Chapter 5

Canonical Field Quantization for Fermions

In the previous chapter we worked out with the help of the functional derivative the classical field theory for bosons. Its canonical field quantization then allowed to derive the equal-time commutation relations for the bosonic field operators. Here we show that a corresponding derivation is also possible in view of the equal-time anti-commutation relations for the fermionic field operators. But in order to obtain a proper classical field theory for fermions, one needs anti-commuting Grassmann fields. Therefore, we start this chapter with introducing the concept of anti-commuting Grassmann numbers and fields, which was developed by the mathematician Hermann Grassmann in the middle of the 19th century.

5.1 Grassmann Fields

The classical analogue of the Pauli exclusion principle is not realizable within the realm of the usual numbers like real or complex numbers but needs the new mathematical concept of Grassmann numbers.

5.1.1 Grassmann Numbers

The entity of anti-commuting Grassmann numbers is called the Grassmann algebra. Each element of a Grassmann algebra of dimension n can be represented by a set of n generators or Grassmann variables ψ_i, where the index i runs from 1 to n. The Grassmann algebra is defined by postulating the anti-commutation relations

$$\Big[\psi_i, \psi_j\Big]_+ = \psi_i \, \psi_j + \psi_j \, \psi_i = 0 \tag{5.1}$$

for all $i, j = 1, \ldots, n$. As a special case of (5.1) we read off that the square and all higher powers of a generator have to vanish:

$$\psi_i^2 = 0\,. \tag{5.2}$$

This has the consequence that each element of the Grassmann algebra can be expanded in a finite sum over products of generators as follows:

$$\begin{aligned} f(\psi_1, \ldots, \psi_n) &= f^{(0)} + \sum_{i=1}^{n} f_i^{(1)}\,\psi_i + \sum_{i=1}^{n}\sum_{j=1}^{i-1} f_{ij}^{(2)}\,\psi_i\,\psi_j + \ldots \\ &\quad + \sum_{i=1}^{n} f_i^{(n-1)}\,\psi_1\,\cdots\,\psi_{i-1}\,\psi_{i+1}\,\cdots\,\psi_n + f^{(n)}\,\psi_1\,\cdots\,\psi_n\,, \end{aligned} \tag{5.3}$$

where all coefficients $f^{(0)}, f_i^{(1)}, f_{ij}^{(2)}, \ldots, f_i^{(n-1)}, f^{(n)}$ are complex numbers. Due to the anti-commutation relations (5.1) it is sufficient in the sum (5.3) that the indices of the generators appear in ascending order, i.e. $i > j$ in the third term. This reduces correspondingly the number of independent products of p generators to the binomial coefficients

$$n_p = \begin{pmatrix} n \\ p \end{pmatrix}\,. \tag{5.4}$$

For instance, one obtains for $p = 0, 1, 2, \ldots, n-1, n$:

$$\begin{aligned} n_0 = 1 = \begin{pmatrix} n \\ 0 \end{pmatrix}\,, \quad n_1 = \sum_{i=1}^{n} 1 = n = \begin{pmatrix} n \\ 1 \end{pmatrix}\,, \quad n_2 = \sum_{i=1}^{n}\sum_{j=1}^{i-1} 1 = \frac{1}{2}\,n(n-1) = \begin{pmatrix} n \\ 2 \end{pmatrix} \\ ,\ \ldots\,, \quad n_{n-1} = \sum_{i=1}^{n} 1 = n = \begin{pmatrix} n \\ n-1 \end{pmatrix}\,, \quad n_n = 1 = \begin{pmatrix} n \\ n \end{pmatrix}\,. \end{aligned} \tag{5.5}$$

The dimension of the Grassmann algebra, i.e. the maximal number of linear independent terms in the expansion (5.3) amounts to

$$\sum_{p=0}^{n} n_p = \sum_{p=0}^{n} 1^p\,1^{n-p}\,\begin{pmatrix} n \\ p \end{pmatrix} = 2^n \tag{5.6}$$

as (5.4) has to be taken into account.

5.1.2 Grassmann Functions

A Grassmann function maps a Grassmann number (5.3) to another Grassmann number (5.3). Consider as an example the Grassmann algebra of degree 2 with the generators ψ_1 and ψ_2, which has the dimension $2^2 = 4$. A Grassmann number f is then represented as

$$f(\psi_1, \psi_2) = f^{(0)} + f_1^{(1)}\,\psi_1 + f_2^{(1)}\,\psi_2 + f^{(2)}\,\psi_1\,\psi_2\,. \tag{5.7}$$

ordinary variables	Grassmann variables
$\frac{\partial}{\partial x_i} 1 = 0$	$\frac{\partial}{\partial \psi_i} 1 = 0$
$\frac{\partial x_j}{\partial x_i} = \delta_{ij}$	$\frac{\partial \psi_j}{\partial \psi_i} = \delta_{ij}$
$\frac{\partial}{\partial x_i}\Big(x_j\, x_k\Big) = \delta_{ij}\, x_k + \delta_{ik}\, x_j$	$\frac{\partial}{\partial \psi_i}\Big(\psi_j\, \psi_k\Big) = \delta_{ij}\, \psi_k - \delta_{ik}\, \psi_j$
$\frac{\partial}{\partial x_i}\Big[x_j\, f(x_1,\ldots,x_n)\Big] = \delta_{ij}\, f(x_1,\ldots,x_n) + x_j\, \frac{\partial f(x_1,\ldots,x_n)}{\partial x_i}$	$\frac{\partial}{\partial \psi_i}\Big[\psi_j\, f(\psi_1,\ldots,\psi_n)\Big] = \delta_{ij}\, f(\psi_1,\ldots,\psi_n) - \psi_j\, \frac{\partial f(\psi_1,\ldots,\psi_n)}{\partial \psi_i}$
$\left[\frac{\partial}{\partial x_i}, x_j\right]_- = \frac{\partial}{\partial x_i}\, x_j - x_j\, \frac{\partial}{\partial x_i} = \delta_{ij}$	$\left[\frac{\partial}{\partial \psi_i}, \psi_j\right]_+ = \frac{\partial}{\partial \psi_i}\, \psi_j + \psi_j\, \frac{\partial}{\partial \psi_i} = \delta_{ij}$
$\left[\frac{\partial}{\partial x_i}, \frac{\partial}{\partial x_j}\right]_- = \frac{\partial}{\partial x_i}\, \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_j}\, \frac{\partial}{\partial x_i} = 0$	$\left[\frac{\partial}{\partial \psi_i}, \frac{\partial}{\partial \psi_j}\right]_+ = \frac{\partial}{\partial \psi_i}\, \frac{\partial}{\partial \psi_j} + \frac{\partial}{\partial \psi_j}\, \frac{\partial}{\partial \psi_i} = 0$

Figure 5.1: Comparison of calculation rules for differentiation with respect to ordinary and Grassmann variables.

With the help of the Taylor series and (5.1) we obtain, for instance, the following two Grassmann functions:

$$e^{\psi_1+\psi_2} = 1 + \psi_1 + \psi_2 \,, \tag{5.8}$$

$$e^{\psi_1\,\psi_2} = 1 + \psi_1\,\psi_2 \,. \tag{5.9}$$

Does a Grassmann number f only consist of an even number of generators, then it commutes with all Grassmann numbers and one assigns to it the parity $\pi(f) = 0$. In the opposite case that a Grassmann number f consists of an odd number of generators, then it anti-commutes with such Grassmann numbers, which also have an odd number of generators, and one assigns to it the parity $\pi(f) = 1$. Grassmann numbers, which contain both an even and an odd number of generators, do not have any parity. We have, for example, $\pi(\psi_1) = \pi(\psi_2) = 1$ and $\pi(e^{\psi_1\,\psi_2}) = 0$ due to (5.9), but we can assign to $e^{\psi_1+\psi_2}$ no parity due to (5.8).

5.1.3 Differentiation and Integration

Within a Grassmann algebra one can introduce the operations of differentiation and integration. But these are abstract constructions, which have properties differing considerably from the usual differentiation and integration calculus with real or complex numbers. In comparison of a differentiation with respect to an ordinary variable, the differentiation with respect to a Grassmann variable is defined via the rules in Fig. 5.1. As an example we consider again the Grassmann algebra of degree 2. For the respective derivatives of (5.7) we obtain

$$\frac{\partial f(\psi_1,\psi_2)}{\partial \psi_1} = f_1^{(1)} + f^{(2)}\,\psi_2\,, \quad \frac{\partial f(\psi_1,\psi_2)}{\partial \psi_2} = f_2^{(1)} - f^{(2)}\,\psi_1\,, \tag{5.10}$$

$$\frac{\partial^2 f(\psi_1,\psi_2)}{\partial \psi_1^2} = \frac{\partial^2 f(\psi_1,\psi_2)}{\partial \psi_2^2} = 0\,, \quad \frac{\partial^2 f(\psi_1,\psi_2)}{\partial \psi_1 \partial \psi_2} = -f^{(2)} = -\frac{\partial^2 f(\psi_1,\psi_2)}{\partial \psi_2 \partial \psi_1}\,. \tag{5.11}$$

ordinary variable	Grassmann variable
$\int_{-\infty}^{\infty} dx \Big[\alpha f(x) + \beta g(x)\Big] = \alpha \int_{-\infty}^{\infty} dx f(x) + \beta \int_{-\infty}^{\infty} dx g(x)$	$\int d\psi \Big[\alpha f(\psi) + \beta g(\psi)\Big] = \alpha \int d\psi f(\psi) + \beta \int d\psi g(\psi)$
$\int_{-\infty}^{\infty} dx f(x + x_0) = \int_{-\infty}^{\infty} dx f(x)$	$\int d\psi f(\psi + \psi_0) = \int d\psi f(\psi)$

Figure 5.2: Linearity and translational invariance as defining properties of integration with respect to Grassmann variables in comparison to integration with respect to ordinary variables.

Correspondingly the derivatives of (5.8) and (5.9) yield

$$\frac{\partial e^{\psi_1+\psi_2}}{\partial \psi_1} = 1\,, \qquad \frac{\partial e^{\psi_1+\psi_2}}{\partial \psi_2} = 1\,, \tag{5.12}$$

$$\frac{\partial e^{\psi_1\,\psi_2}}{\partial \psi_1} = \psi_2\,, \qquad \frac{\partial e^{\psi_1\,\psi_2}}{\partial \psi_2} = -\psi_1\,. \tag{5.13}$$

Introducing an integration with respect to a Grassmann variable one has to abstain from various usual properties. For instance, the integration with respect to Grassmann variables can not be defined via a Riemann sum as there does not exist any concrete interpretation for an area under a curve. But the integration can also not be defined by inverting the differentiation as integration boundaries do not make any sense. Let us consider at first the case of a single Grassmann variable ψ with the property

$$\Big[\psi, \psi\Big]_+ = 0\,. \tag{5.14}$$

Then a Grassmann function f of this Grassmann variable ψ is given by

$$f(\psi) = a + b\,\psi\,. \tag{5.15}$$

The integral $\int d\psi\, f(\psi)$ is determined according to Fig. 5.2 such that its properties are similar to those of a definite integral $\int_{-\infty}^{+\infty} dx\, f(x)$ of ordinary functions $f(x)$, which vanish at infinity. Demanding linearity and translational invariance of integration according to Fig. 5.2, we conclude

$$\int d\psi\, \Big[a + b\,(\psi + \psi_0)\Big] = \int d\psi\, \Big(a + b\,\psi\Big) + b\left(\int d\psi\, 1\right)\psi_0 = \int d\psi \Big(a + b\,\psi\Big)\,, \tag{5.16}$$

from which we can read off the following important integration rule:

$$\int d\psi\, 1 = 0\,. \tag{5.17}$$

This is integration rule is complemented by the arbitrary normalization

$$\int d\psi\, \psi = 1\,. \tag{5.18}$$

Those integration rules (5.17), (5.18) have to be compared with the corresponding differentiation rules, see Fig. 5.1:

$$\frac{d}{d\psi}\, 1 = 0\,, \qquad \frac{d}{d\psi}\, \psi = 1\,. \tag{5.19}$$

Thus, one can conclude that in the space of Grassmann numbers integration and differentiation are surprisingly identical. For instance, we get for the function (5.15):

$$\int d\psi\, f(\psi) = b\,, \qquad \frac{d}{d\psi}\, f(\psi) = b\,. \tag{5.20}$$

The generalization of the integration rules (5.17), (5.18) to the case of higher-dimensional Grassmann algebra with generators ψ_i for $i = 1, \ldots, n$ is given by

$$\int d\psi_i\, 1 = 0\,, \qquad \int d\psi_i\, \psi_j = \delta_{ij}\,, \tag{5.21}$$

which corresponds to the differentiation rules in Fig. 5.1. Multiple integrals are calculated in the usual way by performing successively the respective one-dimensional integrals. As an example we determine the integral over the function (5.7):

$$\int d\psi_2 \int d\psi_1\, f(\psi_1, \psi_2) = f^{(2)}\,. \tag{5.22}$$

Thus, a multiple integration has the effect of projecting the corresponding coefficient in the expansion (5.3) of the Grassmann function

$$\int d\psi_n \ldots \int d\psi_1\, f(\psi_1, \ldots, \psi_n) = f^{(n)}\,. \tag{5.23}$$

5.1.4 Complex Grassmann Numbers

In view of dealing with a quantum many-body problem with an arbitrary number of fermions it is reasonable to also introduce complex Grassmann numbers. To this end one deals with two disjunct sets of Grassmann numbers $\psi_1, \ldots, \psi_n$ and $\psi_1^*, \ldots, \psi_n^*$, which anti-commute:

$$\Big[\psi_i, \psi_j\Big]_+ = \Big[\psi_i^*, \psi_j^*\Big]_+ = \Big[\psi_i, \psi_j^*\Big]_+ = 0\,. \tag{5.24}$$

Those generators constitute together a $2n$-dimensional Grassmann algebra. Both sets $\psi_1, \ldots, \psi_n$ and $\psi_1^*, \ldots, \psi_n^*$ are interconnected via the operation of conjugation:

$$(\psi_i)^* = \psi_i^*\,, \quad (\psi_i^*)^* = \psi_i\,, \quad (\psi_{i_1}\, \psi_{i_2} \cdots \psi_{i_n})^* = \psi_{i_n}^* \cdots \psi_{i_2}^*\, \psi_{i_1}^*\,, \quad (\lambda\, \psi_i)^* = \lambda^*\, \psi_i^*\,, \tag{5.25}$$

where λ denotes a complex number. Differentiation and integration are the defined in such a way that both sets $\psi_1, \ldots, \psi_n$ and $\psi_1^*, \ldots, \psi_n^*$ are treated as independent numbers.

5.1.5 Grassmann Fields

Finally, in order to apply complex Grassmann numbers in the realm of classical field theory for fermions, we have to introduce also anti-commuting fields, which amounts to the continuum limit $\psi_i \to \psi(x)$ and $\psi_i^* \to \psi^*(x)$. Thus, the anti-commutation relations (5.24) go over to

$$\Big[\psi(x), \psi(x')\Big]_+ = \Big[\psi^*(x), \psi^*(x')\Big]_+ = \Big[\psi(x), \psi^*(x')\Big]_+ = 0\,. \tag{5.26}$$

With this the anti-commuting fields $\psi(x)$ and $\psi^*(x)$ are the generators of an infinite-dimensional Grassmann algebra. An arbitrary element of this algebra then represents a functional $f[\psi^*, \psi]$, which can be expanded in generalization to (5.3) according to

$$f[\psi^*(\bullet), \psi(\bullet)] = f^{(0)} + \int dx_1 \, \Big\{ f_1^{(1)}(x_1)\psi^*(x_1) + f_2^{(1)}(x_1)\psi(x_1) \Big\} + \int dx_1 \int dx_2$$
$$\times \Big\{ f_1^{(2)}(x_1, x_2)\psi^*(x_1)\psi^*(x_2) + f_2^{(2)}(x_1, x_2)\psi^*(x_1)\psi(x_2) + f_3^{(2)}(x_1, x_2)\psi(x_1)\psi(x_2) \Big\} + \ldots\,. \tag{5.27}$$

In this continuum limit the differentiation with respect to Grassmann variables becomes the functional derivative with respect to complex Grassmann fields, which obey the rules

$$\frac{\delta\psi(x)}{\delta\psi(x')} = \frac{\delta\psi^*(x)}{\delta\psi^*(x')} = \delta(x - x')\,, \qquad \frac{\delta\psi(x)}{\delta\psi^*(x')} = \frac{\delta\psi^*(x)}{\delta\psi(x')} = 0\,. \tag{5.28}$$

5.2 Lagrange Field Theory for Fermions

Now we develop a classical field theory for fermions and assume to this end that the Schrödinger fields $\psi^*(\mathbf{x}, t)$ and $\psi(\mathbf{x}, t)$ are anti-commuting complex Grassmann fields. As in the bosonic case (4.8)–(4.10) the action is a space-time integral

$$\mathcal{A} = \int dt \, L \left[\psi^*(\bullet, t), \frac{\partial\psi^*(\bullet, t)}{\partial t}; \psi(\bullet, t), \frac{\partial\psi(\bullet, t)}{\partial t} \right] \tag{5.29}$$

of the Lagrange function

$$L = \int d^3x \, \mathcal{L} \left(\psi^*(\mathbf{x}, t), \boldsymbol{\nabla}\psi^*(\mathbf{x}, t), \frac{\partial\psi^*(\mathbf{x}, t)}{\partial t}; \psi(\mathbf{x}, t), \boldsymbol{\nabla}\psi(\mathbf{x}, t), \frac{\partial\psi(\mathbf{x}, t)}{\partial t} \right)\,, \tag{5.30}$$

where the Lagrange density is given by

$$\mathcal{L} = i\hbar \, \psi^*(\mathbf{x}, t) \, \frac{\partial\psi(\mathbf{x}, t)}{\partial t} - \frac{\hbar^2}{2M} \, \boldsymbol{\nabla}\psi^*(\mathbf{x}, t) \cdot \boldsymbol{\nabla}\psi(\mathbf{x}, t) - V_1(\mathbf{x})\psi^*(\mathbf{x}, t)\psi(\mathbf{x}, t)\,. \tag{5.31}$$

Instead of the bosonic Hamilton principle of the Lagrange field theory (4.37), (4.38) we obtain now the corresponding fermionic version:

$$\delta\mathcal{A} = \int dt \int d^3x \, \left\{ \delta\psi^*(\mathbf{x}, t) \, \frac{\delta\mathcal{A}}{\delta\psi^*(\mathbf{x}, t)} + \delta\psi(\mathbf{x}, t) \, \frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x}, t)} \right\} = 0\,. \tag{5.32}$$

As the variations of the complex Grassmann fields $\delta\psi^*(\mathbf{x},t)$ and $\delta\psi(\mathbf{x},t)$ are considered to be independent, we obtain from (5.32) like in (4.38):

$$\frac{\delta\mathcal{A}}{\delta\psi^*(\mathbf{x},t)} = 0\,, \qquad \frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)} = 0\,. \tag{5.33}$$

Calculating the functional derivatives of the action (5.29) with respect to the complex Grassmann fields $\psi^*(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$ yields the same Euler-Lagrange equations like in the bosonic case (4.42) and (4.43):

$$\frac{\delta\mathcal{A}}{\delta\psi^*(\mathbf{x},t)} = \frac{\delta L}{\delta\psi^*(\mathbf{x},t)} - \frac{\partial}{\partial t}\,\frac{\delta L}{\delta\,\dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}}\,, \tag{5.34}$$

$$\frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)} = \frac{\delta L}{\delta\psi(\mathbf{x},t)} - \frac{\partial}{\partial t}\,\frac{\delta L}{\delta\,\dfrac{\partial\psi(\mathbf{x},t)}{\partial t}}\,. \tag{5.35}$$

Also the respective functional derivatives of the Lagrange function (5.30) with respect to the complex Grassmann fields $\psi^*(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$ formally coincide with the bosonic calculation (4.44), (4.45):

$$\frac{\delta L}{\delta\psi^*(\mathbf{x},t)} = \frac{\partial\mathcal{L}}{\partial\psi^*(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial\mathcal{L}}{\boldsymbol{\nabla}\psi^*(\mathbf{x},t)}\,, \qquad \frac{\delta L}{\delta\,\dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}} = \frac{\partial\mathcal{L}}{\partial\,\dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}}\,, \tag{5.36}$$

$$\frac{\delta L}{\delta\psi(\mathbf{x},t)} = \frac{\partial\mathcal{L}}{\partial\psi(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial\mathcal{L}}{\boldsymbol{\nabla}\psi(\mathbf{x},t)}\,, \qquad \frac{\delta L}{\delta\,\dfrac{\partial\psi(\mathbf{x},t)}{\partial t}} = \frac{\partial\mathcal{L}}{\partial\,\dfrac{\partial\psi(\mathbf{x},t)}{\partial t}}\,. \tag{5.37}$$

Thus, also the Euler-Lagrange equations for the complex Grassmann fields have formally the same structure as in the bosonic case (4.46), (4.47)

$$\frac{\partial\mathcal{L}}{\partial\psi^*(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial\mathcal{L}}{\boldsymbol{\nabla}\psi^*(\mathbf{x},t)} - \frac{\partial\mathcal{L}}{\partial\,\dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}} = 0\,, \tag{5.38}$$

$$\frac{\partial\mathcal{L}}{\partial\psi(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial\mathcal{L}}{\boldsymbol{\nabla}\psi(\mathbf{x},t)} - \frac{\partial\mathcal{L}}{\partial\,\dfrac{\partial\psi(\mathbf{x},t)}{\partial t}} = 0\,. \tag{5.39}$$

A difference between the Schrödinger field theory for bosons and fermions only occurs once the partial derivatives of the Lagrange density (5.31) are determined:

$$\frac{\partial\mathcal{L}}{\partial\psi^*(\mathbf{x},t)} = -V_1(\mathbf{x})\psi(\mathbf{x},t) + i\hbar\,\frac{\partial\psi(\mathbf{x},t)}{\partial t}\,, \frac{\partial\mathcal{L}}{\boldsymbol{\nabla}\psi^*(\mathbf{x},t)} = -\frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\psi(\mathbf{x},t)\,, \frac{\partial\mathcal{L}}{\partial\,\dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}} = 0\,, \tag{5.40}$$

$$\frac{\partial\mathcal{L}}{\partial\psi(\mathbf{x},t)} = V_1(\mathbf{x})\psi(\mathbf{x},t)\,, \quad \frac{\partial\mathcal{L}}{\boldsymbol{\nabla}\psi(\mathbf{x},t)} = \frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\psi^*(\mathbf{x},t)\,, \quad \frac{\partial\mathcal{L}}{\partial\,\dfrac{\partial\psi(\mathbf{x},t)}{\partial t}} = -i\hbar\psi^*(\mathbf{x},t)\,. \tag{5.41}$$

Namely, whereas (4.49) and (5.40) have the same signs, we observe different signs in (4.50) and (5.41). Despite of that we obtain in the fermionic case from (5.38)–(5.41) formally the same equations of motion for the Schrödinger Grassmann fields

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \psi(\mathbf{x},t)\,, \tag{5.42}$$

$$-i\hbar \frac{\partial \psi^*(\mathbf{x},t)}{\partial t} = \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \psi^*(\mathbf{x},t)\,. \tag{5.43}$$

as in the bosonic case (4.1) and (4.2).

5.3 Hamilton Field Theory for Fermions

Going over from the Lagrange to the Hamilton formulation of field theory one needs the momentum fields, which are canonically conjugated to the anti-commuting Schrödinger fields $\psi^*(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$. From (5.36), (5.37) as well as from (5.40), (5.41) we conclude:

$$\pi^*(\mathbf{x},t) = \frac{\delta L}{\delta \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} = 0\,, \tag{5.44}$$

$$\pi(\mathbf{x},t) = \frac{\delta L}{\delta \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} = -i\hbar\psi^*(\mathbf{x},t)\,. \tag{5.45}$$

Thus, $\pi^*(\mathbf{x},t)$ vanishes and the momentum field $\pi(\mathbf{x},t)$, which is canonically conjugated to the Grassmann field $\psi(\mathbf{x},t)$, turns out be also a Grassmann field as it is given by $\psi^*(\mathbf{x},t)$. Furthermore, we remark that a comparison of (4.52) with (5.45) reveals a sign change. The Legendre transformation between the Lagrange function L and the Hamilton function H reads

$$L = \int d^3x \left\{ \frac{\partial \psi^*(\mathbf{x},t)}{\partial t}\,\pi^*(\mathbf{x},t) + \frac{\partial \psi(\mathbf{x},t)}{\partial t}\,\pi(\mathbf{x},t) \right\} - H\Big[\pi(\bullet,t);\psi(\bullet,t)\Big]\,. \tag{5.46}$$

Note that here the order of the Grassmann fields $\partial\psi(\mathbf{x},t)/\partial t$ and $\pi(\mathbf{x},t)$ and their complex conjugate is chosen in such a way that the Legendre transformation (5.46) is consistent with the definition of the canonical conjugated momentum fields in (5.44) and (5.45). Taking into account (5.30), (5.31) as well as (5.44) and (5.46), the Hamilton function turns out to be of the form

$$H = \int d^3x\, \mathcal{H}\left(\pi(\mathbf{x},t), \boldsymbol{\nabla}\pi(\mathbf{x},t); \psi(\mathbf{x},t), \boldsymbol{\nabla}\psi(\mathbf{x},t)\right)\,, \tag{5.47}$$

where the Hamilton density $\mathcal{H}$ is given by

$$\mathcal{H} = -\frac{\hbar}{2Mi}\,\boldsymbol{\nabla}\pi(\mathbf{x},t)\cdot\boldsymbol{\nabla}\psi(\mathbf{x},t) - \frac{V_1(\mathbf{x})}{i\hbar}\pi(\mathbf{x},t)\psi(\mathbf{x},t)\,. \tag{5.48}$$

Note that the fermionic Hamilton density (5.48) has the opposite sign of the bosonic Hamilton density (4.55). Furthermore, we remark that, in order to derive (5.48), we used the anti-commutativity of the Grassmann fields so that two terms proportional to $[\partial\psi(\mathbf{x},t)/\partial t]\pi(\mathbf{x},t)$

and $\pi(\mathbf{x},t)[\partial\psi(\mathbf{x},t)/\partial t]$ just cancel each other. Taking into account the relation (5.45) between $\pi(\mathbf{x},t)$ and $\psi^*(\mathbf{x},t)$ yields

$$H = \int d^3x \left\{ \frac{\hbar^2}{2M} \boldsymbol{\nabla}\psi^*(\mathbf{x},t) \cdot \boldsymbol{\nabla}\psi(\mathbf{x},t) + V_1(\mathbf{x})\psi^*(\mathbf{x},t)\psi(\mathbf{x},t) \right\} , \tag{5.49}$$

so a subsequent partial integration then converts (5.49) to the standard form

$$H = \int d^3x \, \psi^*(\mathbf{x},t) \left\{ -\frac{\hbar^2}{2M} \Delta + V_1(\mathbf{x}) \right\} \psi(\mathbf{x},t) \, . \tag{5.50}$$

Thus, we conclude that the two sign changes in (5.45) and (5.48) in comparison to the bosonic case compensate each other and the Hamilton function of anti-commuting Schrödinger fields (5.49) finally coincides formally with the corresponding one of commuting Schrödinger fields in (4.56).

The Hamilton principle of classical field theory reads in the Hamilton formulation

$$\delta\mathcal{A}\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right] = \int dt \int d^3x \left\{ \delta\pi(\mathbf{x},t) \, \frac{\delta\mathcal{A}}{\delta\pi(\mathbf{x},t)} + \delta\psi(\mathbf{x},t) \, \frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)} \right\} = 0 \, . \tag{5.51}$$

As the variations of the Grassmann fields $\delta\pi(\mathbf{x},t)$ and $\delta\psi(\mathbf{x},t)$ can be arbitrary, we obtain

$$\frac{\delta\mathcal{A}}{\delta\pi(\mathbf{x},t)} = 0 \, , \qquad \frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)} = 0 \, . \tag{5.52}$$

Due to (5.29) and (5.46) the action $\mathcal{A}$ depends on the Hamilton function H as follows:

$$\mathcal{A} = \int dt \int d^3x \, \frac{\partial\psi(\mathbf{x},t)}{\partial t} \, \pi(\mathbf{x},t) - \int dt \, H\left[\pi(\bullet,t);\psi(\bullet,t)\right] \, . \tag{5.53}$$

Performing the functional derivatives (5.52) of the action (5.53) then leads to the Hamilton equations of the anti-commuting Schrödinger fields:

$$\frac{\delta\mathcal{A}}{\delta\pi(\mathbf{x},t)} = -\frac{\partial\psi(\mathbf{x},t)}{\partial t} - \frac{\delta H}{\delta\pi(\mathbf{x},t)} = 0 \, , \tag{5.54}$$

$$\frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)} = -\frac{\partial\pi(\mathbf{x},t)}{\partial t} - \frac{\delta H}{\delta\psi(\mathbf{x},t)} = 0 \, . \tag{5.55}$$

Note that the first term of the Hamilton equation equation (5.54) has an opposite sign in comparison with the corresponding bosonic case in (4.61). As the Hamilton function H is of the form (5.47), the respective functional derivatives in (5.54) and (5.55) yield

$$\frac{\delta H}{\delta\pi(\mathbf{x},t)} = \frac{\partial\mathcal{H}}{\partial\pi(\mathbf{x},t)} - \boldsymbol{\nabla} \, \frac{\partial\mathcal{H}}{\partial\boldsymbol{\nabla}\pi(\mathbf{x},t)} \, , \tag{5.56}$$

$$\frac{\delta H}{\delta\psi(\mathbf{x},t)} = \frac{\partial\mathcal{H}}{\partial\psi(\mathbf{x},t)} - \boldsymbol{\nabla} \, \frac{\partial\mathcal{H}}{\partial\boldsymbol{\nabla}\psi(\mathbf{x},t)} \, , \tag{5.57}$$

which formally agree with the corresponding formulas of the bosonic case (4.63) and (4.64). Thus, inserting (5.56), (5.57) into (5.54), (5.55) the Hamilton equations of the Grassmann field theory have the form

$$\frac{\partial \psi(\mathbf{x},t)}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \pi(\mathbf{x},t)} + \boldsymbol{\nabla}\,\frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\pi(\mathbf{x},t)}\,, \tag{5.58}$$

$$\frac{\partial \pi(\mathbf{x},t)}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \psi(\mathbf{x},t)} + \boldsymbol{\nabla}\,\frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\psi(\mathbf{x},t)}\,. \tag{5.59}$$

Due to the Hamilton density of the Schrödinger theory (5.47) the respective partial derivatives read

$$\frac{\partial \mathcal{H}}{\partial \pi(\mathbf{x},t)} = -\frac{V_1(\mathbf{x})}{i\hbar}\psi(\mathbf{x},t)\,, \qquad \frac{\partial \mathcal{H}}{\boldsymbol{\nabla}\pi(\mathbf{x},t)} = -\frac{\hbar}{2Mi}\,\boldsymbol{\nabla}\psi(\mathbf{x},t)\,, \tag{5.60}$$

$$\frac{\partial \mathcal{H}}{\partial \psi(\mathbf{x},t)} = \frac{V_1(\mathbf{x})}{i\hbar}\pi(\mathbf{x},t)\,, \qquad \frac{\partial \mathcal{H}}{\boldsymbol{\nabla}\psi(\mathbf{x},t)} = \frac{\hbar}{2Mi}\,\boldsymbol{\nabla}\pi(\mathbf{x},t)\,. \tag{5.61}$$

Thus, we recover from (5.58)–(5.61) due to (5.45) the Schrödinger equations for the Grassmann fields (5.42) and (5.43), which formally agree with the Schrödinger equations of the bosonic case (4.1) and (4.2).

5.4 Poisson Brackets

Also in the classical field theory of anti-commuting Schrödinger fields one can introduce Poisson brackets. For two Grassmann functionals $F\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right]$ and $G\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right]$ their Poisson bracket is defined as

$$\Big\{F,G\Big\}_+ = (-1)^{\pi(F)}\int d^3x\left(\frac{\delta F}{\delta\psi(\mathbf{x},t)}\,\frac{\delta G}{\delta\pi(\mathbf{x},t)} + \frac{\delta F}{\delta\pi(\mathbf{x},t)}\,\frac{\delta G}{\delta\psi(\mathbf{x},t)}\right)\,, \tag{5.62}$$

where $\pi(F)$ denotes the parity of the Grassmann functional F. For instance, the anti-commuting Schrödinger fields $\psi(\mathbf{x},t)$ and $\pi(\mathbf{x},t)$ have an odd parity $\pi = 1$, whereas the Lagrange function (5.30), (5.31) or the Hamilton function (5.47), (5.48) have an even parity $\pi = 0$. Now we investigate the symmetry of the Poisson bracket (5.62), which leads to three cases:

1. case: $\pi(F) = \pi(G) = 0$

$$\begin{aligned}\Big\{F,G\Big\}_+ &= \int d^3x\left(\frac{\delta F}{\delta\psi(\mathbf{x},t)}\,\frac{\delta G}{\delta\pi(\mathbf{x},t)} + \frac{\delta F}{\delta\pi(\mathbf{x},t)}\,\frac{\delta G}{\delta\psi(\mathbf{x},t)}\right)\\ &= -\int d^3x\left(\frac{\delta G}{\delta\pi(\mathbf{x},t)}\,\frac{\delta F}{\delta\psi(\mathbf{x},t)} + \frac{\delta G}{\delta\psi(\mathbf{x},t)}\,\frac{\delta F}{\delta\pi(\mathbf{x},t)}\right) = -\Big\{G,F\Big\}_+\end{aligned} \tag{5.63}$$

2. case: $\pi(F) = 0$, $\pi(G) = 1$

$$\begin{aligned}\Big\{F,G\Big\}_+ &= \int d^3x\left(\frac{\delta F}{\delta\psi(\mathbf{x},t)}\,\frac{\delta G}{\delta\pi(\mathbf{x},t)} + \frac{\delta F}{\delta\pi(\mathbf{x},t)}\,\frac{\delta G}{\delta\psi(\mathbf{x},t)}\right)\\ &= \int d^3x\left(\frac{\delta G}{\delta\pi(\mathbf{x},t)}\,\frac{\delta F}{\delta\psi(\mathbf{x},t)} + \frac{\delta G}{\delta\psi(\mathbf{x},t)}\,\frac{\delta F}{\delta\pi(\mathbf{x},t)}\right) = -\Big\{G,F\Big\}_+\end{aligned} \tag{5.64}$$

   Note that the case $\pi(F) = 1$, $\pi(G) = 0$ follows from reading (5.64) in the opposite direction and exchanging F and G.

3. case: $\pi(F) = \pi(G) = 1$

$$\begin{aligned}
\left\{F, G\right\}_+ &= -\int d^3x \left(\frac{\delta F}{\delta\psi(\mathbf{x},t)} \frac{\delta G}{\delta\pi(\mathbf{x},t)} + \frac{\delta F}{\delta\pi(\mathbf{x},t)} \frac{\delta G}{\delta\psi(\mathbf{x},t)} \right) \\
&= -\int d^3x \left(\frac{\delta G}{\delta\pi(\mathbf{x},t)} \frac{\delta F}{\delta\psi(\mathbf{x},t)} + \frac{\delta G}{\delta\psi(\mathbf{x},t)} \frac{\delta F}{\delta\pi(\mathbf{x},t)} \right) = \left\{G, F\right\}_+ \qquad (5.65)
\end{aligned}$$

Thus, the Poisson bracket is symmetric for two odd Grassmann fields, otherwise it is anti-symmetric provided that the involved functionals do have a specific parity.

With the help of the Poisson bracket (5.62), the Hamilton equations (5.54), (5.55) for Grassmann fields read

$$\left\{\psi(\mathbf{x},t), H\right\}_+ = -\frac{\delta H}{\delta\pi(\mathbf{x},t)} = \frac{\partial\psi(\mathbf{x},t)}{\partial t}\,, \qquad (5.66)$$

$$\left\{\pi(\mathbf{x},t), H\right\}_+ = -\frac{\delta H}{\delta\psi(\mathbf{x},t)} = \frac{\partial\pi(\mathbf{x},t)}{\partial t}\,. \qquad (5.67)$$

Thus, the Hamilton equations of the fermionic and bosonic case (5.66), (5.67) and (4.70), (4.71), respectively, have the same general structure and only differ by the used Poisson bracket. Also the temporal change of a Grassmann functional $F\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right]$ can be formulated with the help of a Poisson bracket. At first we obtain with the chain rule of functional differentiation:

$$\frac{\partial F}{\partial t} = \int d^3x \left(\frac{\partial\pi(\mathbf{x},t)}{\partial t} \frac{\delta F}{\delta\pi(\mathbf{x},t)} + \frac{\partial\psi(\mathbf{x},t)}{\partial t} \frac{\delta F}{\delta\psi(\mathbf{x},t)} \right)\,, \qquad (5.68)$$

which reduces due to the Hamilton equations (5.54), (5.55) to

$$\begin{aligned}
\frac{\partial F}{\partial t} &= -\int d^3x \left(\frac{\delta H}{\delta\psi(\mathbf{x},t)} \frac{\delta F}{\delta\pi(\mathbf{x},t)} + \frac{\delta H}{\delta\pi(\mathbf{x},t)} \frac{\delta F}{\delta\psi(\mathbf{x},t)} \right) \\
&= (-1)^{\pi(F)} \int d^3x \left(\frac{\delta F}{\delta\psi(\mathbf{x},t)} \frac{\delta H}{\delta\pi(\mathbf{x},t)} + \frac{\delta F}{\delta\pi(\mathbf{x},t)} \frac{\delta H}{\delta\psi(\mathbf{x},t)} \right) = \left\{F, H\right\}_+\,. \qquad (5.69)
\end{aligned}$$

Thus, the formulation of the Hamilton equations in form of Poisson brackets according to (5.66), (5.67) represent a special case of (5.69). Furthermore, we obtain for the fundamental Poisson brackets:

$$\left\{\psi(\mathbf{x},t), \psi(\mathbf{x}',t)\right\}_+ = -\int d^3x'' \left(\frac{\delta\psi(\mathbf{x},t)}{\delta\psi(\mathbf{x}'',t)} \frac{\delta\psi(\mathbf{x}',t)}{\delta\pi(\mathbf{x}'',t)} - \frac{\delta\psi(\mathbf{x},t)}{\delta\pi(\mathbf{x}'',t)} \frac{\delta\psi(\mathbf{x}',t)}{\delta\psi(\mathbf{x}'',t)} \right) = 0\,. \qquad (5.70)$$

$$\left\{\pi(\mathbf{x},t), \pi(\mathbf{x}',t)\right\}_+ = -\int d^3x'' \left(\frac{\delta\pi(\mathbf{x},t)}{\delta\psi(\mathbf{x}'',t)} \frac{\delta\pi(\mathbf{x}',t)}{\delta\pi(\mathbf{x}'',t)} - \frac{\delta\pi(\mathbf{x},t)}{\delta\pi(\mathbf{x}'',t)} \frac{\delta\pi(\mathbf{x}',t)}{\delta\psi(\mathbf{x}'',t)} \right) = 0\,. \qquad (5.71)$$

$$\left\{\psi(\mathbf{x},t), \pi(\mathbf{x}',t)\right\}_+ = -\int d^3x'' \left(\frac{\delta\psi(\mathbf{x},t)}{\delta\psi(\mathbf{x}'',t)} \frac{\delta\pi(\mathbf{x}',t)}{\delta\pi(\mathbf{x}'',t)} - \frac{\delta\psi(\mathbf{x},t)}{\delta\pi(\mathbf{x}'',t)} \frac{\delta\pi(\mathbf{x}',t)}{\delta\psi(\mathbf{x}'',t)} \right) = -\delta(\mathbf{x}-\mathbf{x}')\,. \qquad (5.72)$$

Note the additional minus sign in (5.72) in comparison with (4.76).

5.5 Canonical Field Quantization

No we implement the canonical field quantization for fermions in the Heisenberg picture by going over from the anti-commuting Schrödinger fields $\psi(\mathbf{x},t)$ and $\pi(\mathbf{x},t)$ to corresponding second quantized field operators $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\pi}(\mathbf{x}, t)$. Here the question arises whether the Poisson bracket (5.62) corresponds to a commutator or to an anti-commutator. We show now that this depends upon which parity the Grassmann functions F and G have.

In case of the fundamental Poisson brackets (5.70)–(5.72) we observe that they are all symmetric. Therefore we postulate in case of symmetric Poisson brackets (5.65) a transition to anti-commutators, which are also symmetric:

$$\pi(F) = \pi(G) = 1 : \qquad \Big\{F, G\Big\}_+ \qquad \Longrightarrow \qquad \frac{1}{i\hbar}\Big[\hat{F}, \hat{G}\Big]_+ . \tag{5.73}$$

In this way, the fundamental Poisson brackets (5.70)–(5.72) go over into equal-time anti-commutation relations

$$\Big[\hat{\psi}(\mathbf{x}, t), \hat{\psi}(\mathbf{x}', t)\Big]_- = \Big[\hat{\pi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t)\Big]_- = 0\,, \qquad \Big[\hat{\psi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t)\Big]_- = -i\hbar\,\delta(\mathbf{x} - \mathbf{x}')\,. \tag{5.74}$$

As (5.45) implies that the momentum field operator $\hat{\pi}(\mathbf{x}, t)$ is given by the adjoint field operator $\hat{\psi}^\dagger(\mathbf{x}, t)$ via

$$\hat{\pi}(\mathbf{x}, t) = -i\hbar\,\hat{\psi}^\dagger(\mathbf{x}, t)\,, \tag{5.75}$$

we recognize that the previous equal-time anti-commutation relations (3.87) between the field operators $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\psi}^\dagger(\mathbf{x}, t)$ follow from (5.74).

Afterwards, we consider the Hamilton equations (5.66), (5.67), where the involved Poisson brackets are anti-symmetric. Therefore we postulate in case of (5.64))that the Poisson brackets go over to commutators, which are also anti-symmetric:

$$\pi(F) = 1,\ \pi(G) = 0 : \qquad \Big\{F, G\Big\}_+ \qquad \Longrightarrow \qquad \frac{1}{i\hbar}\Big[\hat{F}, \hat{G}\Big]_- . \tag{5.76}$$

Then we obtain from the Hamilton equations (5.66), (5.67) the corresponding Heisenberg equations

$$i\hbar\,\frac{\partial\hat{\psi}(\mathbf{x}, t)}{\partial t} = \Big[\hat{\psi}(\mathbf{x}, t), \hat{H}\Big]_-\,, \tag{5.77}$$

$$i\hbar\,\frac{\partial\hat{\pi}(\mathbf{x}, t)}{\partial t} = \Big[\hat{\pi}(\mathbf{x}, t), \hat{H}\Big]_-\,. \tag{5.78}$$

Due to (5.75) they turn out to agree with the Heisenberg equations of motion of the fields operators $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\psi}^\dagger(\mathbf{x}, t)$ in (3.68) and (3.73). And the Hamilton function (5.50) is converted within the canonical field quantization to the Hamilton operator (3.67) in the Heisenberg picture without the 2-particle interaction.