Boundary Quantum Mechanics*

Pavel Krtouš†

Institute of Theoretical Physics,
Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 180 00 Prague 8,
Czech Republic

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A reformulation of a physical theory in which measurements at the initial and final moments of time are treated independently is discussed, both on the classical and quantum levels. Methods of the standard quantum mechanics are used to quantize boundary phase space to obtain boundary quantum mechanics — a theory that does not depend on the distinction between the initial and final moments of time, a theory that can be formulated without reference to the causal structure. As a supplementary material, the geometrical description of quantization of a general (e.g. curved) configuration space is presented.

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†e-mail: Pavel.Krtous@mff.cuni.cz
Introduction

Motivation

In this work we formulate boundary quantum mechanics — a modification of the standard quantum mechanics where states at the initial and final moments of time are treated independently.

Our primary motivation for building the boundary quantum mechanics was an observation that in a field theory one usually has to define similar structures (such as e.g., Fock bases, vacuum states, coherent states, field and momentum observables) both for the initial and final moments of time and these structures only differ in the time at which they are defined. An effort to simplify handling of different structures at the initial and final time led to a unified picture in which both time boundaries play a completely equivalent role.

The main idea is to treat both the initial and final states of a physical system in an independent way, as if they would be states of different systems. The Hilbert space of boundary quantum mechanics is thus given as a tensor product of the initial and final Hilbert spaces. The dynamics of the boundary quantum mechanics is given by specifying a special physical state $|\text{phys}\rangle$ that contains all information about dynamical correlations.

Surprisingly, the resulting theory does not need to distinguish between the initial and final states — it can be formulated in a way in which we do not need to split the boundary of a (space)time domain on which we study the system to the initial and final parts. The consequence of this fact is that we can use the formalism of boundary quantum mechanics in situations when we do not have a reasonable causal structure which would allow us to identify the “initial” and “final” moments of time, particularly, we can use the formalism in the Euclidian form of a theory.

The material presented here is based on some parts of Ref. [1]. The work [1] was concerned mainly with a study of the relation between quantizations of a scalar field theory and relativistic particle theory. Boundary quantum mechanics was used for an alternative description of the scalar field theory. The general framework leading to boundary quantum mechanics was scattered in several places in Ref. [1]. Here, the material is presented in a modified and more compact form with an emphasis on the construction of the general formulation of the boundary mechanics.

After boundary quantum mechanics was constructed and used in Ref. [1] the author has found out that similar ideas have been pursued in the context of quantum gravity [2,3], however, in these works the idea of treating the different moments of time independently has been extended much farther — here “all moments of time” are treated independently, hence, the constructed Hilbert space of the theory is given by some kind of a continuous tensor product of Hilbert spaces for each time.

Plan of work

The explanation of the formalism is divided to three chapters. In Chapter 1 a classical analogue of boundary quantum mechanics is constructed, namely the boundary phase space is defined and its connection to standard phase spaces is studied. This chapter formulates the theory on a very general level. It allows to define the
boundary phase space without a reference to the causal structure. However, these
details are not necessary for the following chapters — if one is not interested in the
causal (in)dependence of the boundary phase space, it is sufficient to understand
the boundary phase space on the level explained in the overview and summary of
Chapter 1. The way of treating the general dynamical theory has been mainly
inspired by Ref. [4].

The material presented in Chapter 2 is actually independent of the main sub-
ject — of boundary quantum mechanics. In this chapter we present a geometrical
formulation of quantization for a system with a phase space with cotangent bundle
structure $T^*V$ over some configuration space $V$. This is a generalization of the
standard quantum mechanical methods of quantization of the position and mo-
mentum variables to the situation when the space of “positions” $V$ does not have a
linear structure — when it is a general manifold. Only a construction of “position”
and “momentum” observables and their position representation is presented here,
dynamical questions are not discussed.

Finally, boundary quantum mechanics is formulated in Chapter 3. First, the
theory is built on the basis of the usual quantum mechanics. Afterwards, it is
shown that boundary quantum mechanics can be constructed immediately from the
boundary phase space without reference to quantum mechanics at a given time. At
the end the issue of dynamics is discussed.

The main text is supplemented by three appendices in which some of the ge-
ometrical notions are reviewed. Appendix C defines the notion of densities of a
general (complex) weight on a manifold. Appendices A, B contain a geometri-
cal formulation of symplectic geometry. Most of this material is well known (see,
e.g., [5, 6]) and it is included mainly to fix the notation and remind the reader of
properties of different introduced objects. However, let us note that Appendix B
also defines covariant partial derivatives on tangent and cotangent bundles — a
notion which, to the author’s knowledge, is not defined elsewhere.

**Notation**

We use abstract indices to denote the tensor structure of different tensor objects
(see e.g. [7]). They indicate which space the object is from and allow us to write
down a contraction in the tensor algebra by the usual repetition of the indices. We
distinguish tensors with abstract indices from their coordinate representation. We
use bold letters for the abstract indices and normal letters for coordinate indices
(but you can hardly find them here). Hence, choosing a base $e^a_b$ and dual base $e^a_b$,
a = 1, 2, ... , we can write $A^a_b_\ldots = A^a_b_\ldots c^a_b_\ldots$, and $A^a_b_\ldots = A^a_b_\ldots e^a_b_\ldots$. Here $A^a_b_\ldots$ is a tensor object and $A^a_b_\ldots$ is a “bunch” of numbers depending on the base.

Because it can be tiresome to write indices all the time (but it is sometimes
inescapable), we drop them if it is clear what structure the object has. (In fact, we
view the abstract indices as some kind of a “dress” of the tensor object which serves
to specify tensor operations.) We also use an alternative notation for contraction
using an infix operator dot (we use different dots for different spaces), i.e., for
example, $a \cdot \omega = \omega \cdot a = a^m \omega_n$ or $(a \cdot g)_n = a^m g^m_n$. 


1 Boundary, canonical, and covariant phase spaces

Overview

The main goal of this chapter is to define a boundary phase space — a kinematical area of the classical counterpart of boundary quantum mechanics. We will start our construction on a very general level and we will see that the boundary phase space can be introduced for a very broad class of theories. However, after this general introduction we turn to a more specific theory to grasp the meaning of the boundary phase space and to understand its relation to standard phase spaces used in physics. We represent it as a cotangent bundle over the boundary value space and, at the end, we introduce special types of observables that will be quantized in the next chapter.

Before turning to a discussion of a general situation let us note that the basic idea lying behind the boundary phase space is very simple. The boundary phase space is a space of canonical data ("values" and "momenta") at both the initial and final time with a symplectic structure induced from canonical phase spaces at the initial and final moment of time. The main nontrivial output of the general discussion below is a construction of the boundary phase space without reference to the causal structure, without necessity of splitting the boundary data to the initial and final parts.

The space of histories and the action

A physical theory can be specified by a space of elementary histories $H$ and a dynamical structure on it. Elementary histories represent a wide class of potentially imaginable evolutions of the system, not necessarily realized in the nature.

Examples of the spaces of histories are the space of all possible trajectories in the spacetime (theory of a relativistic particle), the space of all possible field configuration on the spacetime (field theory), the space of all possible connections on a spacetime (gauge field theory) or the space of all maps from one manifold to another (target manifold (strings, membranes, ...). The space of histories of a general nonrelativistic system is a space of trajectories in a configuration space $V_o$ — in space of "positions".

We restrict ourselves to theories that are local on some inner manifold $N$ and we pay attention to this dependence. Generally, histories of such local theories can be represented as sections of some fibre bundle over the inner manifold. We use $x, y, \ldots$ as tensor indices for objects from tangent tensor spaces $TH$ and the dot $\cdot$ for contraction in these spaces. Let us note that "vectors" from $TH$ are again sections of some bundles over the inner manifold, i.e., they are essentially functions (or distributions), and their tensor indices $x, \ldots$ denote also the inner manifold dependence. The contraction $\cdot$ thus includes integration over the inner manifold.

Almost all known theories can be reformulated in this way. For example, elementary histories of a general nonrelativistic system can be viewed as mapping from a one dimensional inner manifold $N$ ("time-line" manifold) to the so-called target manifold $V_o$, i.e., as sections of the trivial fibre bundle $N \times V_o$ over $N$. The realization of a field theory is even more straightforward — the inner manifold is
spacetime and histories are sections of some bundle over it. We will restrict ourselves mainly to these two cases. Typical examples are a particle in a curved space and the scalar field theory (see [1] for a discussion of the latter case).

We assume that we are able to restrict the theory to any domain $\Omega$ in the inner manifold $N$. It means that we are able to speak about space of histories $\mathcal{H}[\Omega]$ on the domain $\Omega$. We will see that the domain of dependence plays an important role in the dynamics.

On the general level, we admit any sufficiently bounded domain $\Omega$ with a smooth boundary $\partial \Omega$. We need to deal with a bounded domain to assure that the action functional is well defined on a sufficiently wide set of histories. Generally, if the domain is compact, the action is defined for all smooth histories. However, we can also allow domains that are not compact “in some insignificant directions”. A typical example is a sandwich domain in a globally hyperbolic spacetime between two non-intersecting non-compact Cauchy surfaces. Such a domain is unbounded in the spatial direction and this fact has to be compensated by a restriction of the set of histories to those that fall-off sufficiently fast at spatial infinity. We cannot do the same thing in the temporal direction because we would exclude physically interesting histories — specifically, the solutions of the classical equations of motion. In case of a nonrelativistic system the domain $\Omega$ is simply a compact interval in the one dimensional inner manifold $N$.

The localization of histories on the domain $\Omega$ also gives us a localization of elements of the tangent spaces $T\mathcal{H}$, i.e., we can speak about a space $T\mathcal{H}[\Omega]$. We call these tangent vectors linearized histories. As we said, the tangent space at $h$ can be represented as a vector bundle over the inner manifold (or over the domain $\Omega$).

The dynamics of the system is given by a domain-dependent action $S[\Omega]$

$$S[\Omega] : \mathcal{H} \to \mathbb{R}.$$ \hspace{1cm} (1.1)

Let us note that we cannot generalize the action to a functional $S[N]$ on the whole inner manifold — it would be infinite for most physically interesting histories.

The action is local, i.e., for any $\Omega$

$$S[\Omega](h_1) = S[\Omega](h_2) \quad \text{if} \quad h_1 = h_2 \text{ on } \Omega,$$ \hspace{1cm} (1.2)

and additive under smooth joining of domains, i.e.,

$$S[\Omega](h) = S[(\Omega_1)(h) + S[\Omega_2](h),$$ \hspace{1cm} (1.3)

where $\Omega = \Omega_1 \cup \Omega_2$ is a domain and $\Omega_1 \cap \Omega_2$ is a submanifold without boundary which is a subset of both $\partial \Omega_1$ and $\partial \Omega_2$.

The equation of motion

In general, we work with smooth histories and smooth domains with a boundary, unless stated otherwise. We assume sufficient smoothness of the action but we skip the discussion of this issue.

However, we explicitly assume that the action is essentially of the first-order. In short, this means that the action leads to second-order equations of motion. On a
general level, this can be formulated by a condition that the variation of the action (keeping the domain $\Omega$ fixed) can be written in the following way

$$dS[\Omega](h) = \chi[\Omega] \delta S(h) - \mathfrak{P}[\partial \Omega](h) . \quad (1.4)$$

This relation represents an “integration by parts” usually employed in the variation of the action. A description of individual terms follows.

We use the gradient operator $d_x$ on the space of histories $\mathcal{H}$ to denote the variation. It is defined by the usual relation

$$\delta h \bullet dS[\Omega](h) = \frac{d}{d\varepsilon} S[\Omega](h_\varepsilon) \bigg|_{\varepsilon=0} , \quad (1.5)$$

where $h_\varepsilon$ is a curve in $\mathcal{H}$ with a tangent vector $\delta h x$ and, as mentioned above, the contraction $\bullet$ also includes integration over the domain $\Omega$ in the inner manifold.

$\delta S_x$ represents the variation of the action on the entire inner manifold. It is a 1-form on the space of histories $\mathcal{H}$ and we will refer to its tensor index $x$ as to a variational argument. We require that $\delta S(h)$ contain at most second-order inner space derivatives of the history $h$ and it is smooth in the variational argument. Thanks to this smoothness, multiplication by $\chi[\Omega]$ is well defined.

$\chi[\Omega]$ is the characteristic function of the domain $\Omega$ (i.e., $\chi[\Omega] = 1$ inside $\Omega$ and zero outside). We will also use a bi-distribution ($\chi[\Omega] \delta$) which projects (“cuts-off”) smooth functions to functions with a support on $\Omega$ (cf. Appendix C).

$\mathfrak{P}_x[\partial \Omega]$ is the generalized momentum on the boundary $\partial \Omega$. It is localized on the boundary in both its history dependence and in the variational argument (the momentum is a 1-form on $\mathcal{H}$ and by variational argument we again mean the $x$-dependence). We require that it can contain at most the first derivative in the direction normal to the boundary and cannot contain any normal derivatives in the variational argument. Hence, it can be represented as a distribution on boundary values of the linearized histories. Later (cf. Eqs. (1.13) and (1.14)) we clarify a relation of the generalized momentum to the usual definition of the momentum in the Lagrangian formalism.

The classical equations of motion are given by the condition

$$\delta S(h) = 0 , \quad (1.6)$$

and we denote the space of their solutions by $\mathcal{S}$ — it is the space of classical solutions.

The linearized equation of motion selects the linearized histories tangent to $\mathcal{S}$. It has the form

$$\tilde{\delta} S(h) \bullet \delta h = 0 , \quad (1.7)$$

where $\delta h$ is a linearized history (tangent vector to $\mathcal{H}$) at a classical history $h$ and the second variation of the action $\tilde{\delta}^2 S_{xy}$, given by

$$\tilde{\delta}^2 S_{xy}(h) = \mathcal{D}_y \delta S_x(h) , \quad (1.8)$$

$^a$The symbol “$\delta$” does not represent any operation here; it should be understood as a part of the symbol $\delta S$. 

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is a derivative of the form $\delta S$ using an ultralocal connection $D$. It is easy to check that for a classical history $h$, thanks to (1.6), the second variation of the action $\delta^2 S(h)$ does not depend on the choice of the connection $D$. We define $\delta^2 S_{xy} = \delta^2 S_{yx}$ and

$$\delta^2 S[\Omega] = (\chi[\Omega]) \cdot \delta^2 S, \quad \delta^2 S[\Omega] = \delta^2 S \cdot (\chi[\Omega]),$$

satisfying again $\delta^2 S_{xy}[\Omega] = \delta^2 S_{yx}[\Omega]$.

We assume that the equation of motion has a well-defined boundary problem on the domain $\Omega$, i.e., we assume the existence of a unique solution from $\mathcal{S}$ for a given restriction of a history to the boundary. Moreover, we assume that the linearized equation of motion has a well-formulated Dirichlet and Neumann boundary problem, i.e., there is a unique solution to the linearized equation of motion for a given linearized value on the boundary or linearized momentum on the boundary. This requires some generality of the action — for example we exclude a massless scalar field. More serious is the restriction that we must also exclude theories with local symmetries — see [4] for some details on this case.

When working with the manifold $\mathcal{S}$, we use $\mathbf{A}, \mathbf{B}, \ldots$ for tangent tensor indices.

**Boundary phase space**

Next we define the boundary symplectic structure $d\mathcal{P}[\partial \Omega]$ to be the external derivative of the generalized momentum 1-form $\mathcal{P}[\partial \Omega]$, which turns out to be the Wronskian of the second variation of the action (see (1.8)),

$$d\mathcal{P}[\partial \Omega] = \delta^2 S - \delta^2 S.$$

We say that two histories are canonically equivalent on the boundary if they have the same restriction on the boundary and the same momentum $\mathcal{P}$. We call the quotient of the space $\mathcal{H}$ with respect to this equivalence the boundary phase space $\mathcal{B}[\partial \Omega]$. A point from the boundary phase space thus represents values and momenta on the entire boundary $\partial \Omega$, i.e., at both the initial and final time.

We use $\mathbf{A}, \mathbf{B}, \ldots$ as tensor indices for tensors from the tangent spaces $T \mathcal{B}[\partial \Omega]$.

It is straightforward to check that vectors tangent to the orbits of equivalence are degenerate directions of the boundary symplectic form $d\mathcal{P}[\partial \Omega]$ and therefore we can define its action on the space $\mathcal{B}[\partial \Omega]$. We will require that the form $d\mathcal{P}[\partial \Omega]$ is non-degenerate on the boundary phase space. Because the external derivative of this form is zero, it is indeed a symplectic form in the sense of Appendix [A] and it gives a symplectic space structure to the space $\mathcal{B}[\partial \Omega]$, thus justifying the name boundary phase space.

The space $\mathcal{S}$ is a submanifold of $\mathcal{H}$ and, therefore, it defines a submanifold of the space $\mathcal{B}[\partial \Omega]$, which we denote by the same letter $\mathcal{S}$.
Lagrangian density

Until now, we have been developing the formalism on a very general level. In the following we restrict to theories with the action given by

\[ S(\Omega)(h) = \int_{\Omega} L(h, Dh) , \quad (1.11) \]

where \( L \) is the Lagrangian density — density on the inner manifold \( N \) — ultralocally dependent on the value of the history and “velocities”, i.e., inner space derivatives of the history.\(^6\)

In general, we need some additional structure on the fibre bundle \( \mathcal{H} \) to define the “velocity” (an inner space derivative of the history) — we need, for example, a connection on the bundle. There can exist a natural connection (e.g. if we can identify fibres of the bundle) or a choice of the connection can be equivalent to a specification of an external field (a gauge field of Yang-Mills theories). In the following we will have in mind mainly a general nonrelativistic system, where we do not need any additional structure — the velocity can be simply understood as a derivative of the trajectory \( h : N \to \mathcal{V}_o \) with respect to the “proper time” (a preferred coordinate on \( N \)).

In this simple case the variation of the action and an integration by parts gives us the decomposition \([12]\) with \( \delta S \) and \( \Psi[\partial \Omega] \) as follows:

\[ \delta S(h) = \nabla L(h, \dot{h}) - \left( \frac{\partial L}{\partial \dot{h}}(h, \dot{h}) \right) , \quad (1.12) \]

\[ \Psi[\partial \Omega](h) = \frac{\partial L}{\partial \dot{h}}(h, \dot{h}) \delta[\partial \Omega] . \quad (1.13) \]

Here \( \delta[\partial \Omega] \) is a delta function localized on the boundary \( \partial \Omega \), i.e., with a support at the end points of the time interval \( \Omega \). A similar expression for the general case when the inner manifold is not one dimensional and a thorough discussion of the scalar field case can be found in \([1]\).

Space of boundary values

We call the restriction of the history to the boundary \( \partial \Omega \) the boundary value of the history. We emphasize that the boundary values do not include any inner space derivatives of the histories in the direction normal to the boundary. The space of all boundary values \( \mathcal{V}[\partial \Omega] \) can be represented as a fibre bundle with the boundary \( \partial \Omega \) as the base manifold. We use \( x, y, \ldots \) as tensor indices for tensors from the tangent spaces \( T \mathcal{V}[\partial \Omega] \) and the dot \( \cdot \) for contraction in these spaces. In general, the boundary \( \partial \Omega \) is a manifold and the contraction \( \cdot \) includes integration over the boundary.

Let us note that the choice of notation is adjusted to the scalar field theory. In this case the inner manifold is spacetime, the target manifold are real numbers \( \mathbb{R} \),

\(^6\)The formalism developed until now is more general — it covers for example the case of the Einstein-Hilbert action for gravity for which the Lagrangian density contains second spacetime derivatives of the metric. But this dependence is degenerate and it is possible to satisfy the above conditions if a proper boundary term is chosen.
the space of histories $H$ is the space of functions on spacetime, and the indices $x, \ldots$ used for vectors from $T \mathcal{H}$ actually represent points in spacetime. Similarly, the space $V[\partial \Omega]$ is the space of functions on the boundary $\partial \Omega$ of a spacetime domain $\Omega$ and indices $x, \ldots$ represent points on the boundary. In case of the target manifold being not so simple, all these indices also carry information about a direction in the target manifold.

Another simple case is the nonrelativistic system where the inner manifold is one dimensional. In this case the linearized history $\delta h^x$ represents a time dependent target-manifold-vector-valued function, i.e., the index $x$ represents a time variable and a direction in the target manifold. The boundary $\partial \Omega$ consists only of two points from $N$ and the boundary value $x$ of a trajectory $h$ is a pair of end points $x = [x_f, x_i]$. The space of boundary values $V[\partial \Omega]$ is thus isomorphic to $V_o \times V_o$ and the tangent space $T V[\partial \Omega]$ to a direct sum $T V_o \oplus T V_o$. Therefore, the tensor indices $x, \ldots$ correspond to pairs of directions in the target manifold and the contraction $\cdot$ reduces to a contraction over finite dimensional vector spaces.

We denote the projection from $H$ to $V[\partial \Omega]$ by $x[\partial \Omega]$. We already said that the condition that the generalized momentum does not contain inner space derivatives normal to the boundary in its variational argument ensures that $x[\partial \Omega]$ can be realized as a distribution (in the $x$ argument) on the boundary values of the linearized histories — we do not need any other information about a linearized history $\delta h^x$ except its value on the boundary to compute $\delta h^x x[\partial \Omega]$. Translation between linearized histories and its boundary values is, of course, the differential $D x[\partial \Omega]$ of the projection $x[\partial \Omega]$. Hence, we can represent the generalized momentum in the following form:

$$\mathcal{P}_x[\partial \Omega] = p_x[\partial \Omega] D x[\partial \Omega] .$$

Here $p[\partial \Omega](h)$ is from the cotangent bundle $T^* x(h) V[\partial \Omega]$. The differential $D x[\partial \Omega]$ understood as a distribution (in the $x$ argument) is actually a delta function with a support on the boundary (multiplied by a (finite dimensional) unit tensor on the target manifold).

$x[\partial \Omega](h)$ and $p[\partial \Omega](h)$ represent the values and the momenta of the history $h$ at both the initial and final time. The meaning of $x[\partial \Omega](h)$ is clear from its definition; the meaning of $p[\partial \Omega](h)$ can be seen — at least in case of a one dimensional inner manifold — by comparing Eq. (1.14) and Eq. (1.13). The same interpretation holds in the general case, too (see [1] for the details of the scalar field case). In the following, we drop the boundary dependence of $x$ and $p$.

Next we define the classical history $\bar{h}(x)$ with a given boundary value $x$

$$\delta S(\bar{h}(x)) = 0 , \quad x(\bar{h}(x)) = x$$

and the classical action

$$\bar{S}[\Omega](x) = S[\Omega](\bar{h}(x)) .$$

We use $\bar{h}$ also for the induced map from the space $V[\partial \Omega]$ to the boundary phase space $B[\partial \Omega]$, and $x$ and $p$ for the induced maps from the boundary phase space $B[\partial \Omega]$ to the spaces $V[\partial \Omega]$ and $T^* V[\partial \Omega]$. This suggests that we can represent the boundary phase space $B[\partial \Omega]$ as a cotangent bundle $T^* V[\partial \Omega]$. Indeed, the
canonical symplectic structure of the cotangent bundle \(B.7\) does coincide with \(d\mathcal{P}[^\partial\Omega]\):

\[
\nabla_A p_x \wedge D^k_a x = d_A(p_x D^k_a x) = d_A \mathcal{P}_b.
\]

The space \(\mathcal{S}\) as a submanifold of \(\mathcal{B}[\partial\Omega]\) can be characterized using the condition

\[
p = -d\bar{S}(x),
\]

which follows from

\[
d_x \bar{S} = D^x_x \bar{h} \, d_x S(\bar{h}) = D^x_x \bar{h} \left( \delta S_x[^\Omega](\bar{h}) - \mathcal{P}_x[^\partial\Omega](\bar{h}) \right) = -D^x_x \bar{h} \left( D^x_x x(\bar{h}) \right) p_y(\bar{h}) = -p_x(\bar{h}).
\]

Linearization of Eq. (1.18) gives

\[
D^x_x \bar{h} = \nabla^x_x - (\nabla_x d_y \bar{S}) \frac{\partial}{\partial p_y}
\]

(see Appendix B for definitions of objects used here, especially Eq. \(B.6\)).

**Causal structure**

Until now we have not needed any time flow in the underlying inner manifold \(N\). It could be spacetime, an inner sheet of a string, or a one dimensional time-line — in all these cases we do have some kind of time flow. However, the formalism also works in a more general situation. We can use it, for example, for the Euclidian form of the theory, where we do not have any time direction. Now, we will use the time flow for the first time and we will add an additional causal structure that will allow us to define concepts such as canonical and covariant phase spaces.

All what we will use is an assumption that the boundary of the domain can be split into two disjoint parts without a boundary

\[
\partial \Omega = \partial \Omega_f \cup \partial \Omega_i = -\Sigma_f \cup \Sigma_i,
\]

\[
\partial \Omega_f = -\Sigma_f, \quad \partial \Omega_i = \Sigma_i,
\]

(1.21)

each of them carrying a full set of data (see the condition below). Here the minus sign suggests an opposite choice of the normal direction orientation for one part of the boundary. Clearly, we have in mind two Cauchy hypersurfaces that define a sandwich domain in a globally hyperbolic spacetime, or two end points of the interval in the one dimensional inner manifold \(N\) in the case of a non-relativistic system. The decomposition in (1.21) allows us to write

\[
\mathcal{V}[\partial \Omega] = \mathcal{V}[\Sigma_f] \times \mathcal{V}[\Sigma_i],
\]

\[
\mathcal{B}[\partial \Omega] = -\mathcal{B}[\Sigma_f] \oplus \mathcal{B}[\Sigma_i],
\]

\[
T \mathcal{V}[\partial \Omega] = T \mathcal{V}[\Sigma_f] \oplus T \mathcal{V}[\Sigma_i],
\]

(1.22)

and we will use shorthands \(\mathcal{V}, \mathcal{V}_f, \mathcal{V}_i\) and \(\mathcal{B}, \mathcal{B}_f, \mathcal{B}_i\).

In case of field theory, the space \(\mathcal{V}_f\) (or \(\mathcal{V}_i\), respectively) represents the space of field configurations on the final (or the initial) Cauchy hypersurface. In case of particle theory, spaces \(\mathcal{V}_f, \mathcal{V}_i\) represent positions of the particle at the final or
init time, i.e., $V_f = V_i = V_o$. Similarly $B_f$ (or $B_i$) represent canonical data (values and momenta) at the final (or initial) time.

We require that both parts contain a full set of boundary data — there should exist a unique classical history for a given element from $B_f$ or $B_i$.

Thanks to the locality, we can decompose the symplectic structure $d\mathcal{P}[\partial\Omega]$ as

$$d\mathcal{P}[\partial\Omega] = -d\mathcal{P}[\Sigma_f] + d\mathcal{P}[\Sigma_i] .$$

(1.23)

$d\mathcal{P}[\Sigma_f]$ and $d\mathcal{P}[\Sigma_i]$ play the role of the symplectic structure on $B_f$ and $B_i$. We will call these spaces canonical phase spaces. The minus sign in the relations (1.22) reflects the relation of these spaces as symplectic spaces.

The canonical phase spaces can be again represented as cotangent bundles $\mathcal{T} V_f$ and $\mathcal{T} V_i$ through the maps $x_f, p_f$ and $x_i, p_i$. Let us note that $p_f$ takes into account the opposite orientation of the normal direction to $\Sigma_f$ and $\partial\Omega f$, so that $p = -p_f \oplus p_i$.

(1.24)

Finally, we can also give a phase space structure to the space of classical histories $\mathcal{S}$. First we note that, thanks to (1.10), solutions $\xi_1, \xi_2 \in T \mathcal{S}$ of linearized equations of motion (1.7) satisfy

$$\xi_1 \cdot d\mathcal{P}[\partial\Omega] \cdot \xi_2 = 0 .$$

(1.25)

Therefore, it follows from (1.23) that $d\mathcal{P}[\Sigma_f]$ and $d\mathcal{P}[\Sigma_i]$ have the same restriction $\psi$ on the space $\mathcal{S}$.

$$\xi_1^A \psi_{AB} \xi_2^B = \xi_1 \cdot d\mathcal{P}[\Sigma_f] \cdot \xi_2 = \xi_1 \cdot d\mathcal{P}[\Sigma_i] \cdot \xi_2 .$$

(1.26)

In the same way, we check that the same expression for $\psi$ holds for any future-oriented Cauchy hypersurface $\Sigma$. It means that we have equipped the space of classical histories $\mathcal{S}$ with the symplectic structure $\psi$. We will call this space the covariant phase space. From Eq. (1.17) follows that the $\mathcal{V}_f, \mathcal{V}_i$ and $T^* \mathcal{V}_f, T^* \mathcal{V}_i$-valued observables $x_f, x_i$ and $p_f, p_i$ are canonically conjugate on this space (cf. Appendix A):

$$\psi_{AB} = \nabla_A p_i x_f \land \nabla_A p_i x_f = \nabla_A p_i x_f \land \nabla_A p_i x_f .$$

(1.27)

We can invert the symplectic form $\psi$ to get $\psi^{-1}$:

$$\psi^{-1} A M \psi_{BM} = \psi^{-1} A M \psi_{MB} = \delta^A_B .$$

(1.28)

If we view $\mathcal{S}$ as a subspace of the boundary phase space $\mathcal{B}$ we can understand $\psi^{-1}$ as a tensor from $T^2 \mathcal{B}$ tangent to $\mathcal{S}$ in both indices. Because the differential $D\bar{h}$ of the map $\bar{h} : \mathcal{V} \to \mathcal{B}$ (it is a restriction of the map (1.15) to $\mathcal{B}$) plays the role of a projector of vectors from $T \mathcal{V}$ to vectors from $T \mathcal{B}$ tangent to $\mathcal{S}$, we can write

$$\psi^{-1} = D\bar{h} \cdot g_c \cdot D\bar{h} .$$

(1.29)

with an antisymmetric tensor $g_c \in T^2 \mathcal{V}$. Using (1.24), (1.25), and (1.27) we get

$$g_c \cdot (d_i d_t \bar{S} - d_i d_t \bar{S}) = \delta^A .$$

(1.30)
This means that

\[ g_c = g_{i\ell} - g_{i\bar{\ell}}, \quad g_{i\ell}^{xy} = g_{i\bar{\ell}}^{xy}, \]

\[ g_{i\ell} \cdot d_i d_\ell \delta S = \delta \mathcal{V}_i, \quad g_{i\bar{\ell}} \cdot d_i d_{\bar{\ell}} \delta \bar{S} = \delta \mathcal{V}_i, \]  

(1.31)

and, using Eq. (1.20) again, we get

\[ \bar{\omega}^{-1} = \left( \frac{\nabla_x}{\partial x} - \frac{\partial}{\partial p_{iu}} (\nabla_{u} d_{iu} \bar{S}) \right) g_c^{xy} \left( \frac{\nabla_y}{\partial x} - (\nabla_y d_y \bar{S}) \frac{\partial}{\partial p_c} \right) = \]

\[ = \left( \frac{\partial}{\partial p_{iu}} \frac{\nabla_u}{\partial x_i} - \frac{\nabla_u}{\partial x_{i}} \frac{\partial}{\partial p_{iu}} \right) + \left( \frac{\partial}{\partial p_{iu}} \frac{\nabla_u}{\partial x_i} - \frac{\nabla_u}{\partial p_{iu}} \frac{\partial}{\partial x_i} \right) + \]

\[ + \left( \frac{\partial}{\partial p_{ix}} \frac{\nabla_x}{\partial x} \right) + \]

\[ + \left( \frac{\partial}{\partial p_{ix}} \left( (\nabla_{ix} d_{iu} \bar{S}) g_{i\ell}^{uv} (\nabla_{iv} d_{iy} \bar{S}) - d_{ix} d_{iy} \bar{S} \right) \frac{\partial}{\partial p_{iy}} \right) \]

(1.32)

\[ = \frac{\partial}{\partial p_{iy}} \left( (\nabla_{ix} d_{iu} \bar{S}) g_{i\ell}^{uv} (\nabla_{ix} d_{iu} \bar{S}) - d_{ix} d_{iy} \bar{S} \right) \frac{\partial}{\partial p_{iy}} \right) + \]

\[ + \frac{\nabla_x}{\partial x_i} \frac{\nabla_x^{xy}}{\partial x} \frac{\partial}{\partial p_{iu}} - \frac{\nabla_x}{\partial p_{iu}} \frac{\nabla_x^{xy}}{\partial x_i} \frac{\partial}{\partial p_{iu}} \]

\[ + \left( \frac{\nabla_x}{\partial x_i} \frac{\nabla_x^{xy}}{\partial x} \frac{\partial}{\partial p_{iu}} - \frac{\nabla_x}{\partial p_{iu}} \frac{\nabla_x^{xy}}{\partial x_i} \right). \]

Here, \( \nabla \) is any covariant derivative on the value space \( \mathcal{V} \), \( \mathcal{V}_i \) and \( \mathcal{V}_i \) are its restrictions to \( \mathcal{V}_i \) and \( \mathcal{V}_i \), and \( d_i \), \( d_i \) are gradients on \( \mathcal{V}_i \) and \( \mathcal{V}_i \).

Or, if we view \( \mathcal{S} \) as a subspace of the space of histories \( \mathcal{H} \) we can understand \( \bar{\omega}^{-1} \) as a tangent tensor from \( T^2 \mathcal{H} \) that satisfies the linear equation of motion in both indices. We call this representation the causal Green function \( G_c \)

\[ G_c^{xy} = D_{x}^{x} \bar{g}_{y}^{xy} D_{y}^{y} \bar{g}_{x}^{xy}, \]  

(1.33)

where we now understand \( \bar{g} \) as a map from \( \mathcal{V} \) to \( \mathcal{H} \). In the space \( T \mathcal{H} \), Eq. (1.28) takes the form

\[ G_c \cdot d_{\mathfrak{P}}[\Sigma] = -D_C[\Sigma], \]  

(1.34)

where \( D_C[\Sigma] \) is a Cauchy projector on a history on the linearized classical history with the same value and momentum on the surface \( \Sigma \). It is, of course, an identity on \( T \mathcal{S} \).

Similarly to Eq. (1.33) we can introduce \( g_{i\ell} \) and \( G_{i\ell} \), which turn out to be the advanced and retarded Green functions, \( g_c \), \( g_{i\ell} \), and \( g_{i\ell} \) are thus the corresponding Green functions evaluated on the boundary \( \partial \Omega \).

Poisson brackets

The Poisson brackets of two observables on a phase space are defined by \( \{ A, B \} \mathcal{S} = d_x A G_c^{xy} d_y B \) on \( \mathcal{S} \).

(1.35)
For observables depending only on the boundary values and momenta — i.e., for observables on \( \mathcal{B} \) — we can define the Poisson brackets in the sense of the boundary phase space
\[
\{A, B\}_\mathcal{B} = d_a A \, d^{-1} \omega \, d_u B = \frac{\partial A}{\partial x} \nabla_x B - \frac{\partial B}{\partial x} \nabla_x A + \nabla_x A \, \frac{\partial B}{\partial p_x} - \frac{\partial A}{\partial p_x} \nabla_x B.
\] (1.36)

With the help of (1.32), we find that the covariant Poisson brackets for such observables are given by
\[
\{A, B\}_\mathcal{S} = d_a A \, d^{-1} \omega \, d_u B = 
\frac{\partial A}{\partial p_{lu}} \nabla_{x_i} \frac{\partial B}{\partial p_{lu}} + \nabla_x A \, \frac{\partial B}{\partial p_{lu}} + \frac{\partial B}{\partial p_{lu}} \nabla_x A + \nabla_x A \, \frac{\partial B}{\partial p_{lu}}.
\] (1.37)

Moreover, for observables localized only on \( \Sigma_1 \) or \( \Sigma_2 \) we have
\[
\{A_1, B_1\}_\mathcal{B} = -\{A_1, B_1\}_\mathcal{S} = \{A_1, B_1\}_\mathcal{S},
\] (1.38)

**Observables at most linear in momenta**

During the quantization we will be interested in a special kind of observables on the boundary phase space \( \mathcal{B} \) (or, in general, on any phase space with the cotangent bundle structure). We will investigate observables dependent only on the value and observables linear in the momentum. We define the following observables for a function \( f \) and a vector field \( a \) on \( \mathcal{V} \)
\[
F_f = f(x),
\] (1.39)
\[
G_a = a^x(x) p_x.
\] (1.40)

The Poisson brackets of these observables are
\[
\{F_{f_1}, F_{f_2}\}_\mathcal{B} = 0,
\] (1.41)
\[
\{F_f, G_a\}_\mathcal{B} = -F_a df,
\] (1.41)
\[
\{G_{a_1}, G_{a_2}\}_\mathcal{B} = G_{[a_1, a_2]}.
\]

Here \([a_1, a_2]\) is the Lie bracket of the vector fields \( a_1, a_2 \). In the sense of the covariant phase space we have
\[
\{F_{f_1}, F_{f_2}\}_\mathcal{S} = F_{df_1, g_{[a_1, a_2]} df_2} \text{ on } \mathcal{S}
\] (1.42)
and from the condition (1.18) we get
\[ G_a = F_a \, dS \quad \text{on} \quad S. \]  

(1.43)

Summary

Canonical phase spaces \( \mathcal{B}_1, \mathcal{B}_i \) or the covariant phase space \( S \) are commonly used phase spaces of the classical theory. The dynamical evolution is described as a canonical transformation of \( \mathcal{B}_i \) to \( \mathcal{B}_1 \) (the Schrödinger picture of the classical theory) or as an evolution of observables on \( S \) (Heisenberg picture on the classical level).

If we could use experimental devices localized only on the boundary of the investigated domain (i.e., if we could perform experiments only at the initial and final moments of time), the boundary phase space \( \mathcal{B} \) would be sufficient for a description of our system. It is enough to investigate observables defined using canonical variables at the beginning and at the end. The dynamics of the system is hidden in the definition of the special subspace — of the physical phase space \( S \) that tells us the relation between the initial value and momentum and the final value and momentum for a physical solution of the equation of motion. In other words, the space \( \mathcal{B} \) represents all possible values of canonical observables at the initial and the final time without knowledge of the equations of motion. The subspace \( S \) represents values of canonical observables correlated via the dynamical development of the system. The advantage of the boundary phase space \( \mathcal{B} \) is that we do not need any causal structure to define it. Hence, we can construct it even for a Euclidian theory. This advantage will be even more appealing in the quantum case.
2 Configuration quantization

Overview

In this chapter we describe a construction of quantum observables at most linear in momenta for a general system with a phase space $\mathcal{G}$. This chapter is completely independent of the previous one. The starting point is a phase space with a cotangent bundle structure, i.e., with the phase space built over a general configuration space $\mathcal{V}$. We will introduce a special type of quantum observables, that are generalizations of the classical position and momentum observables of the standard quantum mechanics on a linear configuration space, and we will find their position representation. The main idea is to understand the momentum observable as a shift operator along some “direction” in the configuration space. On a general manifold, however, we have to be careful, because the “direction” is specified by a vector field that is, in general, position dependent; and, of course, the position and momentum observables don’t commute.

Ideas of quantization

Quantization is a heuristic procedure of constructing a quantum theory for a given classical theory. Let us have a classical system with a kinematical area given by a phase space $\mathcal{G}$ and a symplectic structure $\omega$. Observables are functions on $\mathcal{G}$, and the Poisson brackets are given by Eq. (A.5). Quantization tells us how to assign to (at least some) classical observables quantum observables — operators on a quantum Hilbert space $\mathcal{H}$. We will use letters with a hat to denote quantum observables and we denote $\mathcal{O}$ the algebra they obey. They should satisfy the same algebraic relations as the classical observables and the commutation relations generated by Poisson brackets. Specifically, if the quantum versions of classical observables $A, B,$ and $C = \{A, B\}$ are $\hat{A}, \hat{B}, \hat{C}$, they should be related by

$$[\hat{A}, \hat{B}] = -i\hat{C},$$

(2.1)$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ being the commutator of operators. It is well known that the procedure described above cannot be carried out for all classical observables. Because quantum observables do not commute we have an “ordering problem” for observables given by a product of non-commuting observables.

The usual quantization procedure tries to quantize a specific class of classical observables and construct physically interesting observables from them. Even in this case the operator ordering ambiguity is encountered. But we have to expect this — a quantum theory is not fully determined by the classical counterpart.

We will discuss quantization for a general example of a classical theory given on a phase space $\mathcal{G}$ that has a cotangent bundle structure $T^*\mathcal{V}$. The mathematical structure of such a phase space is reviewed in Appendices \[\text{\text{A}}\] and \[\text{\text{B}}\]. The main goal is not to solve a dynamical problem here, but to formulate the quantization procedure in a geometrically covariant way. We will define quantum observables of the position and momentum in the case of a general configuration space $\mathcal{V}$ (i.e., without the usual assumption of linearity of the configuration space). This procedure will be applied to quantization of the boundary phase space in the next section.
Let us note that the procedure described below has a well-defined meaning for a finite-dimensional configuration space $\mathcal{V}$. Of course, this is not the case of, e.g., the scalar field theory, where the configuration space is the space of functions on the space manifold $\Sigma$. Technical problems with a generalization to an infinite dimensional case is one of the reasons why this kind of quantization is not usually employed to quantize a field theory, but see [1] and the end of this section for an additional discussion. However, in the following we will consider mainly a finite dimensional non-relativistic system, for example a particle in a curved space.

**Algebra of observables**

At the end of the last chapter we introduced two special kinds of observables on the phase space with a cotangent bundle structure. We defined the observables $\tilde{F}_f$ depending only on the “position” (Eq. (1.39)) and the observables $\tilde{G}_a$ linear in momentum (Eq. (1.40)). Their Poisson brackets are given in Eq. (1.41). Now, we will quantize these observables. First, we formulate more carefully what conditions we are imposing on the quantum versions of these observables.

We are looking for maps $\hat{F}$ and $\hat{G}$ from the test functions and test vector fields on the configuration space $\mathcal{V}$ to the space of quantum observables $O$

\[
\hat{F}_f \in O \quad \text{for} \quad f \in \mathfrak{F} \mathcal{V}, \\
\hat{G}_a \in O \quad \text{for} \quad a \in \mathfrak{T} \mathcal{V},
\]

(2.2)

that should be hermitian (for real $f$ and $a$)

\[
\hat{F}_f' = \hat{F}_f, \quad \hat{G}_a' = \hat{G}_a,
\]

(2.3)

and should satisfy commutation relations motivated by the Poisson brackets (1.41)

\[
[\hat{F}_f, \hat{F}_{f'}] = 0, \quad \text{(2.4)}
\]

\[
[\hat{F}_f, \hat{G}_a] = i\hat{F}_a \cdot df, \quad \text{(2.5)}
\]

\[
[\hat{G}_{a_1}, \hat{G}_{a_2}] = -i\hat{G}_{[a_1, a_2]} \quad \text{(2.6)}
\]

Next, we have to formulate the condition that the quantum observables satisfy “the same algebraic relations as the classical ones”. For the observables $\tilde{F}_f$ this is straightforward because they commute — we require that we be able to take out any algebraic operation $g(\ldots)$ from the argument of the observable and perform the same operation on the observables:

\[
\hat{F}_g(f_1, f_2, \ldots) = g(\hat{F}_{f_1}, \hat{F}_{f_2}, \ldots). \quad \text{(2.7)}
\]

With the $\tilde{G}_a$ we have to be more careful — they do not commute with each other and with the $\tilde{F}_f$ observables. But we are interested in observables linear in momentum, so we need to investigate only the vector-field dependence of the $\tilde{G}_a$. We require

\[
\hat{G}_{a_1 + \alpha a_2} = \hat{G}_{a_1} + \alpha \hat{G}_{a_2} \quad \text{for} \quad \alpha \in \mathbb{R}, \quad \text{(2.8)}
\]

\[
\hat{G}_{fa} = \hat{F}_{f' - a}, \hat{G}_a \hat{F}_{f' + a} \quad \text{for} \quad \gamma \in \mathbb{R}. \quad \text{(2.9)}
\]

The last condition is equivalent to the classical expression $G_{fa} = F_f G_a$, but it specifies the ordering of the quantum theory. We have chosen the exponents of
the function \( f \) in the special forms \((\frac{1}{2} - i\gamma)\) and \((\frac{1}{2} + i\gamma)\) to satisfy the hermiticity condition. The ordering condition can be rewritten as
\[
\hat{G}_{fa} = \left(\frac{1}{2} - i\gamma\right) \hat{F}_f \hat{G}_a + \left(\frac{1}{2} + i\gamma\right) \hat{G}_a \hat{F}_f = \frac{1}{2}(\hat{F}_f \hat{G}_a + \hat{G}_a \hat{F}_f) + \gamma \hat{F}_a \hat{d}_f .
\] (2.10)

Finally, we require that the position observables \( \hat{F}_f \) form a complete set of commuting observables
\[
\forall f \quad [\hat{F}_f, \hat{A}] = 0 \quad \Rightarrow \quad \exists g \quad \hat{A} = \hat{F}_g .
\] (2.11)

Let us note that from these conditions it follows that
\[
\hat{F}_\alpha = \alpha \hat{1} \quad \text{for} \quad \alpha \in \mathbb{R},
\] (2.12)
\[
\forall f, a \quad [\hat{F}_f, \hat{A}] = 0 \quad [\hat{G}_a, \hat{A}] = 0 \quad \Rightarrow \quad \exists \alpha \in \mathbb{R} \quad \hat{A} = \alpha \hat{1} .
\] (2.13)

**Position representation**

Next, we construct a position base in \( \mathcal{H} \) on which the action of the operators \( \hat{F}_f \) and \( \hat{G}_a \) has a simple representation. Or, in other words, we find a realization of the operators \( \hat{F}_f \) and \( \hat{G}_a \), which satisfies the conditions formulated above, as operators on the space of densities on the configuration manifold \( \mathcal{V} \).

We have, of course, immediately a candidate for such a base. The observables \( \hat{F}_f \) form a complete set of commuting observables, so there exists a base of eigenvectors labeled by the position in the configuration space \( \mathcal{V} \) such that
\[
\hat{F}_f |\text{pos}: x\rangle = f(x) |\text{pos}: x\rangle .
\] (2.14)

Strictly speaking, \( |\text{pos}: x\rangle \) are not vectors from the Hilbert space \( \mathcal{H} \) but generalized vectors that can be defined, for example, by the condition that the projectors to these states form an operator-valued density on the configuration space. It will be convenient later to give these vectors the character of a density of some (generally complex) weight \( \alpha \in \mathbb{C} \) (see Appendix \C\ for short review of densities on a manifold). I.e., we assume
\[
|\text{pos}: x\rangle \in \mathcal{H} \otimes \hat{C}_x^\alpha \mathcal{V} .
\] (2.15)

The base of eigenvectors is orthogonal, but we need to be careful when writing down a normalization condition. Because of the distributional character of the vectors we can normalize them only to a delta-distribution. And to get the right normalization we need to choose a volume element \( \mu \) on the value space. With such a volume element we can write the orthonormality relation
\[
\langle \text{pos}: x | \text{pos}: y \rangle = (\mu^{2 \Re \alpha - 1} \delta)(x|y) .
\] (2.16)

The completeness relation is
\[
\hat{1} = \int_{\mathcal{V}} |\text{pos}: \rangle \langle \text{pos}: | \mu^{1 - 2 \Re \alpha} .
\] (2.17)

Let us note that the conditions above do not fix the base \( |\text{pos}: x\rangle \) uniquely — they fix the base up to an \( x \)-dependent phase factor. We will deal with this ambiguity below.
For any vector \(|\text{state}\rangle \in \mathcal{H}\) we can define a wave function — a density of the weight \(\alpha^*\) on the configuration space \(\mathcal{V}\)

\[
\Psi_{|\text{state}\rangle}(x) = \langle \text{pos} : x | \text{state} \rangle . \tag{2.18}
\]

The density \(\mu\) defines the scalar product on this space which is an isomorphic to the product on the quantum space

\[
\langle \text{st}_1 | \text{st}_2 \rangle = (\Psi_{|\text{st}_1\rangle}, \Psi_{|\text{st}_2\rangle})_\mu = \int_{\mathcal{V}} \Psi_{|\text{st}_1\rangle}^* \Psi_{|\text{st}_2\rangle} \mu^{1-2 \Re \alpha} , \tag{2.19}
\]

and it induces the hermitian conjugation \(\dagger\) on operators acting on densities of weight \(\alpha\)

\[
(A\dagger \psi_1, \psi_2)_\mu = (\psi_1, A\psi_2)_\mu . \tag{2.20}
\]

We define the position representation of a quantum observable \(\hat{A}\) as an operator \(\hat{A}\) on wave functions

\[
\hat{A} \Psi_{|\text{state}\rangle} = \Psi_{\hat{A}|\text{state}\rangle} . \tag{2.21}
\]

Clearly,

\[
\hat{F}_f = f \delta , \tag{2.22}
\]

which can be also written as

\[
\hat{F}_f = \int_{\mathcal{V}} f \langle \text{pos} : . \rangle \langle \text{pos} : . | \mu^{1-2 \Re \alpha} . \tag{2.23}
\]

Phase fixing

Now we proceed to find the position representation of the momentum observables \(\hat{G}_a\). In this section we show that there exists a unique choice of the weight \(\alpha\), namely \(\alpha = (\frac{1}{2} - i \gamma)\), and of the phase of the position base \(|\text{pos} : x\rangle\), for which

\[
\hat{G}_a = -i \mathcal{L}_a , \tag{2.24}
\]

where \(\mathcal{L}_a\) is the Lie derivative along the vector field \(a\) acting to the right.

First we define the position shift operator along a vector field \(a\) on the configuration space \(\mathcal{V}\) as

\[
\hat{U}_a(\varepsilon) = \exp(-i \varepsilon \hat{G}_a) . \tag{2.25}
\]

The commutation relation gives us

\[
\hat{U}_a \hat{F}_f \hat{U}_a^{-1} = \hat{F}_{u_a f} . \tag{2.26}
\]

Here \(u_a(\varepsilon)\) is a diffeomorphism on \(\mathcal{V}\) induced by the vector field \(a\)

\[
\frac{d}{d\varepsilon} u_a = a , \quad u_a(\varepsilon_1 + \varepsilon_2) = u_a(\varepsilon_1) u_a(\varepsilon_2) , \tag{2.27}
\]
and \( u^*_a \) is a map induced by the diffeomorphism on objects defined on the configuration space. The equation \( \hat{F}_f \hat{U}_a \) gives us

\[
\hat{F}_f \hat{U}_a |\text{pos} : x \rangle = \hat{U}_a \hat{F}_{u^*_a}^{-1} f |\text{pos} : x \rangle \quad \Rightarrow \quad \hat{U}_a |\text{pos} : x \rangle \text{ is proportional to } |\text{pos} : u_a x \rangle.
\]

(2.28)

Here we have to be careful about the proportionality coefficient because vectors \(|\text{pos} : x \rangle\) and \(|\text{pos} : u_a x \rangle\) are also densities in different points \(x\) and \(u_a x\). Because \( \hat{U}_a(\varepsilon) \) forms a commuting one-dimensional group for \( \varepsilon \in \mathbb{R} \) we can write the proportionality relation as follows

\[
\begin{align*}
\hat{U}_a(\varepsilon) \Psi_a(x) |\text{pos} : x \rangle &= \Psi_a(u_a x) |\text{pos} : u_a x \rangle,
\end{align*}
\]

(2.29)

where \( \Psi_a \) is a density on \( V \) that is defined up to a density invariant under the action of the diffeomorphism \( u_a \).

Next we prove that \( \Psi_a \) can be chosen as a density of weight \( \left( \frac{1}{2} - \alpha \right) \) in the form

\[
\Psi_a = \mu \frac{1}{2} - \alpha \exp(-i\phi_a),
\]

(2.30)

where \( \phi_a \) is a real function on \( W \) defined up to a function constant on the orbits of \( u_a \).

We write \( \Psi_a \) as a density of the weight \( \left( \frac{1}{2} - \alpha \right) \) in the form

\[
\Psi_a = \mu \frac{1}{2} - \alpha \rho_a \exp(-i\phi_a),
\]

(2.31)

with \( \rho_a, \phi_a \) real functions. Remembering Eq. \( \text{(2.25)} \), the differential form of equation \( \text{(2.29)} \), gives

\[
\hat{G}_a \left( \mu \frac{1}{2} - \alpha \rho_a \exp(-i\phi_a) |\text{pos} : x \rangle \right) = i \mathcal{L}_a \left( \mu \frac{1}{2} - \alpha \rho_a \exp(-i\phi_a) |\text{pos} : x \rangle \right).
\]

(2.32)

From this, it follows that the position representation of the \( \hat{G}_a \) observables:

\[
\hat{G}_a = -i \mathcal{L}_a - i \left( \frac{1}{2} - \alpha^* \right) \frac{1}{\mu} \mathcal{L}_a \mu + \frac{1}{\rho_a} \mathcal{L}_a \rho_a + i a \cdot d\phi_a \delta.
\]

(2.33)

The definition \( \text{(2.21)} \) gives us

\[
\mathcal{L}_a^\dagger = -\mathcal{L}_a + \left( 2 \Re \alpha - 1 \right) \frac{1}{\mu} \mathcal{L}_a \mu \delta.
\]

(2.34)

The hermiticity condition \( \text{(2.3)} \) implies \( \hat{G}_a = \hat{G}_a^\dagger \). Substituting to this condition we obtain

\[
\frac{1}{\rho_a} \mathcal{L}_a \rho_a = 0,
\]

(2.35)

which means \( \rho_a \) should be constant, e.g., \( \rho_a = 1 \). It proves the statement \( \text{(2.30)} \).
Finally we show that the function \( \phi_a \) in equation (2.30) has the form
\[
\phi_a = \varphi + \tilde{\phi}_a ,
\]
\[
\tilde{\phi}_a(u_a(\varepsilon)x) - \tilde{\phi}_a(x) = \gamma \int_0^\varepsilon \frac{1}{\mu}(\mathcal{L}_a \mu) d\varepsilon ,
\]  
where \( \varphi \) is a real function independent of the vector field \( a \).

Let us define a function
\[
\lambda_a = a \cdot d\phi_a - \frac{\gamma}{\mu} \mathcal{L}_a \mu .
\]  
This allows us to write \( \tilde{G}_a \) as
\[
\tilde{G}_a = \tilde{G}_a' + \lambda_a \delta ,
\]
\[
\tilde{G}_a' = -i\mathcal{L}_a - i(\frac{1}{2} + i\gamma - \alpha^*) \frac{1}{\mu}(\mathcal{L}_a \mu) \delta .
\]

It is easy to check that the operators \( \tilde{G}_a' \) have the same properties as the operators \( \tilde{G}_a \). Using the consequences of the properties (2.8), (2.9), and (2.6), we get conditions on \( \lambda_a \):
\[
\lambda_{a_1 + a_2} = \lambda_{a_1} + f \lambda_{a_2} ,
\]
\[
\lambda_{[a_1, a_2]} = a \cdot d\lambda_{a_2} - a_2 \cdot d\lambda_{a_1} .
\]

The first condition implies that \( \lambda_a = a \cdot \lambda \) for some form \( \lambda \) on the configuration space \( \mathcal{V} \) and the second condition implies that this form is closed: \( d\lambda = 0 \). So, if we ignore topological problems (see some of the comments below), we can rewrite relation (2.37) as
\[
a \cdot d\phi_a = a \cdot d\varphi + \frac{\gamma}{\mu} \mathcal{L}_a \mu
\]  
for a real function \( \varphi \). Integrating along orbits of \( u_a \), we get the desired expression (2.36).

If we redefine our position base by the phase factor \( \exp(-i\varphi) \), we obtain the position representation for the momentum observables \( \tilde{G}_a \) in the form (2.39). We see that if we choose the density weight of our position base to be
\[
\alpha = \frac{1}{2} - i\gamma ,
\]
the position representation reduces to the simple form (2.24). This also allows us to write the action of \( \hat{G}_a \) in the position base:
\[
\hat{G}_a|_{\text{pos}} : \rangle = i\mathcal{L}_a|_{\text{pos}} : \rangle .
\]

Let us note that for this choice of \( \alpha \) we do not need any volume element on \( \mathcal{V} \) because the normalization and completeness conditions (2.16) and (2.17) reduce to
\[
\langle \text{pos} : x|\text{pos} : y \rangle = \delta(x|y) , \quad \mathbf{i} = \int_\mathcal{V} |\text{pos} : \rangle \langle \text{pos} : | .
\]  

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Uniqueness of the quantization

Now we ask the question whether all realizations of our quantization of the basic observables $F_f$ and $G_a$ are unitarily equivalent. Let us assume we have two quantum versions of the basic observables $\hat{F}_f, \hat{G}_a$ and $\hat{F}'_f, \hat{G}'_a$ that both satisfy all the conditions formulated above. Clearly, we can construct a unitary operator mapping the position base of the first pair to the position base of the second pair, except that we do not require a proper phase fixing. Such a unitary operator essentially identifies the position observables but not necessarily the momentum observables.

Therefore, we will investigate the relation between the observables $\hat{G}_a$ and $\hat{G}'_a$ that both, together with the common position observables $\hat{F}_f$, satisfy all the conditions above. The commutation relation (2.44) together with the completeness condition (2.11) gives

$$\hat{G}'_a - \hat{G}_a = \hat{F}_a \lambda_a$$

for an $a$-dependent real function $\lambda_a$. The linearity (2.45) and the ordering condition (2.9) give

$$\lambda_{a_1 + a_2} = \lambda_{a_1} + f \lambda_{a_2} \quad \Rightarrow \quad \lambda_a = \lambda \cdot a$$

for some form $\lambda$ on $\mathcal{V}$. The commutation relation (2.6) implies

$$[a_1, a_2] \cdot \lambda = a_1 \cdot d(a_2 \cdot \lambda) - a_2 \cdot d(a_1 \cdot \lambda) \quad \Rightarrow \quad d\lambda = 0.$$ (2.47)

If the configuration space $\mathcal{V}$ is sufficiently topologically trivial (precisely, if the first cohomology group is trivial), it follows from the last equation that the form $\lambda$ is a gradient of some function $\varphi$. In this case we can write

$$\hat{G}'_a = \exp(-i\hat{F}_\varphi)\hat{G}_a \exp(i\hat{F}_\varphi),$$

and we see that $\hat{G}'_a$ and $\hat{G}_a$ are unitary equivalent. If the configuration space is not topologically trivial and closed forms are not the same as exact forms, we can have unitarily inequivalent realizations of the basic quantum variables. We ignored this possibility when constructing the position base and we will not investigate it further here.

Relation between different orderings

Here we will investigate a relation between different orderings of the momentum observables. Let us assume that $\gamma_1 \hat{G}$ and $\gamma_2 \hat{G}$ together with the position observables $\hat{F}_f$ satisfy the above conditions with the parameter $\gamma_1$ or $\gamma_2$ in the ordering condition (2.9). Similary to the previous discussion we get

$$\gamma_1 \hat{G}_a - \gamma_2 \hat{G}_a = \hat{F}_a \tilde{\lambda}_a,$$

$$\tilde{\lambda}_{a_1 + a a_2} = \tilde{\lambda}_{a_1} + \alpha \tilde{\lambda}_{a_2} \quad \text{for} \quad \alpha \in \mathbb{R},$$

$$\tilde{\lambda}_f a = f \tilde{\lambda}_a + (\gamma_1 - \gamma_2) a \cdot df.$$ (2.51)

If we write the function $\tilde{\lambda}_a$ using a density $\mu$ on $\mathcal{V}$ as

$$\tilde{\lambda}_a = (\gamma_1 - \gamma_2) \frac{1}{\mu} \mathcal{L}_a \mu + \lambda_a,$$ (2.52)
we find that $\lambda_a$ has the same properties as in the previous section, i.e., it represents the freedom of the quantization of $G_a$ with the given ordering parameter. Because we have discussed it already, we ignore it now. Thus, we found that different orderings of the momentum observable can be written in the form

$$\gamma G_a = 0 \hat{G}_a + \gamma \hat{F}_{\mu} \Lambda_{\alpha \mu}.$$  

(2.53)

It is easy to check that the $\mu$ dependence for a fixed $\gamma$ is of the form discussed in the previous section.

**Observables quadratic in momentum**

Until now we only discussed quantization of observables independent of momentum and linear in momentum. We saw that these observables were sufficient for the construction of the natural base in the quantum Hilbert space $\mathcal{H}$. But they are not usually sufficient for the construction of the dynamics of the theory. A typical Hamiltonian is quadratic in momenta. Therefore, it is necessary to address the issue of quantization of such observables. I.e., we want to quantize classical observables of the form

$$K_k(x, p) = p \cdot k^{-1}(x) \cdot p,$$  

(2.54)

where $k$ is a metric on $\mathbf{V}$ and we have restricted ourself to the case of a non-degenerate $k$.

We can formulate conditions similar to those above for $\hat{F}_f$ and $\hat{G}_a$. With a suitable choice of simplicity and covariance requirements it is possible to show that there is a one-dimensional freedom in the ordering for the quadratic observables (labeled by a parameter $\xi \in \mathbb{R}$) and that the position representation $\hat{K}_k$ of the quadratic observable is

$$\hat{K}_k = L_k + \xi R_k,$$  

(2.55)

where $L_k$ and $R_k$ are the Laplace operator and scalar curvature of the metric $k$.

**Linear theory**

The situation simplifies significantly if the configuration space $\mathbf{V}$ is linear. This is usually assumed in simple quantum mechanical models and it is essential in the quantum field theory. For a linear theory, the formalism reduces to the standard canonical quantization. We will shortly illustrate the correspondence with the usual formalism using a notation borrowed from the the scalar field theory. However, these notes apply for any linear theory.

In the scalar field theory, the configuration space $\mathbf{V}[\Sigma]$ represents the space of all field configurations on a Cauchy hypersurface $\Sigma$ and the phase space $\mathcal{B}[\Sigma]$ has the structure of a cotangent bundle $T^* \mathbf{V}[\Sigma]$ that can be identified with the dual space $\mathbf{V}[\Sigma]^*$. The dual can be realized as the space of densities $\mathbf{V}[\Sigma]$ of the weight 1 on the hypersurface $\Sigma$. This brings good and bad news. As we said, the value space $\mathbf{V}[\Sigma]$ is linear, but it is infinite-dimensional. Let’s ignore the infinite dimension and do some formal manipulation first.
Linearity allows us to define the observables of value and momentum $\hat{\varphi}$ and $\hat{\pi}$ (roughly speaking operators $\hat{x}$ and $\hat{p}$ in the previous notations). These are, of course, not well defined objects in the general non-linear case but in the case of a linear space $\mathbf{V}$ it is possible to define them as objects from the spaces $\mathbf{V} \otimes \mathcal{O}$ and $\bar{\mathbf{V}} \otimes \mathcal{O}$. They are connected with the general observables $\hat{F}_f, \hat{G}_a$ of the previous sections as

$$\hat{F}_f = f(\hat{\varphi}) ,$$

$$\hat{G}_a = (\frac{1}{2} - i\gamma) a(\hat{\varphi}) \cdot \hat{\pi} + (\frac{1}{2} + i\gamma) \hat{\pi} \cdot a(\hat{\varphi}) ,$$

(2.56)

where we used the natural identification of the tangent space $T\mathbf{V}$ with $\mathbf{V}$ itself.

The value and momentum observables satisfy the canonical commutation relations

$$[\hat{\varphi}, \hat{\pi}] = i\delta_\mathbf{V} \mathbb{I} .$$

(2.57)

We can construct the value base normalized to a “constant measure” $\Omega$ on the configuration space $\mathbf{V}$

$$\varphi|val : \varphi\rangle = \varphi|val : \varphi\rangle \text{ for } \varphi \in \mathbf{V} ,$$

$$\hat{\pi}|val : \varphi\rangle = i d|val : \varphi\rangle ,$$

$$\langle val : \varphi_1|val : \varphi_2\rangle = (\Omega^{-1}) (\varphi_1|\varphi_2\rangle ,$$

$$\mathbb{I} = \int_{\varphi \in \mathbf{V}} \Omega|val : \varphi\rangle\langle val : \varphi| .$$

(2.58)

The wave functional for a state $|\text{state}\rangle$ has the form

$$\Psi_{|\text{state}\rangle}(\varphi) = \langle val : \varphi|\text{state}\rangle ,$$

(2.59)

the scalar product on wave functions is

$$\langle \text{st1}|\text{st2}\rangle = \int_{\mathbf{V}} \Psi^*_{|\text{st1}\rangle} \Psi_{|\text{st2}\rangle} \Omega ,$$

(2.60)

and the value representations of the observables $\hat{\varphi}$ and $\hat{\pi}$ are

$$\hat{\varphi} \Psi_{|\text{state}\rangle}(\varphi) = \varphi \Psi_{|\text{state}\rangle}(\varphi) ,$$

$$\hat{\pi} \Psi_{|\text{state}\rangle}(\varphi) = -i d\Psi_{|\text{state}\rangle}(\varphi) .$$

(2.61)

The problem is that in the infinite-dimensional case there is no such thing as a “constant measure” $\Omega$ on the space $\mathbf{V}$ and we do not have a Hilbert space generated by a scalar product on wave functions. The solution to these technical difficulties lies in a restriction of the possible wave functions to those that are falling off sufficiently fast so the functional integral (2.60) has a meaning even if the measure $\Omega$ itself does not have one. Such wave functions have to be suppressed, for example, by a Gaussian exponent — so the integral (2.60) turns into a Gaussian integration that is well defined even for infinite-dimensional spaces.
3 Boundary Quantum Mechanics

Introduction

In this chapter we will finally develop boundary quantum mechanics — a variation of quantum mechanics based on quantization of the boundary phase space. Here we present a general formulation of the method, an application to scalar field theory can be found in [1].

Let us start with the quantum theory described in the previous section. We quantized the observables \( F_f \) and \( G_a \) on a phase space with the cotangent bundle structure, we found quantum operators \( \hat{F}_f \) and \( \hat{G}_a \), and we constructed the special position base \( |\text{pos}: x_f\rangle \). We did not formulate the dynamical part of the theory; we will touch this issue now.

We are interested in a situation when we study the system only at the “beginning” and at the “end”. More precisely, we are interested in observables with a support only on the boundary of the domain \( \Omega \). It means that in the case of the field theory, when the inner manifold is a globally hyperbolic spacetime, observables are localized only on the initial and final hypersurfaces of the sandwich domain \( \Omega = (\Sigma_f, \Sigma_i) \). In case of a one-dimensional inner space manifold, the boundary of \( \Omega \) reduces to the initial and final moment of time. In these cases we can quantize the initial and final canonical phase spaces \( \mathcal{B}_i = \mathcal{B}[\Sigma_i] \) and \( \mathcal{B}_f = \mathcal{B}[\Sigma_f] \) — i.e. we construct the quantum observables \( \hat{F}_{f_i} \), \( \hat{G}_{f_i} \) and \( \hat{F}_{f_f} \), \( \hat{G}_{f_f} \) on a quantum space \( \mathcal{H} \) satisfying the conditions with the ordering parameters \( \gamma_i = -\gamma_i \), and the corresponding position bases \( |\text{pos}: x_i\rangle \) and \( |\text{pos}: x_f\rangle \) in the space \( \mathcal{H} \). The dynamics reduces to the investigation of relations between these two sets of observables or relations between objects generated by them, for example, of the position bases. We can state we solved the dynamical problem if we find in-out transition amplitudes \( \langle f\text{pos}: x_f|\text{pos}: x_i \rangle \) for all \( x_f \in \mathcal{V}[\Sigma_f] \) and \( x_i \in \mathcal{V}[\Sigma_i] \).

We do not attempt to find the transition amplitudes in a general situation. Instead, we reformulate this setting in a slightly different language.

Construction of the boundary quantum space

We represented the quantization of both \( \mathcal{B}_i \) and \( \mathcal{B}_f \) on a common quantum Hilbert space \( \mathcal{H} \). Let us construct another representation on the boundary quantum space

\[
\mathcal{H}_B = \mathcal{H}^\dagger \otimes \mathcal{H}
\]

(the space of tensor products of covector and vector elements of the form \( \langle f | \otimes | i \rangle \), i.e., essentially operators on \( \mathcal{H} \)). We use the notation \( |\text{state}\rangle \) for vectors from \( \mathcal{H}_B \).

\[\hat{F}_{f_i} = \int_{x_i \in \mathcal{V}[\Sigma_i]} |\text{pos}: x_i\rangle \langle \text{pos}: x_i | \hat{F}_{f_i} |\text{pos}: x_i \rangle \langle \text{pos}: x_i |. \]

\[\text{(3.1)}\]
and we use the accent to denote observables on this space.

We interpret the boundary quantum space in the following way: we assign a vector \(|f_i\) from \(\mathcal{H}_B\) to any pair of \(f\)-dependent and \(i\)-dependent vectors \(|f\rangle\) and \(|i\rangle\) by

\[ |f_i\rangle = (f \otimes i) \]  (3.2)

Here, the description \(f\)-dependent vector suggests that the vector is identified using quantum observables on \(\Sigma_f\); but, of course, it can be any vector from \(\mathcal{H}\). Particularly, we define a vector in \(\mathcal{H}_B\) for any \(x = [x_T, x_i] \in \mathbf{V}[\partial \Omega] = \mathbf{V}[\Sigma_f] \times \mathbf{V}[\Sigma_i]:

\[ |\text{pos} : x\rangle = (f \text{pos} : x_T) \otimes (i \text{pos} : x_i) \]  (3.3)

This allows us to “lift” any \(f\)-dependent or \(i\)-dependent operator \(\hat{A}_f\) or \(\hat{A}_i\) on \(\mathcal{H}\) to an operator on the boundary quantum space \(\mathcal{H}_B\)

\[ \hat{A}_f = \hat{A}_f^f \otimes \hat{1}_i \quad \hat{A}_i = \hat{1}_f \otimes \hat{A}_i \]

(3.4)

Using these definitions, we find

\[ [\hat{A}_f, \hat{A}_i] = 0 \]  (3.5)

We apply this method to construct the observables \(\hat{F}_{f_i}, \hat{G}_{a_i}\) and \(\hat{F}_{f_i}, \hat{G}_{i_a}\) for any functions and vector fields \(f_1, a_1\) or \(f_i, a_i\) on the value spaces \(\mathbf{V}[\Sigma_i]\) or \(\mathbf{V}[\Sigma_i]\). Next we want to construct a generalization of these observables \(\hat{F}_f\) and \(\hat{G}_a\) for any function \(f\) and vector field \(a\) on the value space \(\mathbf{V}[\partial \Omega] = \mathbf{V}[\Sigma_i] \times \mathbf{V}[\Sigma_i]\). Thanks to (2.4) for both \(\hat{F}_{f_i}\) and \(\hat{F}_{f_i}\) and to equation (3.5), we do not have ordering problems with \(\hat{F}_f\) for \(f(x) = f(x_T, x_i)\)

\[ \hat{F}_f = \int \frac{|\text{pos} : x_T\rangle \langle f \text{pos} : x_T| \otimes |i \text{pos} : x_i\rangle \langle i \text{pos} : x_i| f(x_T, x_i) =}{x_T \in \mathbf{V}[\Sigma_f] \quad x_i \in \mathbf{V}[\Sigma_i]} \]

(3.6)

\[ = \int |\text{pos} : x\rangle \langle f(x)| f(x) \]  \(x \in \mathbf{V}[\partial \Omega]\)

Similarly, for any vector field \(a(x) = a_f(x_T) \oplus a_i(x_i)\) on \(\mathbf{V}[\partial \Omega]\) where \(a_f \in \mathbf{T}[\mathbf{V}[\Sigma_f]]\) and \(a_i \in \mathbf{T}[\mathbf{V}[\Sigma_i]]\), motivated by (1.24), we can write

\[ \hat{G}_a = -\hat{G}_{a_1} + \hat{G}_{i_a} \]  (3.7)

It is straightforward to check that \(\hat{F}_f, \hat{G}_a\) are quantizations of the observables \(F_f, G_a\) on the boundary phase space \(\mathcal{B}[\partial \Omega]\); i.e. they satisfy (1.24) with the ordering parameter \(\gamma = \gamma_f = \gamma_i\). Note that a different orientation of the boundary \(\partial \Omega\) and the final hypersurface \(\Sigma_f\), which translates to the different sign of the symplectic structures (1.24) and to the definition of the momenta (1.24), is compensated by the covector representation of \(f\)-dependent vectors.

Let us summarize: quantization of the basic observables on the final and initial hypersurfaces \(\Sigma_f\) and \(\Sigma_i\) induces quantization of the basic observables \(F_f, G_a\) on
the entire boundary $\partial \Omega$. Hence, we are able to formulate the “kinematics” of the theory using quantization of the boundary phase space $\mathcal{B}[\partial \Omega]$ — which we call *boundary quantum mechanics*. The boundary quantum space $\mathcal{H}_B$ represents all possible quantum states at the beginning and at the end chosen independently of the real evolution of the system. Essentially, we are treating the initial and final experiments as experiments on independent systems. States in $\mathcal{H}_B$ represent outputs of measurements understood in this way.

Before we turn to the dynamics let us list some properties of the space $\mathcal{H}_B = \mathcal{H}^\dagger \otimes \mathcal{H}$. For vectors and operators in the “product” form $|f\rangle = \langle f| \otimes |i\rangle$, $\hat{A}_B f = \hat{A}_B^\dagger f \otimes \hat{A}_i$, $\hat{A}_B \hat{B}_i |f\rangle = \hat{A}_B^\dagger \hat{B}_i f \otimes \hat{A}_i$, we can write

$$(fistor|f_{\text{in}}) = \langle f_{\text{out}}|f\rangle \otimes \langle i_{\text{out}}|i\rangle \stackrel{\text{Tr}}{=} \text{Tr}_{\mathcal{H}_B}(\langle f_{\text{out}}|f\rangle \otimes \langle i_{\text{out}}|i\rangle) ,$$

$$\hat{A}_B f = \hat{A}_B^\dagger f \otimes \hat{A}_i ,$$

(3.8)

### Dynamics in the boundary quantum space

Of course, much more interesting is the dynamical part of a theory. We have to ask the question whether we are able to translate the dynamically interesting quantities to the language of boundary quantum mechanics. As we outlined, the dynamical information is hidden in the in-out transition amplitudes $\langle f|i\rangle$. Such an amplitude can be written as

$$\langle f|i\rangle = \text{Tr}_{\mathcal{H}}(\hat{I}^\dagger \langle i| \langle f|) = (\text{phys}|fi) ,$$

where $|fi\rangle$ is as in (3.8) and the physical state $|\text{phys}\rangle$ is given by

$$|\text{phys}\rangle = \sum_k \langle k| \otimes |k\rangle = \hat{I}$$

(3.10)

for a complete orthonormal base $|k\rangle$ in $\mathcal{H}$.

This means that there exists a preferred physical state $|\text{phys}\rangle$ in the boundary quantum space $\mathcal{H}_B$ that determines the dynamics of the theory. Specifically, if we set up some initial and final experiments that determine the quantum state $|\text{state}\rangle \in \mathcal{H}_B$, the physical transition amplitude corresponding to this state is given by

$$A(\text{state}) = (\text{phys}|\text{state}) .$$

(3.12)

For example, for the position base $|\text{pos}:x\rangle$ we get

$$A_{\text{pos}}(x) = A_{\text{pos}}(x_1|x_2) = (\text{phys}|\text{pos}:x) = \langle f\text{pos}:x_i|\text{pos}:x_i\rangle .$$

(3.13)

We will call $A_{\text{pos}}(x)$ the *position transition amplitude*.

The physical state $|\text{phys}\rangle$ is actually an entangled quantum state that carries all information about the dynamical correlations between the initial and final moment of time without reference to particular initial or final conditions.
Boundary quantum mechanics

In the previous subsections we constructed the boundary quantum space and observables on it using quantization based on the initial and final phase spaces. But it is clear that we can skip the splitting of the boundary into two pieces and quantize directly the basic observables \( F_f, G_a \) on the boundary phase space \( B[\partial \Omega] \). It is a phase space with a cotangent bundle structure, so we can apply the general formalism and obtain the quantum observables \( \hat{F}_f \) and \( \hat{G}_a \). We can also construct the position base \( |\text{pos} : x\rangle \). And we do not need any causal information for this; we do not need any global time flow on the underlying inner manifold or a causal decomposition of the boundary.

It means that we can build boundary quantum mechanics even in situations where we do not have any natural splitting of the boundary into two pieces, for example in Euclidian theories. Therefore, we could call boundary quantum mechanics also time-symmetric quantum mechanics.

However, in this setting we have to find the physical state \( |\text{phys}\rangle \) without reference to the initial and final causal decomposition.\(^6\) Again, we cannot expect an answer on a general level — this is a question equivalent to solving the quantum evolution. But we suggest methods determining the physical state — we formulate a dynamical equation for boundary quantum mechanics.

The classical evolution in the boundary phase space \( B[\partial \Omega] \) is determined by a specification of the physical phase space \( S \) as a subspace of \( B[\partial \Omega] \). It can be done, for example, via condition (1.18), or, expressed using observables \( F_f, G_a \), by the condition

\[
G_a + F_a \cdot d\hat{S} = 0 \quad \text{for all} \quad a \in TV[\partial \Omega].
\]

Hence, on the classical level we specified physical states by imposing constraints in the phase space. In the usual quantum mechanics one quantizes the constrained subspace \( S \). In boundary quantum mechanics we quantize the entire boundary phase space, but we have to impose conditions on the physical state inspired by the classical constraints

\[
(G_a + F_a \cdot d\hat{S})|\text{phys}\rangle = 0
\]

for, at least, some vector fields \( a \) on the value space \( V[\partial \Omega] \).

We cannot expect the condition above to be satisfied for all vector fields \( a \) due to the noncommutativity of the position and momentum observables (\( G_a \) is some ordering of the “\( a(x) \cdot \hat{p} \)” observable). We will see that such a strong requirement would be inconsistent. It will turn out that the choice of the class of vector fields for which the condition (3.15) is required to hold (i.e. the choice of a preferred operator ordering) is equivalent to the solution of the dynamical problem. So, if we have some preferred vector fields, it can provide us with a method for finding the transition amplitudes we are looking for.

\(^6\)More precisely, in the Heisenberg picture, which we are using, the physical state \( |\text{phys}\rangle \) is a fixed dynamically independent state and the dynamics is hidden in the relations of the basic observables \( F_f, G_a \) to this state. But we will be a bit vague and speak about a determination of the physical state \( |\text{phys}\rangle \) because it is more intuitive and does not influence any computation.
Let us look at the position representation of the constraint conditions. Using (2.14) and (2.43) we find
\[
(\text{phys}|(G_a + F_a \cdot d\mathcal{S})|\text{pos}:.) = (i\mathcal{L}_a + a \cdot d\mathcal{S})(\text{phys}|\text{pos}:.) = 0 . \tag{3.16}
\]
If we represent the position transition amplitude as
\[
A_{\text{pos}}(x) = a(x) \exp(i\mathcal{S}(x)) \tag{3.17}
\]
with \(a(x)\) a density of the weight \(\frac{1}{2} - i\gamma\), the condition above translates to
\[
\mathcal{L}_a a = 0 . \tag{3.18}
\]
This confirms that the constraint conditions cannot be satisfied for all vector fields \(a\) — it would require \(a = 0\).

If a linearly complete set of vector fields for which the constraint conditions should be satisfied is specified, the density \(a\) is determined completely up to a constant multiplicative factor (this remaining freedom of choice is, of course, equivalent to the choice of a global normalization and phase factor). In case of a linear non-interacting theory,\(^7\) such a set of vectors exists — if we require the condition \(3.15\) be satisfied for globally parallel vector fields\(^9\) we obtain that \(a\) is a constant and we recover the known fact that the quantum amplitudes for a non-interacting theory are given by the classical action through \(3.17\).

In a general case, the density \(a\) contains all quantum corrections to the transition amplitude \(A_{\text{pos}}\). It indicates that a choice of the “right” vector fields in the case of a general interacting theory can be difficult or even impossible. Therefore, we turn to another way of specifying the physical state \(|\text{phys}\rangle\) or physical amplitudes \(A(\text{state})\).

Path integral

There exists another approach to the quantization. This is the path integral quantization, which gives essentially a prescription for the position transition amplitude on the basis of a completely different calculation — through a sum of elementary amplitudes over all possible histories with fixed boundary values,
\[
\langle f \text{ pos } : x_f | i \text{ pos } : x_i \rangle = A_{\text{pos}}(x_f|x_i) = \int_{h \in \mathcal{H}} \mathcal{M}^F(h) \exp(iS(h)) . \tag{3.19}
\]
However, this amplitude is exactly the wave function of the physical state \(|\text{phys}\rangle\), i.e., the dynamics of boundary quantum mechanics can be specified by the path integral
\[
(\text{phys}) = \int_{h \in \mathcal{H}} \mathcal{M}^F(h) \exp(iS(h)) \langle pos : x(h) | . \tag{3.20}
\]
\(^7\)Motivated by the field theory, by non-interacting theory we mean a Hamiltonian quadratic in momenta and positions.
\(^9\)The notion of global parallelism is defined thanks to the linearity.
Let us add some comments about the advantages and problems of this approach. The integral over the space of histories faces serious problems due to the infinite dimension of the space of histories and the oscillatory character of the integrand. A technical solution usually leads to the computation of some Euclidian equivalent of the integral, which is usually better defined, followed by some “Wick rotation” — a transformation from the Euclidian to the physical theory. We can view this “Euclidian business” as a mere technical detour without a physical interpretation. Only after computing the integral we are able to identify the results with the transition amplitudes of quantum mechanics. In the usual framework, we do not even know what would be the quantum mechanics of the Euclidian formulation of the theory — the usual quantum mechanics essentially uses the causal structure to define the initial and final states.

However, the formalism developed above gives us a hope for another option. We can formulate boundary quantum mechanics even for a Euclidian version of the theory — it does not need the causal structure, it can be formulated without splitting of the boundary phase space to the initial and final part. Therefore we could make the connection with the path integral already in the Euclidian formulation

\[ (\text{phys}|\text{pos}: x) = A_{\text{pos}}(x) = \int_{\mathcal{H}}^{h \in \mathcal{H}} x(h) = x \mathcal{M}^F(h) \exp(-I(h)), \quad (3.21) \]

\( I(h) \) being the Euclidian action.\(^b\) For the physical version of the theory, this reduces to the relations (3.20) above. In the Euclidian case, this relation would give an interpretation for the path integral amplitude in terms of transition amplitudes of boundary quantum mechanics.

Unfortunately, the situation is not so straightforward. Even in case of a linear non-interacting theory, the form of boundary quantum mechanics formulated above applied to the Euclidian version of the theory does not correspond exactly to the Euclidian path integral. The problem is hidden in the method of quantization we used. The translation of the Poisson brackets of the classical theory to the commutators of the quantum theory

\[ \{, \} \rightarrow i[ , ] \quad (3.22) \]

intrinsically contains reference to the physical signature. The imaginary unit in this translation can be traced to be the cause of the imaginary unit in the exponent of the transition amplitude (3.17) computed in boundary quantum mechanics independently of the physical or Euclidian version of the theory. For the Euclidian theory it would be more appropriate to construct “Euclidian quantum mechanics” based on the commutation relation generated by the rule

\[ \{, \} \rightarrow [ , ] \quad (3.23) \]

with observables represented, probably, on a real Hilbert space. We do not attempt to build such quantum mechanics here. However, escaping the necessity of a causal structure in the usual quantum mechanics through the method of quantization of the boundary phase space is the first step towards Euclidian quantum mechanics.

\(^b\) \( I(h) \) is real for “Euclidian” histories. For physical histories we have \( iS(h) = -I(h) \).
A Symplectic geometry

This appendix is a review of the standard geometrical formulation of the symplectic geometry (see, e.g., [5, 6]).

The phase space is a manifold $\mathcal{G}$ of an even dimension $2n$ with a symplectic form $\omega$ that satisfies

$$\omega^T = -\omega, \quad \omega \in T^*_2 \mathcal{G},$$

$$\omega$$ is non-degenerate,

$$\omega$$ is closed (i.e. $d\omega = 0$) .  

(A.1)

We can invert it $^1$

$$\omega^{-1} \circ \omega = -\delta_{\mathcal{G}}$$ \hspace{1cm} (A.2)

and define a canonical vector field associated with a function $H$ on $\mathcal{G}$

$$X_H = (dH) \circ \omega^{-1} .$$ \hspace{1cm} (A.3)

This canonical vector field generates a canonical transformation on $\mathcal{G}$ that does not change the symplectic structure:

$$\mathcal{L}_{X_H} \omega = 0 .$$ \hspace{1cm} (A.4)

We can define the Poisson brackets of functions on $\mathcal{G}$ as

$$\{A, B\} = X_A \circ dB = X_A \circ \omega \circ X_B = (dA) \circ \omega^{-1} \circ (dB) .$$ \hspace{1cm} (A.5)

We have

$$\frac{dB}{dt} \overset{\text{def}}{=} \mathcal{L}_{X_H} B = \{H, B\} ,$$ \hspace{1cm} (A.6)

$$[X_A, X_B] = X_{(A, B)} ,$$ \hspace{1cm} (A.7)

where $[,]$ are the Lie brackets on vector fields. The symplectic structure also induces a volume element on $\mathcal{G}$

$$d\Gamma = (2\pi)^{-n} \frac{1}{n!} |\omega \wedge \omega \wedge \cdots \wedge \omega| = \left(\text{Det} \frac{\omega}{2\pi}\right)^{\frac{n}{2}} .$$ \hspace{1cm} (A.8)

Finally, if we choose coordinates $(x^a, p_a)$ for $a = 1, \ldots, n$ such that

$$\omega = dp_a \wedge dx^a ,$$ \hspace{1cm} (A.9)

we get

$$\{x^a, p_b\} = -\delta^a_b$$ \hspace{1cm} (A.10)

and $(x^a, p_a)$ are canonical coordinates.

$^1$The dot $\circ$ indicates the contraction in $T \mathcal{G}$.
B Tangent and cotangent bundle geometry

In this appendix we discuss the geometry of tangent bundles of a manifold \( V \). We define “partial derivatives” of observables on these spaces in a covariant way. We also show that the cotangent bundle has the structure of a symplectic manifold. We use \( a, b, \ldots \) as indices for tensors on the manifold \( V \) and indices \( A, B, \ldots \) for tensors from tangent spaces of the cotangent bundle \( G = T^* V \).

Functions such as the Lagrangian \( L(x, v) \) and the Hamiltonian \( H(x, p) \) are functions on the tangent and cotangent bundle, respectively, of a configuration space \( V \).

Because velocities \( v \) (or momenta \( p \)) are vectors (covectors) from different fibers for different position \( x \) (\( T_x V \neq T_y V \) for \( x \neq y \)), we have to be careful to use a partial derivative with respect of the position \( x \). There is no problem with the definition \( \frac{\partial L}{\partial v^a}(x, v) \):

\[
\delta v^n \frac{\partial L}{\partial v^n}(x, v) = \frac{d}{d\varepsilon} L(x, v + \varepsilon \delta v)|_{\varepsilon = 0} \quad (B.1)
\]

— a partial derivative with \( x \) constant — but to define the derivative with \( v \) constant we need a connection \( \nabla \) on \( V \):

\[
\frac{\nabla}{\partial x}(x, v) : \quad \delta x^n \frac{\nabla}{\partial x}(x, v) = \frac{d}{d\varepsilon} L(x, v + \varepsilon \delta v)|_{\varepsilon = 0} , \quad (B.2)
\]

where \( x_\varepsilon \) is a curve starting from \( x \) in a direction \( \delta x \) and \( v_\varepsilon \) is the parallel transport of \( v \) along \( x_\varepsilon \) in the sense of the connection \( \nabla \) (i.e. \( \nabla_x v_\varepsilon = 0 \)). Similarly, for a function on the cotangent bundle,

\[
\frac{\partial H}{\partial p^a}(x, p) : \quad \delta p^b \frac{\partial H}{\partial p^b}(x, p) = \frac{d}{d\varepsilon} H(x, p + \varepsilon \delta p)|_{\varepsilon = 0} , \quad (B.3)
\]

where again \( \nabla_x p_\varepsilon = 0 \).

We want to show that the cotangent bundle \( G = T^* V \) has the structure of a phase space. It will be useful to define a covariant generalization of “coordinate” vector fields and forms

\[
\frac{\partial^A}{\partial p^a} \quad \text{a vector field on } G \text{ for which } \frac{\partial^A}{\partial p^a} d_\lambda H = \frac{\partial H}{\partial p^a} , \quad (B.4)
\]

\[
\frac{\nabla^A}{\partial x} \quad \text{a vector field on } G \text{ for which } \frac{\nabla^A}{\partial x} d_\lambda H = \frac{\nabla \lambda H}{\partial x} ,
\]

\( \frac{\partial}{\partial p} \) is actually the natural identification of the vector space \( T_p^* V \) with its tangent space \( T_p V \) and \( \nabla_x \) is the horizontal shift of the connection \( \nabla \). Form fields dual to these vector fields

\[
D^a_A x , \quad \text{differential of the bundle projection } x : T V \rightarrow V , \quad p|_x \rightarrow x , \quad (B.5)
\]

\[
\nabla_A p_a ,
\]

are defined by

\[
\frac{\nabla^A}{\partial x} D^b_A x = \delta^b_a , \quad \frac{\partial^A}{\partial p^b} \nabla_A p_a = \delta^b_a , \quad \frac{\nabla^A}{\partial x} \nabla_A p_a = 0 , \quad \frac{\partial^A}{\partial p^a} D^b_A x = 0 , \quad (B.6)
\]

\[
\frac{\nabla^A}{\partial x} D^A_n x + \frac{\partial^A}{\partial p^a} \nabla_A p_a = \delta^A_n .
\]
Now we can write down the canonical cotangent bundle symplectic form

$$\omega_{ab} = \nabla_a p_b \wedge D_b^a x = \nabla_a p_b \, D_b^a x - D_a^b x \nabla_a p_b ,$$  \hspace{1cm} (B.7)

and we can even explicitly write the symplectic potential

$$\omega_{ab} = \delta_a \theta_b , \quad \theta_a = p_n D_n^a x .$$  \hspace{1cm} (B.9)

The canonical vector fields and Poisson brackets are

$$X^a_F = \frac{\partial F}{\partial p_n} \partial_a - \frac{\partial F}{\partial x_n} \partial_p ,$$  \hspace{1cm} (B.10)

$$\{A,B\} = \frac{\partial A}{\partial p_n} \frac{\partial B}{\partial x_n} - \frac{\partial A}{\partial x_n} \frac{\partial B}{\partial p_n} .$$  \hspace{1cm} (B.11)

If we change the connection to another one,

$$\tilde{\nabla} = \nabla \oplus \Gamma , \hspace{1cm} \tilde{\nabla}_a^b = \nabla_a^b + \Gamma^b_{ac} a^c , \hspace{1cm} \tilde{\nabla}_a p_b = \nabla_a p_b - \Gamma^a_{ab} p_n ,$$  \hspace{1cm} (B.12)

we get

$$\frac{\tilde{\nabla}_a^b}{\partial x} (x,p) = \frac{\nabla_a^b}{\partial x} (x,p) + p_r \Gamma^b_{ar} (x) \frac{\partial^b}{\partial p_r} (x,p) ,$$  \hspace{1cm} (B.13)

$$\tilde{\nabla}_a p_b (x,p) = \nabla_a p_b (x,p) - p_r \Gamma^a_{rb} (x) D_b^r x (x,p) .$$

By straightforward calculations, we can check that the quantities $\omega, \theta, X_F,$ and $\{ , \}$ do not depend on the choice of the connection.

Finally, coordinates $x^a$ on $V$ generate coordinates $(x^a, p_n)$ on $G$ by

$$p_n = p_n \frac{\partial}{\partial x^a}$$  \hspace{1cm} (B.14)

and they define the coordinate connection $\partial$ on $V$ for which

$$\partial dx^a = 0 , \quad \partial \frac{x^a}{\partial x^a} = 0 \quad \text{for} \ a = 1, 2, \ldots, n .$$  \hspace{1cm} (B.15)

Using this connection and expressing everything in coordinates, we get the standard relations \cite{5,6}

$$\omega_{ab} = d_a p_n \wedge d_b x^n , \quad \theta_a = p_n d_a x^n ,$$  \hspace{1cm} (B.16)

$$X^a_F = \frac{\partial F}{\partial p_n} \frac{\partial}{\partial x^n} - \frac{\partial F}{\partial x^n} \frac{\partial}{\partial p_n} ,$$  \hspace{1cm} (B.17)

$$\{A,B\} = \frac{\partial A}{\partial p_n} \frac{\partial B}{\partial x^n} - \frac{\partial A}{\partial x^n} \frac{\partial B}{\partial p_n} ,$$  \hspace{1cm} (B.18)

$$\{ x^a, p_b \} = -\delta^a_b .$$  \hspace{1cm} (B.19)
C Densities on a Manifold

In this appendix we shortly review the definition of densities on a manifold and some operations with them.

On any manifold \( M \) we can define a vector bundle of tangent densities of a weight \( \alpha \), that we denote \( \tilde{R}^\alpha M \) and \( \tilde{C}^\alpha M \) if the densities are real and complex, respectively. The space of sections we denote \( \tilde{F}^\alpha M \). The standard fiber of these bundles is the vector space of real or complex numbers. As for any tangent bundle, the density bundle can be defined by a coordinate map from the space of frames of the tangent vector space \( T M \) to the standard fiber \( \mathbb{R} \) (or \( \mathbb{C} \)). The coordinate map has to be a representation of the linear group acting on the space of frames. The coordinate map \( e_a \rightarrow \mu[e_a] \) tells us by what factor is a density \( \mu \) different from the coordinate density \( \epsilon \) given by the base \( e_a \)

\[
\mu[e_a] = \mu \epsilon^1, \quad \epsilon[e_a] = 1. \tag{C.1}
\]

For densities of weight \( \alpha \), the coordinate map is a representation of the linear group of the following type:

\[
\mu[A^\alpha_b e_b] = |\det A|^\alpha \mu[e_a]. \tag{C.2}
\]

Clearly, we can define complex densities even for a complex weight.

Besides the linear operation, we can also define the multiplication and constant powers of densities. These operations map densities of some weight to densities of a different weight. Let us note that a complex conjugation maps the densities of weight \( \alpha \) to densities of weight \( \alpha^* \) and therefore “the absolute value” \( |\mu| = (\mu \mu^*)^{\frac{1}{2}} \) belongs to densities of weight \( \text{Re} \alpha \).

Densities of weight 1 are called volume elements because they can be integrated. Let \( \mu \) be a volume element, then we define locally

\[
\int_\Omega \mu = \int_{x^a(\Omega)} \mu \left[ \frac{\partial}{\partial x^a} \right] d^n x, \tag{C.3}
\]

where \( x^a \) are arbitrary coordinates. On the right hand side the usual coordinate integration is understood. Extension to domains not covered by one coordinate system is done by standard methods \[8\]. The consistency of this definition (independence of a choice of coordinates) follows from the transformation properties \[8\] with \( \alpha = 1 \).

A metric \( g \) or a symplectic form \( \omega \) (see Appendix A) define canonical volume elements:

\[
g^\frac{1}{2} = |\text{Det } g|^{\frac{1}{2}}, \quad d\Gamma = \left| \text{Det } \frac{\omega}{2\pi} \right|^{\frac{1}{2}}, \tag{C.4}
\]

where the operation \( \text{Det } : T^0_2 M \rightarrow \tilde{R}^1 M \) is defined by

\[
(\text{Det } g)[e_a] = \text{det } g_{ab}. \tag{C.5}
\]

We can also define a map from the space of totally antisymmetric forms to the space of volume elements \( \sigma \rightarrow |\sigma| \), such that

\[
|\sigma|[e_a] = |\sigma_{1...n}|, \tag{C.6}
\]

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\( n \) being the dimension of the manifold \( M \). It is easy to check that

Finally, let us note that the delta distribution \( \delta(x|y) \) can be understood as a bi-distribution with a density character in both arguments and of weights \( \alpha, \beta \) such that \( \alpha + \beta = 1 \), i.e., it is a functional on test densities \( \mu, \nu \) of weights \( 1 - \alpha \) and \( 1 - \beta \):

\[
\int \mu(x) \nu(y) \delta(x|y) = \int \mu \nu . \tag{C.7}
\]

If we want to define the “ordinary” delta function that is not a density in any of its arguments, we have to normalize it to some volume element\(^1\) \( \mu \). We call such a distribution \((\mu^{-1}\delta)\). It acts on test densities \( \varphi, \psi \) of weight 1:

\[
\int \varphi(x) \psi(y) (\mu^{-1}\delta)(x|y) = \int \varphi \psi \mu^{-1} . \tag{C.8}
\]

Similarly, for any smooth density \( f \) we can define a bi-distribution \((f\delta)\).

\(^1\)For distributions on \( \mathbb{R}^n \), one usually chooses the canonical volume element \( d^n x \).
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