Chapter 4

Canonical Field Quantization for Bosons

The equal-time commutation relations (3.64) of the field operators $\hat{\psi}(\mathbf{x},t)$ and $\hat{\psi}^\dagger(\mathbf{x},t)$ have so far been introduced heuristically in order to describe a non-relativistic quantum many-body problem. In the following we show that these equal-time commutation relations (3.64) can be systematically derived from first principles within the canonical field quantization formalism for bosons. To this end we have to generalize the recipe how to quantize a system with a finite number of degrees of freedom to a continuum of degrees of freedom. But prior to that it is essential to work out the field theory of non-relativistic quantum mechanics.

4.1 Action of Schrödinger Field

We start with considering the complex Schrödinger field $\psi(\mathbf{x},t)$ and its adjoint $\psi^*(\mathbf{x},t)$ as two independent fields with their respective equations of motion:

$$i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} = \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \psi(\mathbf{x},t)\,, \tag{4.1}$$

$$-i\hbar \frac{\partial \psi^*(\mathbf{x},t)}{\partial t} = \left\{ -\frac{\hbar^2}{2M}\Delta + V_1(\mathbf{x}) \right\} \psi^*(\mathbf{x},t)\,. \tag{4.2}$$

Now we derive a variational principle with an underlying action so that these equations of motion emerge from applying the corresponding Hamilton principle. To this end we multiply (4.1) and (4.2) with the variations $\delta\psi^*(\mathbf{x},t)$ and $\delta\psi(\mathbf{x},t)$, respectively, add both equations together, yielding the spatio-temporal integral

$$\int dt \int d^3x \left\{ i\hbar \left[\delta\psi^*(\mathbf{x},t)\,\frac{\partial \psi(\mathbf{x},t)}{\partial t} - \delta\psi(\mathbf{x},t)\,\frac{\partial \psi^*(\mathbf{x},t)}{\partial t} \right] \right. \tag{4.3}$$
$$\left. + \frac{\hbar^2}{2M}\left[\delta\psi^*(\mathbf{x},t)\Delta\,\delta\psi(\mathbf{x},t) + \delta\psi(\mathbf{x},t)\Delta\,\delta\psi^*(\mathbf{x},t) \right] - V_1(\mathbf{x})\,\delta\left[\psi^*(\mathbf{x},t)\psi(\mathbf{x},t) \right] \right\} = 0\,.$$

Note we have used in the last term the product rule for field variations:

$$\delta\Big[\psi^*(\mathbf{x},t)\psi(\mathbf{x},t)\Big] = \delta\psi^*(\mathbf{x},t)\,\psi(\mathbf{x},t) + \delta\psi(\mathbf{x},t)\,\psi^*(\mathbf{x},t)\,. \tag{4.4}$$

Both terms in (4.3) with the temporal and the spatial derivatives are now partially integrated appropriately. Here we implicitly assume that the variations of the fields $\delta\psi(\mathbf{x},t)$ and $\delta\psi^*(\mathbf{x},t)$ vanish at the respective integration boundaries. Furthermore, we apply the calculational rule that a variation and a partial derivative are independent from each other, so they can be interchanged. With this one partial integration in time leads to

$$\int dt \left[\delta\psi^*(\mathbf{x},t)\frac{\partial\psi(\mathbf{x},t)}{\partial t} - \delta\psi(\mathbf{x},t)\frac{\partial\psi^*(\mathbf{x},t)}{\partial t}\right] = \delta\int dt\,\psi^*(\mathbf{x},t)\frac{\partial\psi(\mathbf{x},t)}{\partial t} \tag{4.5}$$

and two partial integrations in space give, correspondingly:

$$\int d^3x \Big[\delta\psi^*(\mathbf{x},t)\boldsymbol{\nabla}^2\,\delta\psi(\mathbf{x},t) + \delta\psi(\mathbf{x},t)\boldsymbol{\nabla}^2\,\delta\psi^*(\mathbf{x},t)\Big] = -\delta\int d^3x\,\boldsymbol{\nabla}\psi^*(\mathbf{x},t)\,\cdot\,\boldsymbol{\nabla}\psi(\mathbf{x},t)\,. \tag{4.6}$$

Inserting (4.5) and (4.6) into (4.3) we obtain a variational principle of the form

$$\delta\mathcal{A}\left[\psi^*(\bullet,\bullet);\psi(\bullet,\bullet)\right] = 0\,. \tag{4.7}$$

Note that we use here a bullet $\bullet$ in order to emphasize that the action is a functional of both Schrödinger fields $\psi^*(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$. The action $\mathcal{A}$ is defined as a temporal integral over a Lagrange function L according to

$$\mathcal{A} = \int dt\,L\left[\psi^*(\bullet,t),\frac{\partial\psi^*(\bullet,t)}{\partial t};\psi(\bullet,t),\frac{\partial\psi(\bullet,t)}{\partial t}\right] \tag{4.8}$$

and the Lagrange function L represents a spatial integral over the Lagrange density

$$L = \int d^3x\,\mathcal{L}\left(\psi^*(\mathbf{x},t),\boldsymbol{\nabla}\psi^*(\mathbf{x},t),\frac{\partial\psi^*(\mathbf{x},t)}{\partial t};\psi(\mathbf{x},t),\boldsymbol{\nabla}\psi(\mathbf{x},t),\frac{\partial\psi(\mathbf{x},t)}{\partial t}\right)\,. \tag{4.9}$$

In case of the Schrödinger field the Lagrange density reads

$$\mathcal{L} = i\hbar\,\psi^*(\mathbf{x},t)\,\frac{\partial\psi(\mathbf{x},t)}{\partial t} - \frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\psi^*(\mathbf{x},t)\,\cdot\,\boldsymbol{\nabla}\psi(\mathbf{x},t) - V_1(\mathbf{x})\psi^*(\mathbf{x},t)\psi(\mathbf{x},t)\,. \tag{4.10}$$

Conversely, it is also possible to rederive the original equations of motion (4.1) and (4.2) from a variational principle, which is based on the action (4.8)–(4.10). But this necessitates to introduce before the technique of functional derivatives, which we now introduce concisely without mathematical rigour.

4.2 Functional Derivative: Definition

At first we consider a function f of a finite number of degrees of freedom:

$$f = f(q_1,\ldots,q_N)\,. \tag{4.11}$$

The partial derivative of f with respect to the variable q_j, i.e.

$$\frac{\partial f(q_1, \ldots, q_N)}{\partial q_j}, \tag{4.12}$$

then denotes the change of the function with respect to the variable q_j, where all other variables $q_1, \ldots, q_{j-1}, q_{j+1}, \ldots, q_N$ remain constant. The total change of the function f

$$df(q_1, \ldots, q_N) = \sum_{j=1}^{N} \frac{\partial f(q_1, \ldots, q_N)}{\partial q_j}\, dq_j \tag{4.13}$$

is then additive in all possible changes of the function, where always only one variable changes and all the other variables remain constant. Specializing (4.13) to an infinitesimal change in one variable, i.e. $dq_j = \epsilon\delta_{ij}$, yields

$$f(q_1, \ldots, q_i + \epsilon, \ldots, q_N) - f(q_1, \ldots, q_i, \ldots, q_n) = df(q_1, \ldots, q_N) = \epsilon\, \frac{\partial f(q_1, \ldots, q_N)}{\partial q_i}. \tag{4.14}$$

Thus, the partial derivative follows from the limit of a difference quotient:

$$\frac{\partial f(q_1, \ldots, q_N)}{\partial q_i} = \lim_{\epsilon \to 0} \frac{f(q_1, \ldots, q_i + \epsilon, \ldots, q_N) - f(q_1, \ldots, q_i, \ldots, q_n)}{\epsilon}. \tag{4.15}$$

Now we generalize this concept of differentiation from a finite number to a continuum of variables. Therefore, we regard now a functional

$$F = F\big[\phi(\bullet)\big], \tag{4.16}$$

i.e. a mapping of a field $\phi(x)$ to a real or a complex number. The functional derivative

$$\frac{\delta F\big[\phi(\bullet)\big]}{\delta\phi(x)} \tag{4.17}$$

should then describe how the functional F changes provided that the function $\phi(x)$ is only changed at a single point x. Thus, the functional derivative (4.17) becomes in this way an ordinary function, which depends on the variable x. In analogy to (4.13) the total change of the functional F is defined via

$$\delta F\big[\phi(\bullet)\big] = \int dx\, \frac{\delta F\big[\phi(\bullet)\big]}{\delta\phi(x)}\, \delta\phi(x), \tag{4.18}$$

so it is additive with respect to all local changes of the function $\phi(x)$ at all space points x. Similar to the case of a partial derivative also the functional derivative can be determined from the limit of a difference quotient. To this end we introduce a local perturbation of the field $\phi(x)$ at space point y with strength ϵ:

$$\delta\phi(x) = \epsilon\delta(x - y). \tag{4.19}$$

and determine from (4.18)

$$F[\phi(\bullet) + \epsilon\delta(\bullet - y)] - F[\phi(\bullet)] = \delta F[\phi(\bullet)] = \int dx\, \frac{\delta F[\phi(\bullet)]}{\delta\phi(x)}\, \delta\phi(x) = \epsilon\, \frac{\delta F[\phi(\bullet)]}{\delta\phi(y)}. \tag{4.20}$$

In the limit $\epsilon \to 0$ we obtain

$$\frac{\delta F[\phi(\bullet)]}{\delta\phi(y)} = \lim_{\epsilon\to 0} \frac{F[\phi(\bullet)+\epsilon\delta(\bullet - y)] - F[\phi(\bullet)]}{\epsilon} \,. \tag{4.21}$$

From this definition of the functional derivative as a limit of a difference quotient follow several useful calculation rules. At first, we obtain from (4.21) the trivial functional derivative

$$\frac{\delta\phi(x)}{\delta\phi(y)} = \lim_{\epsilon\to 0} \frac{\phi(x)+\epsilon\delta(x-y)-\phi(x)}{\epsilon} = \delta(x-y) \,. \tag{4.22}$$

Then we determine from (4.21) the product rule

$$\begin{aligned}
&\frac{\delta\{F[\phi(\bullet)]G[\phi(\bullet)]\}}{\delta\phi(y)} = \lim_{\epsilon\to 0} \frac{F[\phi(\bullet)+\epsilon\delta(\bullet - y)]G[\phi(\bullet)+\epsilon\delta(\bullet - y)] - F[\phi(\bullet)]G[\phi(\bullet)]}{\epsilon} \\
&= \lim_{\epsilon\to 0} \left\{ \frac{F[\phi(\bullet)+\epsilon\delta(\bullet - y)] - F[\phi(\bullet)]}{\epsilon}\, G[\phi(\bullet)] + F[\phi(\bullet)]\, \frac{G[\phi(\bullet)+\epsilon\delta(\bullet - y)] - G[\phi(\bullet)]}{\epsilon} \right\} \\
&= \frac{\delta F[\phi(\bullet)]}{\delta\phi(y)} G[\phi(\bullet)] + F[\phi(\bullet)] \frac{\delta G[\phi(\bullet)]}{\delta\phi(y)} \,.
\end{aligned} \tag{4.23}$$

And, finally, combining (4.21) and (4.22) yields the chain rule:

$$\frac{\delta f(\phi(x))}{\delta\phi(y)} = \lim_{\epsilon\to 0} \frac{f\left(\phi(x)+\epsilon\delta(x-y)\right) - f(\phi(x))}{\epsilon} = \frac{\partial f(\phi(x))}{\partial\phi(x)}\, \delta(x-y) = \frac{\partial f(\phi(x))}{\partial\phi(x)}\, \frac{\delta\phi(x)}{\delta\phi(y)} \,. \tag{4.24}$$

4.3 Functional Derivative: Application

Now we work out several non-trivial applications of the functional derivative in the realm of second quantization, where it turns out to be a useful tool in order to determine commutators between second quantized operators. We start with the observation that the commutator (3.46) can also be determined from a functional derivative via

$$\left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{x}}\right]_- = \sum_{\nu=1}^{n} \delta(\mathbf{x}-\mathbf{x}_\nu)\, \hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_{\nu+1}}\hat{a}_{\mathbf{x}_{\nu-1}}\cdots\hat{a}_{\mathbf{x}_1} = \frac{\delta}{\delta\hat{a}_{\mathbf{x}}}\, \hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1} \,. \tag{4.25}$$

Let us consider then an arbitrary functional $F[\hat{a}_\bullet]$ of the annihilation operator $\hat{a}_{\mathbf{x}}$:

$$F[\hat{a}_\bullet] = \sum_{n=1}^{\infty} \int d^3x_1 \cdots \int d^3x_n\, F_n(\mathbf{x}_1,\ldots\mathbf{x}_n)\, \hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1} \,. \tag{4.26}$$

Then the functional derivative of this functional (4.26) with respect to the annihilation operator $\hat{a}_{\mathbf{x}}$ can be efficiently determined via a functional derivative due to (4.25):

$$\begin{aligned}
\left[F[\hat{a}_\bullet], \hat{a}^\dagger_{\mathbf{x}}\right]_- &= \sum_{n=1}^{\infty} \int d^3x_1 \cdots \int d^3x_n\, F_n(\mathbf{x}_1,\ldots\mathbf{x}_n)\, \left[\hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1}, \hat{a}^\dagger_{\mathbf{x}}\right]_- \\
&= \sum_{n=1}^{\infty} \int d^3x_1 \cdots \int d^3x_n\, F_n(\mathbf{x}_1,\ldots\mathbf{x}_n)\, \frac{\delta}{\delta\hat{a}_{\mathbf{x}}}\, \hat{a}_{\mathbf{x}_n}\cdots\hat{a}_{\mathbf{x}_1} = \frac{\delta}{\delta\hat{a}_{\mathbf{x}}}\, F[\hat{a}_\bullet] \,.
\end{aligned} \tag{4.27}$$

In a similar manner one also proves

$$\left[\hat{a}_{\mathbf{x}}, F[\hat{a}^{\dagger}_{\bullet}]\right]_{-} = \frac{\delta}{\delta \hat{a}^{\dagger}_{\mathbf{x}}} F[\hat{a}^{\dagger}_{\bullet}] \,. \tag{4.28}$$

In particular, (4.27) and (4.28) allow to reproduce the non-trivial commutation relation in (3.25) with functional derivatives:

$$\left[\hat{a}_{\mathbf{x}}, \hat{a}^{\dagger}_{\mathbf{x}'}\right]_{-} = \frac{\delta \hat{a}_{\mathbf{x}}}{\delta \hat{a}_{\mathbf{x}'}} = \frac{\delta \hat{a}^{\dagger}_{\mathbf{x}'}}{\delta \hat{a}^{\dagger}_{\mathbf{x}}} = \delta(\mathbf{x} - \mathbf{x}') \,. \tag{4.29}$$

And it is even possible to show that both calculational rules (4.27) and (4.28) can also be applied to functionals, which contain creation and annihilation operators in normal order:

$$\left[F[\hat{a}^{\dagger}_{\bullet}, \hat{a}_{\bullet}], \hat{a}^{\dagger}_{\mathbf{x}}\right]_{-} = F[\hat{a}^{\dagger}_{\bullet}, \hat{a}_{\bullet}] \overleftarrow{\frac{\delta}{\delta \hat{a}_{\mathbf{x}}}} \,, \tag{4.30}$$

$$\left[\hat{a}_{\mathbf{x}}, F[\hat{a}^{\dagger}_{\bullet}, \hat{a}_{\bullet}]\right]_{-} = \overrightarrow{\frac{\delta}{\delta \hat{a}^{\dagger}_{\mathbf{x}}}} F[\hat{a}^{\dagger}_{\bullet}, \hat{a}_{\bullet}] \,. \tag{4.31}$$

Here the arrows over the functional derivatives indicate from which side the normal ordered functional of creation and annihilation operators has to be differentiated. With this it is also possible to reproduce the trivial commutation relation in (3.25) with functional derivatives:

$$\left[\hat{a}^{\dagger}_{\mathbf{x}}, \hat{a}^{\dagger}_{\mathbf{x}'}\right]_{-} = \hat{a}^{\dagger}_{\mathbf{x}} \overleftarrow{\frac{\delta}{\delta \hat{a}_{\mathbf{x}'}}} = 0 \,, \qquad \left[\hat{a}_{\mathbf{x}}, \hat{a}_{\mathbf{x}'}\right]_{-} = \overrightarrow{\frac{\delta}{\delta \hat{a}^{\dagger}_{\mathbf{x}}}} \hat{a}_{\mathbf{x}'} = 0 \,. \tag{4.32}$$

Furthermore, the calculational rules (4.30) and (4.31) in the Schödinger picture can be extended correspondingly to the Heisenberg picture:

$$\left[F\left[\hat{\psi}^{\dagger}(\bullet,\bullet)\hat{\psi}(\bullet,\bullet)\right], \hat{\psi}^{\dagger}(\mathbf{x},t)\right]_{-} = F\left[\hat{\psi}^{\dagger}(\bullet,\bullet)\hat{\psi}(\bullet,\bullet)\right] \overleftarrow{\frac{\delta}{\delta \hat{\psi}(\mathbf{x},t)}} \,, \tag{4.33}$$

$$\left[\hat{\psi}(\mathbf{x},t), F\left[\hat{\psi}^{\dagger}(\bullet,\bullet)\hat{\psi}(\bullet,\bullet)\right]\right]_{-} = \overrightarrow{\frac{\delta}{\delta \hat{\psi}^{\dagger}(\mathbf{x},t)}} F\left[\hat{\psi}^{\dagger}(\bullet,\bullet)\hat{\psi}(\bullet,\bullet)\right] . \tag{4.34}$$

With this the Heisenberg equations of motion (3.62) of the fields operators $\hat{\psi}^{\dagger}(\mathbf{x},t)$, $\hat{\psi}(\mathbf{x},t)$ can be formulated with the help of functional derivatives:

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{x},t)}{\partial t} = \left[\hat{\psi}(\mathbf{x},t), \hat{H}_{\mathrm{H}}(t)\right] = \overrightarrow{\frac{\delta}{\delta \hat{\psi}^{\dagger}(\mathbf{x},t)}} \hat{H}_{\mathrm{H}}(t) \,, \tag{4.35}$$

$$i\hbar \frac{\partial \hat{\psi}^{\dagger}(\mathbf{x},t)}{\partial t} = \left[\hat{\psi}^{\dagger}(\mathbf{x},t), \hat{H}_{\mathrm{H}}(t)\right] = -\hat{H}_{\mathrm{H}}(t) \overleftarrow{\frac{\delta}{\delta \hat{\psi}(\mathbf{x},t)}} \,. \tag{4.36}$$

Thus, we conclude that all commutators between second-quantized operators in Sections 3.2–3.4, which have been evaluated via the operator identities (3.10) and (3.43), can also be calculated with appropriate functional derivatives.

4.4 Euler-Lagrange Equations

After this technical excursion to the definition and application of functional derivatives we now return to the question how to determine the underlying equations of motion from the variational principle (4.7). Applying (4.18) to (4.7) we get

$$\delta \mathcal{A} = \int dt \int d^3x \left\{ \frac{\delta \mathcal{A}}{\delta \psi^*(\mathbf{x},t)} \, \delta\psi^*(\mathbf{x},t) + \frac{\delta \mathcal{A}}{\delta \psi(\mathbf{x},t)} \, \delta\psi(\mathbf{x},t) \right\} = 0 \, . \tag{4.37}$$

As the variations of the fields $\delta\psi^*(\mathbf{x},t)$ and $\delta\psi(\mathbf{x},t)$ are considered to be independent, we obtain from (4.37) the following two conditions:

$$\frac{\delta \mathcal{A}}{\delta \psi^*(\mathbf{x},t)} = 0 \, , \qquad \frac{\delta \mathcal{A}}{\delta \psi(\mathbf{x},t)} = 0 \, . \tag{4.38}$$

Thus, the Hamilton principle in Lagrangian field theory states that the fields $\psi^*(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$ are determined from extremizing the action. It remains to explicitly determine the functional derivatives of the action $\mathcal{A}$ with respect to the fields $\psi^*(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$. Due to (4.8) we have to consider the spatial coordinates $\mathbf{x}$ to be fixed and only take only variations with respect to the functional dependencies in time t into account. With the chain rule of functional differentiation (4.24) we get

$$\frac{\delta \mathcal{A}}{\delta \psi^*(\mathbf{x},t)} = \int dt' \left\{ \frac{\delta L}{\delta \psi^*(\mathbf{x},t')} \, \frac{\delta \psi^*(\mathbf{x},t')}{\delta \psi^*(\mathbf{x},t)} + \frac{\delta L}{\delta \dfrac{\partial \psi^*(\mathbf{x},t')}{\partial t'}} \, \frac{\delta \dfrac{\partial \psi^*(\mathbf{x},t')}{\partial t'}}{\delta \psi^*(\mathbf{x},t)} \right\} . \tag{4.39}$$

Interchanging variation and partial derivative allows for a partial integration, where the boundary terms can be ignored, yielding

$$\frac{\delta \mathcal{A}}{\delta \psi^*(\mathbf{x},t)} = \int dt' \left\{ \frac{\delta L}{\delta \psi^*(\mathbf{x},t')} - \frac{\partial}{\partial t'} \, \frac{\delta L}{\delta \dfrac{\partial \psi^*(\mathbf{x},t')}{\partial t'}} \right\} \frac{\delta \psi^*(\mathbf{x},t')}{\delta \psi^*(\mathbf{x},t)} \, . \tag{4.40}$$

From the trivial function derivative (4.22) follows

$$\frac{\delta \psi^*(\mathbf{x},t')}{\delta \psi^*(\mathbf{x},t)} = \delta(t-t') \, , \tag{4.41}$$

so we read off from (4.40)

$$\frac{\delta \mathcal{A}}{\delta \psi^*(\mathbf{x},t)} = \frac{\delta L}{\delta \psi^*(\mathbf{x},t)} - \frac{\partial}{\partial t} \, \frac{\delta L}{\delta \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} \, . \tag{4.42}$$

Correspondingly we obtain

$$\frac{\delta \mathcal{A}}{\delta \psi(\mathbf{x},t)} = \frac{\delta L}{\delta \psi(\mathbf{x},t)} - \frac{\partial}{\partial t} \, \frac{\delta L}{\delta \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} \, . \tag{4.43}$$

Thus, we conclude that (4.38) together with (4.42) and (4.43) represent the underlying Euler-Langrange equations. It remains to determine the respective functional derivatives of the Lagrange function (4.9). To this end we consider, conversely the time t to be fixed and only take only variations with respect to the functional dependencies in the spatial coordinates $\mathbf{x}$ into account. Applying similar techniques of the functional differentiation as before, we obtain

$$\frac{\delta L}{\delta \psi^*(\mathbf{x},t)} = \frac{\partial \mathcal{L}}{\partial \psi^*(\mathbf{x},t)} - \boldsymbol{\nabla} \frac{\partial \mathcal{L}}{\boldsymbol{\nabla} \psi^*(\mathbf{x},t)} \,, \qquad \frac{\delta L}{\delta \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} \,, \tag{4.44}$$

$$\frac{\delta L}{\delta \psi(\mathbf{x},t)} = \frac{\partial \mathcal{L}}{\partial \psi(\mathbf{x},t)} - \boldsymbol{\nabla} \frac{\partial \mathcal{L}}{\boldsymbol{\nabla} \psi(\mathbf{x},t)} \,, \qquad \frac{\delta L}{\delta \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} \,. \tag{4.45}$$

Thus, combining (4.38) with (4.42)–(4.45) yields ultimately the Euler-Lagrange equations of classical field theory:

$$\frac{\partial \mathcal{L}}{\partial \psi^*(\mathbf{x},t)} - \boldsymbol{\nabla} \frac{\partial \mathcal{L}}{\boldsymbol{\nabla} \psi^*(\mathbf{x},t)} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} = 0 \,, \tag{4.46}$$

$$\frac{\partial \mathcal{L}}{\partial \psi(\mathbf{x},t)} - \boldsymbol{\nabla} \frac{\partial \mathcal{L}}{\boldsymbol{\nabla} \psi(\mathbf{x},t)} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} = 0 \,. \tag{4.47}$$

Although we have derived these field equations in two variational steps by taking into account (4.8) and (4.9), they can also be directly determined by considering the action $\mathcal{A}$ as a spatio-temporal integral over the Lagrange density $\mathcal{L}$:

$$\mathcal{A} = \int dt \int d^3x \, \mathcal{L} \left(\psi^*(\mathbf{x},t), \boldsymbol{\nabla}\psi^*(\mathbf{x},t), \frac{\partial \psi^*(\mathbf{x},t)}{\partial t}; \psi(\mathbf{x},t), \boldsymbol{\nabla}\psi(\mathbf{x},t), \frac{\partial \psi(\mathbf{x},t)}{\partial t} \right) . \tag{4.48}$$

Now it remains in (4.46) and (4.47) to evaluate the respective partial derivatives of the Lagrange density $\mathcal{L}$ of the Schrödinger field theory defined in (4.10):

$$\frac{\partial \mathcal{L}}{\partial \psi^*(\mathbf{x},t)} = -V_1(\mathbf{x})\psi(\mathbf{x},t) + i\hbar \frac{\partial \psi(\mathbf{x},t)}{\partial t} \,, \frac{\partial \mathcal{L}}{\boldsymbol{\nabla}\psi^*(\mathbf{x},t)} = -\frac{\hbar^2}{2M} \boldsymbol{\nabla}\psi(\mathbf{x},t) \,, \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi^*(\mathbf{x},t)}{\partial t}} = 0 \,, \tag{4.49}$$

$$\frac{\partial \mathcal{L}}{\partial \psi(\mathbf{x},t)} = -V_1(\mathbf{x})\psi^*(\mathbf{x},t) \,, \quad \frac{\partial \mathcal{L}}{\boldsymbol{\nabla}\psi(\mathbf{x},t)} = -\frac{\hbar^2}{2M} \boldsymbol{\nabla}\psi^*(\mathbf{x},t) \,, \quad \frac{\partial \mathcal{L}}{\partial \dfrac{\partial \psi(\mathbf{x},t)}{\partial t}} = i\hbar\psi^*(\mathbf{x},t) \,. \tag{4.50}$$

Inserting these intermediate results (4.49) and (4.50) into (4.46) and (4.47) yields, indeed, the equations of motion of the Schrödinger theory (4.1) and (4.2).

4.5 Hamilton Field Theory

Now we go over from the Lagrange to the Hamilton formulation of classical field theory. To this end we have to determine at first the momenta fields $\pi^*(\mathbf{x},t)$, $\pi(\mathbf{x},t)$, which are canonically conjugated to the Schödinger fields $\psi^*(\mathbf{x},t)$, $\psi(\mathbf{x},t)$. In close analogy to a classical system with a finite number of degrees of freedom we obtain from (4.44), (4.49), and (4.50):

$$\pi^*(\mathbf{x},t) = \frac{\delta L}{\delta \dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \dfrac{\partial\psi^*(\mathbf{x},t)}{\partial t}} = 0\,, \tag{4.51}$$

$$\pi(\mathbf{x},t) = \frac{\delta L}{\delta \dfrac{\partial\psi(\mathbf{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \dfrac{\partial\psi(\mathbf{x},t)}{\partial t}} = i\hbar\psi^*(\mathbf{x},t)\,, \tag{4.52}$$

Thus, we conclude that $\psi^*(\mathbf{x},t)$ represents the canonically conjugated momentum field of $\psi(\mathbf{x},t)$. The Hamilton function follows via a Legendre transformation from the Lagrange function:

$$H = \int d^3x \left\{ \pi^*(\mathbf{x},t)\,\frac{\partial\psi^*(\mathbf{x},t)}{\partial t} + \pi(\mathbf{x},t)\,\frac{\partial\psi(\mathbf{x},t)}{\partial t} \right\} - L\,. \tag{4.53}$$

Inserting therein (4.9), (4.10) and (4.51), (4.52) the Hamilton function turns out to be of the form

$$H = \int d^3x\, \mathcal{H}\left(\pi(\mathbf{x},t), \boldsymbol{\nabla}\pi(\mathbf{x},t); \psi(\mathbf{x},t), \boldsymbol{\nabla}\psi(\mathbf{x},t)\right)\,, \tag{4.54}$$

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

$$\mathcal{H} = \frac{\hbar}{2Mi}\,\boldsymbol{\nabla}\pi(\mathbf{x},t)\cdot\boldsymbol{\nabla}\psi(\mathbf{x},t) + \frac{V_1(\mathbf{x})}{i\hbar}\pi(\mathbf{x},t)\psi(\mathbf{x},t)\,. \tag{4.55}$$

Thus, taking into account the relation (4.52) between $\pi(\mathbf{x},t)$ and $\psi^*(\mathbf{x},t)$ yields

$$H = \int d^3x \left\{ \frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\psi^*(\mathbf{x},t)\cdot\boldsymbol{\nabla}\psi(\mathbf{x},t) + V_1(\mathbf{x})\psi^*(\mathbf{x},t)\psi(\mathbf{x},t) \right\}\,, \tag{4.56}$$

where a partial integration leads to the standard form

$$H = \int d^3x\, \psi^*(\mathbf{x},t) \left\{ -\frac{\hbar^2}{2M}\,\Delta + V_1(\mathbf{x}) \right\} \psi(\mathbf{x},t)\,, \tag{4.57}$$

Also the Hamilton equations of motion can be obtained in close analogy to the classical mechanics of a finite number of degrees of freedom. To this end one has to consider the action $\mathcal{A}$ as a functional of the fields $\pi(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$. Then the Hamilton principle

$$\delta\mathcal{A}\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right] = \int dt \int d^3x \left\{ \frac{\delta\mathcal{A}}{\delta\pi(\mathbf{x},t)}\,\delta\pi(\mathbf{x},t) + \frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)}\,\delta\psi(\mathbf{x},t) \right\} = 0\,. \tag{4.58}$$

leads because of the arbitrariness of the variations $\delta\pi(\mathbf{x},t)$ and $\delta\psi(\mathbf{x},t)$ to

$$\frac{\delta\mathcal{A}}{\delta\pi(\mathbf{x},t)} = 0\,, \qquad \frac{\delta\mathcal{A}}{\delta\psi(\mathbf{x},t)} = 0\,. \tag{4.59}$$

Due to (4.8) and (4.53) the action $\mathcal{A}$ depends on the Hamilton function H as follows:

$$\mathcal{A} = \int dt \int d^3x\, \pi(\mathbf{x},t)\,\frac{\partial\psi(\mathbf{x},t)}{\partial t} - \int dt\, H\left[\pi(\bullet,t);\psi(\bullet,t)\right]\,. \tag{4.60}$$

With this we can now evaluate the functional derivatives in (4.59), yielding the Hamilton equations of motion of classical field theory:

$$\frac{\delta \mathcal{A}}{\delta \pi(\mathbf{x},t)} = \frac{\partial \psi(\mathbf{x},t)}{\partial t} - \frac{\delta H}{\delta \pi(\mathbf{x},t)} = 0\,, \tag{4.61}$$

$$\frac{\delta \mathcal{A}}{\delta \psi(\mathbf{x},t)} = -\frac{\partial \pi(\mathbf{x},t)}{\partial t} - \frac{\delta H}{\delta \psi(\mathbf{x},t)} = 0\,. \tag{4.62}$$

As the Hamilton function H is of the form (4.56), the respective functional derivatives in (4.61) and (4.62) yield

$$\frac{\delta H}{\delta \pi(\mathbf{x},t)} = \frac{\partial \mathcal{H}}{\partial \pi(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\pi(\mathbf{x},t)}\,, \tag{4.63}$$

$$\frac{\delta H}{\delta \psi(\mathbf{x},t)} = \frac{\partial \mathcal{H}}{\partial \psi(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\psi(\mathbf{x},t)}\,, \tag{4.64}$$

Thus, inserting (4.63) and (4.64) into (4.61), (4.62) the Hamilton equations of classical field theory have the form

$$\frac{\partial \psi(\mathbf{x},t)}{\partial t} = \frac{\partial \mathcal{H}}{\partial \pi(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\pi(\mathbf{x},t)}\,, \tag{4.65}$$

$$\frac{\partial \pi(\mathbf{x},t)}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \psi(\mathbf{x},t)} + \boldsymbol{\nabla}\,\frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\psi(\mathbf{x},t)}\,. \tag{4.66}$$

Due to the Hamilton density of the Schrödinger theory (4.55) the respective partial derivatives read

$$\frac{\partial \mathcal{H}}{\partial \pi(\mathbf{x},t)} = \frac{V_1(\mathbf{x})}{i\hbar}\psi(\mathbf{x},t)\,, \qquad \frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\pi(\mathbf{x},t)} = \frac{\hbar}{2Mi}\,\boldsymbol{\nabla}\psi(\mathbf{x},t)\,, \tag{4.67}$$

$$\frac{\partial \mathcal{H}}{\partial \psi(\mathbf{x},t)} = \frac{V_1(\mathbf{x})}{i\hbar}\pi(\mathbf{x},t)\,, \qquad \frac{\partial \mathcal{H}}{\partial \boldsymbol{\nabla}\psi(\mathbf{x},t)} = \frac{\hbar}{2Mi}\,\boldsymbol{\nabla}\pi(\mathbf{x},t)\,. \tag{4.68}$$

Thus, we recover from (4.65)–(4.68) due to (4.52) the equations of motion of the Schrödinger theory (4.1) and (4.2).

4.6 Poisson Brackets

And, finally, we analyze the role of Poisson brackets in classical field theory. To this end we define for two functionals $F\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right]$ and $G\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right]$ their Poisson bracket via

$$\Big\{F,G\Big\}_- = \int d^3x \left(\frac{\delta F}{\delta \psi(\mathbf{x},t)}\,\frac{\delta G}{\delta \pi(\mathbf{x},t)} - \frac{\delta F}{\delta \pi(\mathbf{x},t)}\,\frac{\delta G}{\delta \psi(\mathbf{x},t)}\right)\,. \tag{4.69}$$

This allows to reexpress the Hamilton equations (4.61), (4.62) with the help of Poisson brackets:

$$\Big\{\psi(\mathbf{x},t),H\Big\}_- = \int d^3x' \left(\frac{\delta \psi(\mathbf{x},t)}{\delta \psi(\mathbf{x}',t)}\,\frac{\delta H}{\delta \pi(\mathbf{x}',t)} - \frac{\delta \psi(\mathbf{x},t)}{\delta \pi(\mathbf{x}',t)}\,\frac{\delta H}{\delta \psi(\mathbf{x}',t)}\right) = \frac{\delta H}{\delta \pi(\mathbf{x},t)} = \frac{\partial \psi(\mathbf{x},t)}{\partial t} \tag{4.70}$$

$$\Big\{\pi(\mathbf{x},t),H\Big\}_- = \int d^3x' \left(\frac{\delta\pi(\mathbf{x},t)}{\delta\psi(\mathbf{x}',t)}\frac{\delta H}{\delta\pi(\mathbf{x}',t)} - \frac{\delta\pi(\mathbf{x},t)}{\delta\pi(\mathbf{x}',t)}\frac{\delta H}{\delta\psi(\mathbf{x}',t)} \right) = -\frac{\delta H}{\delta\psi(\mathbf{x},t)} = \frac{\partial\pi(\mathbf{x},t)}{\partial t} \tag{4.71}$$

Also the temporal change of a functional $F\left[\pi(\bullet,\bullet);\psi(\bullet,\bullet)\right]$ can be formulated with the help of Poisson brackets. At first we obtain with the chain rule of functional differentiation:

$$\frac{\partial F}{\partial t} = \int d^3x \left(\frac{\partial\pi(\mathbf{x},t)}{\partial t}\frac{\delta F}{\delta\pi(\mathbf{x},t)} + \frac{\partial\psi(\mathbf{x},t)}{\partial t}\frac{\delta F}{\delta\psi(\mathbf{x},t)} \right), \tag{4.72}$$

which reduces due to the Hamilton equations (4.61), (4.62) and the Poisson brackets (4.69) to

$$\frac{\partial F}{\partial t} = \int d^3x \left(-\frac{\delta H}{\delta\psi(\mathbf{x},t)}\frac{\delta F}{\delta\pi(\mathbf{x},t)} + \frac{\delta H}{\delta\pi(\mathbf{x},t)}\frac{\delta F}{\delta\psi(\mathbf{x},t)} \right) = \Big\{F,H\Big\}_- . \tag{4.73}$$

Thus, the formulation of the Hamilton equations in form of Poisson brackets according to (4.70) and (4.71) follows immediately from (4.73). Furthermore, we obtain for the fundamental Poisson brackets of the Schrödinger field $\psi(\mathbf{x},t)$ and its canonical momentum field $\pi(\mathbf{x},t)$ at equal times:

$$\Big\{\psi(\mathbf{x},t),\psi(\mathbf{x}',t)\Big\}_- = \int d^3x'' \left(\frac{\delta\psi(\mathbf{x},t)}{\delta\psi(\mathbf{x}'',t)}\frac{\delta\psi(\mathbf{x}',t)}{\delta\pi(\mathbf{x}'',t)} - \frac{\delta\psi(\mathbf{x},t)}{\delta\pi(\mathbf{x}'',t)}\frac{\delta\psi(\mathbf{x}',t)}{\delta\psi(\mathbf{x}'',t)} \right) = 0\,. \tag{4.74}$$

$$\Big\{\pi(\mathbf{x},t),\pi(\mathbf{x}',t)\Big\}_- = \int d^3x'' \left(\frac{\delta\pi(\mathbf{x},t)}{\delta\psi(\mathbf{x}'',t)}\frac{\delta\pi(\mathbf{x}',t)}{\delta\pi(\mathbf{x}'',t)} - \frac{\delta\pi(\mathbf{x},t)}{\delta\pi(\mathbf{x}'',t)}\frac{\delta\pi(\mathbf{x}',t)}{\delta\psi(\mathbf{x}'',t)} \right) = 0\,. \tag{4.75}$$

$$\Big\{\psi(\mathbf{x},t),\pi(\mathbf{x}',t)\Big\}_- = \int d^3x'' \left(\frac{\delta\psi(\mathbf{x},t)}{\delta\psi(\mathbf{x}'',t)}\frac{\delta\pi(\mathbf{x}',t)}{\delta\pi(\mathbf{x}'',t)} - \frac{\delta\psi(\mathbf{x},t)}{\delta\pi(\mathbf{x}'',t)}\frac{\delta\pi(\mathbf{x}',t)}{\delta\psi(\mathbf{x}'',t)} \right) = \delta(\mathbf{x}-\mathbf{x}')\,. \tag{4.76}$$

4.7 Canonical Field Quantization

On the basis of having worked out the classical field theory to such an extent, we can now perform the canonical field quantization in the Heisenberg picture. To this end we associate to the complex Schrödinger field $\psi(\mathbf{x},t)$ and its canonically conjugated momentum field $\pi(\mathbf{x},t)$ corresponding second quantized field operators $\hat\psi(\mathbf{x},t)$ and $\hat\pi(\mathbf{x},t)$. Furthermore, in close analogy to the quantum mechanics for a finite number of degrees of freedom, we postulate that the Poisson bracket between two functionals F and G goes over into a commutator between their corresponding second quantized operators $\hat F$ and $\hat G$ as follows:

$$\Big\{F,G\Big\}_- \qquad \Longrightarrow \qquad \frac{1}{i\hbar}\Big[\hat F,\hat G\Big]_- . \tag{4.77}$$

In this way, the fundamental Poisson brackets (4.74)–(4.76) go over into equal-time commutation relations

$$\Big[\hat\psi(\mathbf{x},t),\hat\psi(\mathbf{x}',t)\Big]_- = \Big[\hat\pi(\mathbf{x},t),\hat\pi(\mathbf{x}',t)\Big]_- = 0\,, \qquad \Big[\hat\psi(\mathbf{x},t),\hat\pi(\mathbf{x}',t)\Big]_- = i\hbar\,\delta(\mathbf{x}-\mathbf{x}')\,. \tag{4.78}$$

As (4.52) 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

$$\hat\pi(\mathbf{x},t) = i\hbar\,\hat\psi^\dagger(\mathbf{x},t)\,, \tag{4.79}$$

we recognize that the previous equal-time commutation relations (3.64) between the field operators $\hat{\psi}(\mathbf{x}, t)$ and $\hat{\psi}^\dagger(\mathbf{x}, t)$ follow from (4.78). Furthermore, the postulate (4.77) converts the Hamilton equations (4.70), (4.71) into

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{x}, t)}{\partial t} = \left[\hat{\psi}(\mathbf{x}, t), \hat{H}\right]_- , \tag{4.80}$$

$$i\hbar \frac{\partial \hat{\pi}(\mathbf{x}, t)}{\partial t} = \left[\hat{\pi}(\mathbf{x}, t), \hat{H}\right]_- . \tag{4.81}$$

Due to (4.79) 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 (4.57) is converted within the canonical field quantization to the Hamilton operator (3.67) in the Heisenberg picture without the 2-particle interaction.