Using again (3.46) we can then evaluate (3.50):

$$\begin{aligned}&\langle 0|\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1},\hat{a}^{\dagger}_{\mathbf{y}_1}\hat{a}^{\dagger}_{\mathbf{y}_2}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{z}_1}\right]_-|\psi(t)\rangle\\ &= \sum_{\nu=1}^{n}\sum_{\mu=1}^{n}\delta(\mathbf{x}_\nu-\mathbf{y}_1)\delta(\mathbf{x}_\mu-\mathbf{y}_2)\langle 0|\hat{a}_{\mathbf{x}_n}\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{z}_1}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_{\mu+1}}\hat{a}_{\mathbf{z}_2}\hat{a}_{\mathbf{x}_{\mu-1}}\cdots\hat{a}_{\mathbf{x}_1}|\psi(t)\rangle\,.\end{aligned} \tag{3.51}$$

Finally, inserting the intermediate results (3.47) and (3.51) into the projected Schrödinger equation (3.40) and the expectation value of the Hamilton operator (3.42) as well as performing the integrations over the delta functions yields the n-particle Schrödinger equation (2.21) with (2.23). Here we take into account that the n-particle wave function $\psi(\mathbf{x}_1,\ldots\mathbf{x}_n;t)$ follows from projecting the state $|\psi(t)\rangle$ upon the basis state (3.30) similar to (2.20):

$$\psi^{+1}(\mathbf{x}_1,\ldots\mathbf{x}_n;t) = {}^{+1}\langle\mathbf{x}_1,\ldots,\mathbf{x}_n|\psi(t)\rangle\,. \tag{3.52}$$

3.4 Field Operators in Heisenberg Picture

So far the non-relativistic many-body theory was formulated in the Schrödinger picture as the local particle creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}$ were time-independent, whereas the many-body state $|\psi(t)\rangle$ from the second quantized Hilbert space was time-dependent. Now we perform the transformation to the Heisenberg picture, where the many-body state is time-independent and the whole time dependence is carried by so-called field operators.

At first we repeat the general procedure in first quantization. To this end we start with the Schrödinger picture and restrict ourselves for the sake of simplicity to the case of a time-independent Hamilton operator $\hat{H}_{\rm S}$. The corresponding equations of motion for both the time-dependent state $|\psi_{\rm S}(t)\rangle$ and a time-independent operator $\hat{O}_{\rm S}$ read

$$i\hbar \frac{\partial}{\partial t} |\psi_{\rm S}(t)\rangle = \hat{H}_{\rm S} |\psi_{\rm S}(t)\rangle , \tag{3.53}$$

$$i\hbar \frac{\partial}{\partial t} \hat{O}_{\rm S} = 0 . \tag{3.54}$$

The formal solution of the Schrödinger equation (3.53) is given by

$$|\psi_{\rm S}(t)\rangle = e^{-i\hat{H}_{\rm S}t/\hbar} |\psi_{\rm S}(0)\rangle . \tag{3.55}$$

Here we identify the initial state $|\psi_{\rm S}(0)\rangle$ in the Schrödinger picture with the state $|\psi_{\rm H}\rangle$ in the Heisenberg picture:

$$|\psi_{\rm S}(0) = |\psi_{\rm H}\rangle . \tag{3.56}$$

Thus, the transformations from the Schrödinger to the Heisenberg picture and vice versa are defined according to the relations

$$|\psi_{\rm S}(t)\rangle = e^{-i\hat{H}_{\rm S}t/\hbar} |\psi_{\rm H}\rangle \qquad \Longleftrightarrow \qquad |\psi_{\rm H}\rangle = e^{i\hat{H}_{\rm S}t/\hbar} |\psi_{\rm S}(t)\rangle . \tag{3.57}$$

From (3.53) and (3.57) we then read off that the state in the Heisenberg picture $|\psi_{\rm H}\rangle$ is time-independent:

$$i\hbar \frac{\partial}{\partial t} |\psi_{\rm H}\rangle = -\hat{H}_{\rm S}\, e^{i\hat{H}_{\rm S}t/\hbar} |\psi_{\rm S}(t)\rangle + e^{i\hat{H}_{\rm S}t/\hbar}\, i\hbar \frac{\partial}{\partial t} |\psi_{\rm S}(t)\rangle = 0 . \tag{3.58}$$

In order to determine the operator $\hat{O}_{\rm H}(t)$ in the Heisenberg picture, we demand that the expectation values do not change once we perform a transformation from the Schrödinger to the Heisenberg picture:

$$\langle\psi_{\rm S}(t)|\hat{O}_{\rm S}|\psi_{\rm S}(t)\rangle = \langle\psi_{\rm H}|\hat{O}_{\rm H}(t)|\psi_{\rm H}\rangle . \tag{3.59}$$

Inserting (3.57) into (3.59) we determine, indeed, formally the time dependence of the operator $\hat{O}_{\rm H}(t)$ in the Heisenberg picture:

$$\begin{aligned} \langle e^{-i\hat{H}_{\rm S}t/\hbar}\,\psi_{\rm H}|\hat{O}_{\rm S}|e^{-i\hat{H}_{\rm S}t/\hbar}\,\psi_{\rm H}\rangle &= \langle\psi_{\rm H}|e^{i\hat{H}_{\rm S}t/\hbar}\,\hat{O}_{\rm S}e^{-i\hat{H}_{\rm S}t/\hbar}|\psi_{\rm H}\rangle = \langle\psi_{\rm H}|\hat{O}_{\rm H}(t)|\psi_{\rm H}\rangle . \\ &\Longrightarrow \quad \hat{O}_{\rm H}(t) = e^{i\hat{H}_{\rm S}t/\hbar}\,\hat{O}_{\rm S}\,e^{-i\hat{H}_{\rm S}t/\hbar} . \end{aligned} \tag{3.60}$$

For instance, for the Hamilton operator $\hat{O}_{\rm S} = \hat{H}_{\rm S}$ we obtain from (3.60) the result that it does not change its form when we perform the transformation from the Schrödinger to the Heisenberg picture:

$$\hat{H}_{\rm H}(t) = e^{i\hat{H}_{\rm S}t/\hbar}\,\hat{H}_{\rm S}\,e^{-i\hat{H}_{\rm S}t/\hbar} = \hat{H}_{\rm S}\,. \tag{3.61}$$

Furthermore, for the operator in the Heisenberg picture $\hat{O}_{\rm H}(t)$ we determine from (3.54), (3.60), and (3.61) the Heisenberg equation of motion:

$$\begin{aligned} i\hbar\,\frac{\partial}{\partial t}\,\hat{O}_{\rm H}(t) &= e^{i\hat{H}_{\rm S}t/\hbar}\left\{-\hat{H}_{\rm S}\hat{O}_{\rm S}+\hat{O}_{\rm S}\hat{H}_{\rm S}\right\}e^{-i\hat{H}_{\rm S}t/\hbar} + e^{i\hat{H}_{\rm S}t/\hbar}\,i\hbar\,\frac{\partial}{\partial t}\,\hat{O}_{\rm S}\,e^{-i\hat{H}_{\rm S}t/\hbar} \\ &\Longrightarrow\; i\hbar\,\frac{\partial}{\partial t}\,\hat{O}_{\rm H}(t) = \left[\hat{O}_{\rm H}(t),\hat{H}_{\rm S}\right]_- = \left[\hat{O}_{\rm H}(t),\hat{H}_{\rm H}(t)\right]_-\,. \end{aligned} \tag{3.62}$$

Now we transfer this procedure to the second quantization. To this end we assign analogous to (3.60) to the local particle creation and annihilation operators $\hat{a}_{\mathbf{x}}^\dagger$ and $\hat{a}_{\mathbf{x}}$ in the Schrödinger picture corresponding time-dependent fields operators in the Heisenberg picture:

$$\hat{\psi}^\dagger(\mathbf{x},t) = \hat{a}_{\mathbf{x}\rm H}^\dagger(t) = e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}^\dagger\,e^{-i\hat{H}t/\hbar}\,, \qquad \hat{\psi}(\mathbf{x},t) = \hat{a}_{\mathbf{x}\rm H}(t) = e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}\,e^{-i\hat{H}t/\hbar}\,. \tag{3.63}$$

At first we determine from (3.25) and (3.63) the equal-time commutator relations of these field operators:

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}(\mathbf{x}',t)\right]_- = \left[\hat{\psi}^\dagger(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\right]_- = 0\,, \quad \left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\right]_- = \delta(\mathbf{x}-\mathbf{x}')\,. \tag{3.64}$$

Thus, the field operators $\hat{\psi}^\dagger(\mathbf{x},t)$, $\hat{\psi}(\mathbf{x},t)$ in the Heisenberg picture fulfill at each time instant t the same commutator relations (3.25) as the local creation and annihilation operators $\hat{a}_{\mathbf{x}}^\dagger$, $\hat{a}_{\mathbf{x}}$ in the Schrödinger picture. This means that $\hat{\psi}^\dagger(\mathbf{x},t)$ and $\hat{\psi}(\mathbf{x},t)$ have the physical interpretation to create and annihilate a boson at space point $\mathbf{x}$ at time t.

Now we transform the Hamilton operator (3.34), (3.36), and (3.37) from the Schrödinger to the Heisenberg picture. Analogous to (3.60) we multiply the Hamilton operator

$$\hat{H} = \int d^3x\,\hat{a}_{\mathbf{x}}^\dagger\left\{-\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x})\right\}\hat{a}_{\mathbf{x}} + \frac{1}{2}\int d^3x\int d^3x'\,\hat{a}_{\mathbf{x}}^\dagger\hat{a}_{\mathbf{x}'}^\dagger\,V_2(\mathbf{x}-\mathbf{x}')\hat{a}_{\mathbf{x}'}\,\hat{a}_{\mathbf{x}} \tag{3.65}$$

from the left with $e^{i\hat{H}t/\hbar}$ and from the right with $e^{-i\hat{H}t/\hbar}$:

$$\begin{aligned} \hat{H}_{\rm H}(t) &= \int d^3x\,e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}^\dagger\,e^{-i\hat{H}t/\hbar}\left\{-\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x})\right\}e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}\,e^{-i\hat{H}t/\hbar} \\ &+\frac{1}{2}\int d^3x\int d^3x'\,e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}^\dagger e^{-i\hat{H}t/\hbar}\,e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}'}^\dagger e^{-i\hat{H}t/\hbar}\,V_2(\mathbf{x}-\mathbf{x}')e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}'}\,e^{-i\hat{H}t/\hbar}\,e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}e^{-i\hat{H}t/\hbar}\,. \end{aligned} \tag{3.66}$$

Using the field operators (3.63) the Hamilton operator reads in the Heisenberg picture:

$$\begin{aligned} \hat{H}_{\rm H}(t) &= \int d^3x\,\hat{\psi}^\dagger(\mathbf{x},t)\left\{-\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x})\right\}\hat{\psi}(\mathbf{x},t) \\ &+\frac{1}{2}\int d^3x\int d^3x'\,\hat{\psi}^\dagger(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t)\,V_2(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x}',t)\,\hat{\psi}(\mathbf{x},t)\,. \end{aligned} \tag{3.67}$$

With this Hamilton operator in the Heisenberg picture we can determine from (3.62) the Heisenberg equation of motion of the field operator $\hat{\psi}(\mathbf{x},t)$:

$$i\hbar\,\frac{\partial\hat{\psi}(\mathbf{x},t)}{\partial t} = \left[\hat{\psi}(\mathbf{x},t),\hat{H}_{\mathrm{H}}(t)\right]_- . \tag{3.68}$$

At first we get

$$i\hbar\,\frac{\partial\hat{\psi}(\mathbf{x},t)}{\partial t} = \int d^3x' \int d^3x''\,\delta(\mathbf{x}-\mathbf{x}')\left\{-\frac{\hbar^2}{2M}\,\Delta'' + V_1(\mathbf{x}'')\right\}\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}(\mathbf{x}'',t)\right]_-$$
$$+\frac{1}{2}\int d^3x' \int d^3x''\,V_2(\mathbf{x}'-\mathbf{x}'')\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}^\dagger(\mathbf{x}'',t)\hat{\psi}(\mathbf{x}'',t)\hat{\psi}(\mathbf{x}',t)\right]_- . \tag{3.69}$$

Here the respective commutators can be evaluated with the help of the identity (3.43) and the commutator relations (3.64), yielding

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}(\mathbf{x}'',t)\right]_- = \delta(\mathbf{x}-\mathbf{x}')\,\hat{\psi}(\mathbf{x}'',t) \tag{3.70}$$

and, correspondingly,

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}^\dagger(\mathbf{x}'',t)\hat{\psi}(\mathbf{x}'',t)\hat{\psi}(\mathbf{x}',t)\right]_-$$
$$= \left\{\delta(\mathbf{x}-\mathbf{x}')\,\hat{\psi}^\dagger(\mathbf{x}'',t) + \delta(\mathbf{x}-\mathbf{x}'')\,\hat{\psi}^\dagger(\mathbf{x}',t)\right\}\hat{\psi}(\mathbf{x}'',t)\hat{\psi}(\mathbf{x}',t) . \tag{3.71}$$

Inserting (3.70) and (3.71) in (3.69) we finally obtain

$$i\hbar\,\frac{\partial\hat{\psi}(\mathbf{x},t)}{\partial t} = \left\{-\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x})\right\}\hat{\psi}(\mathbf{x},t) + \int d^3x'\,V_2(\mathbf{x}-\mathbf{x}')\,\hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}(\mathbf{x}',t)\hat{\psi}(\mathbf{x},t) . \tag{3.72}$$

In the same way also the Heisenberg equation of motion of the adjoint field operator

$$i\hbar\,\frac{\partial\hat{\psi}^\dagger(\mathbf{x},t)}{\partial t} = \left[\hat{\psi}^\dagger(\mathbf{x},t),\hat{H}_{\mathrm{H}}(t)\right]_- \tag{3.73}$$

is evaluated:

$$-i\hbar\,\frac{\partial\hat{\psi}^\dagger(\mathbf{x},t)}{\partial t} = \left\{-\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x})\right\}\hat{\psi}^\dagger(\mathbf{x},t) + \hat{\psi}^\dagger(\mathbf{x},t)\int d^3x'\,V_2(\mathbf{x}-\mathbf{x}')\,\hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}(\mathbf{x}',t) . \tag{3.74}$$

This is, indeed, the adjoint of the Heisenberg equation of motion (3.72). The operator-valued integro-differential equations (3.72) and (3.74) are nonlinear. Due to their complexity it is not possible to obtain exact analytic solutions. Therefore, one has to reside to develop physically reasonable approximate solutions.

3.5 Creation and Annihilation Operators for Fermions

So far we have shown that the symmetric many-body states for bosons can be practically realized with the help of local creation and annihilation operators $\hat{a}_{\mathbf{x}}^\dagger$ and $\hat{a}_{\mathbf{x}}$ in the Schrödinger picture.

Here the symmetry of the many-body states of bosons was ultimately a direct consequence of the commutation relations (3.25). Therefore, the question arises whether there exists a similar formalism also in view of the anti-symmetric many-body states for fermions. To this end we aim for creating an anti-symmetric many-body state for fermions similar to (3.30) via

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^{-1} = \hat{a}^\dagger_{\mathbf{x}_1} \cdots \hat{a}^\dagger_{\mathbf{x}_n} |0\rangle \,. \tag{3.75}$$

But then we have to demand instead of the commutation relations (3.25) corresponding anti-commutation relations

$$\left[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}\right]_+ = \left[\hat{a}^\dagger_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}\right]_+ = 0 \,, \qquad \left[\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}\right]_+ = \delta(\mathbf{x} - \mathbf{x}') \,. \tag{3.76}$$

where the anti-commutator between two quantum mechanical operators $\hat{A}$ and $\hat{B}$ is defined by

$$\left[\hat{A}, \hat{B}\right]_+ = \hat{A}\hat{B} + \hat{B}\hat{A} \,. \tag{3.77}$$

As in the bosonic case in (3.29) we define in addition the vacuum state $|0\rangle$ by the condition that it does not contain any particles:

$$\hat{a}_{\mathbf{x}}|0\rangle = 0 \qquad \Longleftrightarrow \qquad \langle 0|\hat{a}^\dagger_{\mathbf{x}} = 0 \,. \tag{3.78}$$

Indeed, (3.77) and (3.78) turn out to guarantee for the anti-symmetric many-body states (3.75) the orthonormality relations (2.74) for $n = 1$ and $n = 2$ fermions, which are characterized by $\epsilon = -1$. From (2.72), (3.75), (3.76), and (3.78) we obtain at first

$$\begin{aligned} {}^{-1}\langle \mathbf{x}_1 | \mathbf{x}'_1 \rangle^{-1} &= \langle \hat{a}^\dagger_{\mathbf{x}_1} 0 | \hat{a}^\dagger_{\mathbf{x}'_1} 0 \rangle = \langle 0 | \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}'_1} | 0 \rangle \\ &= \langle 0 | -\hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}_{\mathbf{x}_1} + \delta(\mathbf{x}_1 - \mathbf{x}'_1) | 0 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}'_1) = \delta^{-1}(\mathbf{x}_1; \mathbf{x}'_1) \,. \end{aligned} \tag{3.79}$$

Correspondingly, we get then

$$\begin{aligned} &{}^{-1}\langle \mathbf{x}_1, \mathbf{x}_2 | \mathbf{x}'_1, \mathbf{x}'_2 \rangle^{-1} = \langle \hat{a}^\dagger_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}_2} 0 | \hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}^\dagger_{\mathbf{x}'_2} 0 \rangle = \langle 0 | \hat{a}_{\mathbf{x}_2} \hat{a}_{\mathbf{x}_1} \hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}^\dagger_{\mathbf{x}'_2} | 0 \rangle \\ &= \langle 0 | \hat{a}_{\mathbf{x}_2} \big(-\hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}_{\mathbf{x}_1} + \delta(\mathbf{x}_1 - \mathbf{x}'_1) \big) \hat{a}^\dagger_{\mathbf{x}'_2} | 0 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}'_1) \langle 0 | -\hat{a}^\dagger_{\mathbf{x}'_2} \hat{a}_{\mathbf{x}_2} + \delta(\mathbf{x}_2 - \mathbf{x}'_2) | 0 \rangle \\ &- \langle 0 | \big(-\hat{a}^\dagger_{\mathbf{x}'_1} \hat{a}_{\mathbf{x}_2} + \delta(\mathbf{x}'_1 - \mathbf{x}_2) \big) \big(-\hat{a}^\dagger_{\mathbf{x}'_2} \hat{a}_{\mathbf{x}_1} + \delta(\mathbf{x}_1 - \mathbf{x}'_2) \big) | 0 \rangle = \delta(\mathbf{x}_1 - \mathbf{x}'_1) \delta(\mathbf{x}_2 - \mathbf{x}'_2) \\ &- \delta(\mathbf{x}_1 - \mathbf{x}'_2) \delta(\mathbf{x}_2 - \mathbf{x}'_1) = \delta^{-1}(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}'_1, \mathbf{x}'_2) \,. \end{aligned} \tag{3.80}$$

As two local creation operators $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}^\dagger_{\mathbf{x}'}$ anti-commute due to (3.76), we conclude that then the square of the fermionic creation operator $\hat{a}^\dagger_{\mathbf{x}}$ vanishes:

$$\left(\hat{a}^\dagger_{\mathbf{x}}\right)^2 = 0 \,. \tag{3.81}$$

For the anti-symmetric many-body state (3.75) this has the consequence that it vanishes provided that two space coordinates $\mathbf{x}_i$ and $\mathbf{x}_j$ for $i \neq j$ coincide:

$$|\mathbf{x}_1, \ldots, \mathbf{x}_n\rangle^{-1} = 0 \,, \qquad \text{if } \mathbf{x}_i = \mathbf{x}_j \text{ for } i \neq j \,. \tag{3.82}$$

Thus, the anti-commutation relations (3.76) contain automatically the Pauli exclusion principle that two fermions can not be at the same space point.

The properties (3.75) and (3.76) are also sufficient in order to formulate with the help of the second quantized Hamilton operator

$$\hat{H} = \int d^3x\, \hat{a}^\dagger_{\mathbf{x}} \left\{ -\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x}) \right\} \hat{a}_{\mathbf{x}} + \frac{1}{2} \int d^3x \int d^3x'\, \hat{a}^\dagger_{\mathbf{x}} \hat{a}^\dagger_{\mathbf{x}'}\, V_2(\mathbf{x}-\mathbf{x}')\hat{a}_{\mathbf{x}'}\, \hat{a}_{\mathbf{x}} \tag{3.83}$$

the second quantized Schrödinger equation for a fermionic many-body state $|\psi(t)\rangle$:

$$i\hbar\,\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}|\psi(t)\rangle\,. \tag{3.84}$$

Projecting (3.84) to the anti-symmetric basis states (3.75) yields, like in the bosonic case, the corresponding n-body Schrödinger equation (2.21) with (2.23) for the n-particle wave function

$$\psi^{-1}(\mathbf{x}_1, \ldots \mathbf{x}_n; t) = {}^{-1}\langle \mathbf{x}_1, \ldots, \mathbf{x}_n|\psi(t)\rangle\,. \tag{3.85}$$

We leave the detailed proof to the reader, which follows a consideration similar to Section 3.3.

Furthermore, transforming the fermionic creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{a}_{\mathbf{x}}$ from the Schrödinger to the Heisenberg picture yields fermionic field operators

$$\hat{\psi}^\dagger(\mathbf{x},t) = e^{i\hat{H}t/\hbar}\,\hat{a}^\dagger_{\mathbf{x}}\,e^{-i\hat{H}t/\hbar}\,, \qquad \hat{\psi}(\mathbf{x},t) = e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}\,e^{-i\hat{H}t/\hbar}\,, \tag{3.86}$$

which fulfill due to (3.76) equal-time anti-commutation relations:

$$\left[\hat{\psi}(\mathbf{x},t), \hat{\psi}(\mathbf{x}',t)\right]_+ = \left[\hat{\psi}^\dagger(\mathbf{x},t), \hat{\psi}^\dagger(\mathbf{x}',t)\right]_+ = 0\,, \quad \left[\hat{\psi}(\mathbf{x},t), \hat{\psi}^\dagger(\mathbf{x}',t)\right]_+ = \delta(\mathbf{x}-\mathbf{x}')\,. \tag{3.87}$$

Furthermore, we remark that the Hamilton operator in the Heisenberg picture

$$\hat{H}_{\mathrm{H}}(t) = \int d^3x\, e^{i\hat{H}t/\hbar}\,\hat{a}^\dagger_{\mathbf{x}}\,e^{-i\hat{H}t/\hbar} \left\{ -\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x}) \right\} e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}}\,e^{-i\hat{H}t/\hbar} \tag{3.88}$$
$$+\frac{1}{2} \int d^3x \int d^3x'\, e^{i\hat{H}t/\hbar}\,\hat{a}^\dagger_{\mathbf{x}} e^{-i\hat{H}t/\hbar}\, e^{i\hat{H}t/\hbar}\,\hat{a}^\dagger_{\mathbf{x}'} e^{-i\hat{H}t/\hbar}\; V_2(\mathbf{x}-\mathbf{x}') e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}'}\,e^{-i\hat{H}t/\hbar}\,e^{i\hat{H}t/\hbar}\,\hat{a}_{\mathbf{x}} e^{-i\hat{H}t/\hbar}\,.$$

turns out to have the same form as in the bosonic case, see (3.67):

$$\begin{aligned} \hat{H}_{\mathrm{H}}(t) \;&=\; \int d^3x\, \hat{\psi}^\dagger(\mathbf{x},t) \left\{ -\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x}) \right\} \hat{\psi}(\mathbf{x},t) \\ &\quad +\frac{1}{2} \int d^3x \int d^3x'\, \hat{\psi}^\dagger(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t)\, V_2(\mathbf{x}-\mathbf{x}')\hat{\psi}(\mathbf{x}',t)\,\hat{\psi}(\mathbf{x},t)\,. \end{aligned} \tag{3.89}$$

With this the Heisenberg equations of motion of the field operators $\hat{\psi}(\mathbf{x},t)$ and $\hat{\psi}^\dagger(\mathbf{x},t)$

$$i\hbar\,\frac{\partial\hat{\psi}(\mathbf{x},t)}{\partial t} \;=\; \left[\hat{\psi}(\mathbf{x},t), \hat{H}_{\mathrm{H}}(t)\right]_-\,, \tag{3.90}$$

$$i\hbar\,\frac{\partial\hat{\psi}^\dagger(\mathbf{x},t)}{\partial t} \;=\; \left[\hat{\psi}^\dagger(\mathbf{x},t), \hat{H}_{\mathrm{H}}(t)\right]_- \tag{3.91}$$

are evaluated and yield

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{x},t)}{\partial t} = \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \hat{\psi}(\mathbf{x},t) + \int d^3x'\, V_2(\mathbf{x}-\mathbf{x}')\, \hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}(\mathbf{x}',t)\hat{\psi}(\mathbf{x},t) \quad (3.92)$$

as well as its adjoint

$$-i\hbar \frac{\partial \hat{\psi}^\dagger(\mathbf{x},t)}{\partial t} = \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \hat{\psi}^\dagger(\mathbf{x},t) + \hat{\psi}^\dagger(\mathbf{x},t) \int d^3x'\, V_2(\mathbf{x}-\mathbf{x}')\, \hat{\psi}^\dagger(\mathbf{x}',t)\hat{\psi}(\mathbf{x}',t) \quad (3.93)$$

corresponding to the bosonic case, see (3.72) and (3.74). Note that obtaining (3.92) and (3.93) necessitates the operator identity (3.43) and the complementary one

$$\left[\hat{A}, \hat{B}\hat{C}\right]_- = \left[\hat{A}, \hat{B}\right]_+ \hat{C} - \hat{B}\left[\hat{A}, \hat{C}\right]_+ , \quad (3.94)$$

which directly follows from the definitions of both the commutator (2.13) and the anti-commutator (3.77).

3.6 Occupation Number Representation

Let us finally consider the case that the 2-particle interaction vanishes, i.e. $V_2(\mathbf{x}-\mathbf{x}') = 0$, from the point of view of second quantization. We show in this section that then identical particles are described within the so-called occupation number representation. To this end we start with the second quantized Hamilton operator in the Schrödinger picture for non-interacting identical particles

$$\hat{H} = \int d^3x\, \hat{a}^\dagger_{\mathbf{x}} \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \hat{a}_{\mathbf{x}} . \quad (3.95)$$

As we deal at the same time with bosons and fermions, the creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$, $\hat{a}_{\mathbf{x}}$ fulfill either canonical commutation or canonical anti-commutation relations:

$$\left[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}\right]_\mp = \left[\hat{a}^\dagger_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}\right]_\mp = 0 , \qquad \left[\hat{a}_{\mathbf{x}}, \hat{a}^\dagger_{\mathbf{x}'}\right]_\mp = \delta(\mathbf{x}-\mathbf{x}') . \quad (3.96)$$

In the following we assume again that the 1-particle wavefunctions $\psi_{E_\alpha}(\mathbf{x})$ with the quantum numbers α are known as solutions of the time-independent 1-particle Schrödinger equation (2.48), obeying both the orthonormality relation (2.49) and the completeness relation (2.50). Due to the latter the creation and annihilation operators $\hat{a}^\dagger_{\mathbf{x}}$, $\hat{a}_{\mathbf{x}}$ can be expanded in the 1-particle basis:

$$\hat{a}_{\mathbf{x}} = \sum_\alpha \psi_{E_\alpha}(\mathbf{x})\, \hat{a}_\alpha \qquad \Longleftrightarrow \qquad \hat{a}^\dagger_{\mathbf{x}} = \sum_\alpha \psi^*_{E_\alpha}(\mathbf{x})\, \hat{a}^\dagger_\alpha . \quad (3.97)$$

Both expansions are inverted with the help of the orthonormality relation (2.49), yielding

$$\hat{a}_\alpha = \int d^3x\, \psi^*_{E_\alpha}(\mathbf{x})\, \hat{a}_{\mathbf{x}} \qquad \Longleftrightarrow \qquad \hat{a}^\dagger_\alpha = \int d^3x\, \psi_{E_\alpha}(\mathbf{x})\, \hat{a}^\dagger_{\mathbf{x}} . \quad (3.98)$$

With this we deduce the commutation and anti-commutation relations for the operator-valued expansion coefficients $\hat{a}_\alpha^\dagger$, $\hat{a}_\alpha$ by taking into account (3.96):

$$\left[\hat{a}_\alpha, \hat{a}_{\alpha'}\right]_\mp = \left[\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger\right]_\mp = 0 \,, \qquad \left[\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger\right]_\mp = \delta_{\alpha,\alpha'} \,. \tag{3.99}$$

Inserting the expansions of the creation and annihilation operators (3.97) in the second quantized Hamilton operator (3.95), we can express it via the operator-valued expansion coefficients $\hat{a}_\alpha^\dagger$, $\hat{a}_\alpha$ due to (2.48) and (2.49) and end up with

$$\hat{H} = \sum_\alpha E_\alpha \, \hat{n}_\alpha \,, \tag{3.100}$$

where we have introduced the particle number operator

$$\hat{n}_\alpha = \hat{a}_\alpha^\dagger \hat{a}_\alpha \,. \tag{3.101}$$

Note that the useful operator identity

$$\left[\hat{A}\hat{B}, \hat{C}\right]_- = \hat{A}\left[\hat{B}, \hat{C}\right]_\mp \pm \left[\hat{A}, \hat{C}\right]_\mp \hat{B} \,, \tag{3.102}$$

which follows from the definitions of both the commutator (2.13) and the anti-commutator (3.77), complements the bosonic version (3.10) with a corresponding fermionic one. With (3.43) and (3.102) we can then show that the particle operators $\hat{n}_\alpha$ and $\hat{n}_{\alpha'}$ for two quantum numbers α and α' commute:

$$\begin{aligned} \left[\hat{n}_\alpha, \hat{n}_{\alpha'}\right]_- &= \left[\hat{n}_\alpha, \hat{a}_{\alpha'}^\dagger \hat{a}_{\alpha'}\right]_- = \left[\hat{a}_\alpha^\dagger \hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger\right]_- \hat{a}_{\alpha'} + \hat{a}_{\alpha'}^\dagger \left[\hat{a}_\alpha^\dagger \hat{a}_\alpha, \hat{a}_{\alpha'}\right]_- \qquad (3.103) \\ &= \left(\hat{a}_\alpha^\dagger \left[\hat{a}_\alpha, \hat{a}_{\alpha'}^\dagger\right]_\mp \pm \left[\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}^\dagger\right]_\mp \hat{a}_\alpha\right) \hat{a}_{\alpha'} + \hat{a}_{\alpha'}^\dagger \left(\hat{a}_\alpha^\dagger \left[\hat{a}_\alpha, \hat{a}_{\alpha'}\right]_\mp \pm \left[\hat{a}_\alpha^\dagger, \hat{a}_{\alpha'}\right]_\mp \hat{a}_\alpha\right) = 0 \,. \end{aligned}$$

Thus, we conclude that the particle number operator (3.101) commutes with the Hamilton operator (3.100):

$$\left[\hat{n}_\alpha, \hat{H}\right]_- = \sum_{\alpha'} E_{\alpha'} \left[\hat{n}_\alpha, \hat{n}_{\alpha'}\right]_- = 0 \,. \tag{3.104}$$

Due to (3.103) and (3.104) we know that there must exist a set of states, which are eigenstates for both all particle number operators (3.101)and the Hamilton operator (3.100):

$$\hat{n}_\alpha | \ldots, n_\alpha, \ldots \rangle = n_\alpha \, | \ldots, n_\alpha, \ldots \rangle \,, \tag{3.105}$$

$$\hat{H} | \ldots, n_\alpha, \ldots \rangle = \sum_\alpha E_\alpha n_\alpha \, | \ldots, n_\alpha, \ldots \rangle \,. \tag{3.106}$$

In the case of bosons we already know from Section 3.2 that the commutation relations for the operators $\hat{a}_\alpha^\dagger$, $\hat{a}_\alpha$ imply that the eigenvalues of the particle operator $\hat{n}_\alpha$ can have any integer value including zero:

$$\text{bosons:} \qquad n_\alpha = 0, 1, 2, \ldots \,. \tag{3.107}$$

But for fermions it turns out that the anti-commutation relations for the operators $\hat{a}_\alpha^\dagger$, $\hat{a}_\alpha$ lead to an essential restriction for the eigenvalues of the particle operators. Namely we read off from (3.81) and (3.101):

$$(\hat{n}_\alpha)^2 = \hat{a}_\alpha^\dagger \hat{a}_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha = \hat{a}_\alpha^\dagger \hat{a}_\alpha - \left(\hat{a}_\alpha^\dagger\right)^2 (\hat{a}_\alpha)^2 = \hat{n}_\alpha \,. \tag{3.108}$$

Applying (3.108) to the eigenstates $|\ldots, n_\alpha, \ldots\rangle$ we conclude due to the eigenvalue problem (3.105):

$$n_\alpha^2 = n_\alpha \,, \tag{3.109}$$

which yields straightforwardly

$$\text{fermions:} \qquad n_\alpha = 0, 1 \,. \tag{3.110}$$

Thus, each state characterized by the quantum number α can be occupied with at most one fermion in accordance with the Pauli exclusion principle.