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Relationships between Scalar Field and Relativistic Particle Quantizations

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Abstract

The main goal of this work is an investigation of relationships between the quantum theory of a scalar field and the quantum mechanics of a relativistic particle in a general spacetime.

Quantum field theory of a scalar field on a time-bounded domain is formulated using canonical quantization. Special attention is paid to boundary conditions and their implication for the interpretation of the theory. The relationship between configuration, particle and holomorphic representations is found. It is shown that all important structures can be reconstructed from knowledge of Green functions satisfying certain conditions. Transition amplitudes are expressed using such Green functions, and their structure is discussed.

The field theory is also reformulated using boundary quantum mechanics in which initial and final conditions play equivalent roles. This formulation is more suitable for the path integral approach and for the Euclidian version of the theory in which there is no preferred time flow. Also a derivation of transition amplitudes is much more straightforward in this formalism.

Next the quantum mechanics of a relativistic particle is formulated using the sum-over-histories approach. The theory is again investigated in a time-bounded domain, and boundary conditions are discussed. It is shown that the quantum mechanics of a relativistic particle leads to a many-particle theory and that transition amplitudes have the same structure as in the QFT of a scalar field. This connection allows one to identify these two theories. The relationship between boundary conditions needed for QM of a relativistic particle and the particle interpretation of QFT of a scalar field is investigated.

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Introduction

Motivations

One of the main goals of this work is to investigate a relationship between scalar field theory in curved spacetime and quantization of a relativistic particle using the sum-over-histories approach. We have the following motivations to do such a study.

Quantum scalar field theory is widely understood as the theory describing a multi-particle system. Yet, it is a quantization of a completely different system — a quantization of a continuous field on spacetime. It is true that we can identify some states of such system as *particle states* — states with some properties of particles. But is there any other way to make a connection to the particle theory? Is it possible to quantize a classical relativistic particle, and does it gives predictions equivalent to predictions of quantum scalar field theory?

There exists a candidate for the direct quantization of a particle theory — quantization using the sum-over-histories approach. In this approach the transition amplitudes associated with the chosen criteria are computed by summing over amplitudes of all possible multi-particle histories which meet the criteria. It is known that some of these amplitudes (e.g. the propagator) lead in special cases (e.g., in flat spacetime) to quantities which can also be obtained from scalar field theory. The goal of this work is to investigate this correspondence in more detail. We will find in what exact sense we can identify these two theories.

Let us note that there are more reasons for studying relativistic particle theory. One of the attempts to understand the quantization of the gravitational field coupled to matter is to reduce the full gravitation theory to a system with a finite number of degrees of freedom and try to quantize this simplified system. These reduced theories are called minisuperspace models. It is well known that this reduced system is essentially equivalent to a particle theory in a Lorentzian space with (usually) a complicated potential. A common method for the quantization of minisuperspace models is the sum-over-histories approach. A connection of such a method to the better known and thoroughly understood theory — canonical quantized scalar field — could bring a better understanding for of quantization of minisuperspace models.

Another reason for the investigation of scalar field theory in curved spacetime is an interest in the knowledge of the exact dependence of the theory on the spacetime domain in which we study the system. The usual approach is a bit generous on this question — the theory is usually formulated on the whole spacetime with not always clearly formulated special behavior at infinities. In flat spacetime such an approach is justifiable because there exists a preferred behavior at infinities, but in a general curved spacetime we have to be more careful. This problem is usually solved by a choice of positive-negative frequency splitting for particle modes. The aim of this work is to formulate this choice in a covariant way and identify exactly the freedom which we have in the choice of boundary conditions and what is their interpretation.

A similar comment applies to the sum-over-histories approach. The question of boundary conditions is usually completely ignored in the definition of the path integral. We try to formulate the theory in a more careful way and identify its boundary-condition dependence.

Another reason for the necessity of a better understanding of boundary conditions of a theory based on the summation of amplitudes is a better understanding of the definition of the decoherence functional of generalized quantum mechanics. At this moment we lack an exact understanding of the dependence of the decoherence functional on the spacetime domain on which we study the system, its composition properties when we join two domains, etc.. One of the main difficulties are boundary terms in the decoherence functional representing initial and final states, which are not well understood. We hope that the investigation of the sum-over-histories approach to the quantization of relativistic particle, as a representative example of a wide class of theories, could clarify this problem.

Finally, one of the "by-products" of our study will be a reformulation of the theory in a way which does not distinguish between the past and the future. This has great importance for theories where we can have a problem with the identification of time — for example in quantum gravity or a Euclidian version of the theory.

Plan of the work

The plan of our work is the following. In the first three parts we will investigate mostly scalar field theory, and in the last part we will study the sum-over-histories approach to the quantization of a relativistic particle. Besides these main tasks, in the introductory chapters to each part we will present a general framework for the material to be discussed.

The first part reviews the classical formalism on a general level and its application to scalar field theory. Special attention is paid to boundary conditions of the equation of motion.

In the second part we will discuss canonical quantization. The general quantization of the phase space with a cotangent bundle structure will be discussed. Scalar field theory will be quantized using the notion of a particle interpretation. There will be developed a rich covariant formalism for the description of quantum scalar field with emphasis on the dependence on boundary conditions. The main goal will be to compute transition amplitudes between particle states.

In the third part boundary quantum mechanics will be introduced. It is quantum mechanics based on quantization of the boundary phase space. It describes measurements at the initial and final time as experiments on independent systems. The relations of initial and final physical quantities are hidden in a special physical state. The equation for such a state is the dynamical equation of boundary quantum mechanics.

The last part deals with the quantization of a relativistic particle using the sum-over-histories approach. First, the general ideas of such an approach will be discussed. Next, the propagator in a space with boundary will be computed and multi-particle amplitudes will be derived. The discussion of a possible interaction of particles with devices on the boundary of the domain will be carried out.

Finally, we compare both theories.

Part I

Classical Theory

1 Boundary, canonical and covariant phase spaces

The space of histories and the action

In this chapter we will develop a classical formalism for a wide class of physical theories. We will not need this formalism in the following chapters in full generality, but it helps us to see some structures we will use for scalar field theory and for a relativistic particle in a more general context. We will also refer to this chapter in the overview of quantization procedures in chapter 5 and in the introduction to boundary quantum mechanics in chapter 10. The formalism developed here is mainly inspired by [1].

A physical theory can be specified by a space of elementary histories $\boldsymbol{\mathcal{H}}$ 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 all possible trajectories in the spacetime (the theory of a relativistic particle) or all possible field configuration on the spacetime (a matter field theory) or all possible connections on a spacetime (a gauge theory), etc..

We restrict ourself to theories which are local on some *inner manifold* M and we pay an attention to this dependence. Histories of the local theories can be represented as sections of some fibre bundle over the inner manifold. We use $\boldsymbol{x}, \boldsymbol{y}, \ldots$ as tensor indices for objects from tangent spaces $\mathbf{T}\,\boldsymbol{\mathcal{H}}$ and the dot $\bullet$ for contraction in these spaces. It contains, of course, the integration over the inner manifold.

Almost all known theories can be reformulated in this way. For example elementary histories of a particle theory can be viewed as mapping from one dimensional inner manifold M (here the space of a parameter that increases along the particle trajectory) to a target manifold T, i.e. as sections of the trivial fibre bundle $M \times T$ (e.g., spacetime) over M. The realization of field theory is even more straightforward — the inner manifold M is spacetime, and histories are sections of some bundle over it.

We assume that we are able to restrict the theory to any domain in the inner manifold M. I.e., we are able to speak about space of histories $\boldsymbol{\mathcal{H}}[\Omega]$ on a domain Ω. We will see that the domain of dependence will play an important role in the dynamics.

On the general level we admit any sufficiently bounded domain Ω 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. But we allow also domains which do not have to be 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. This section is unbounded in space, and this fact will have to be compensated by a restriction of the set of histories to those which fall off sufficiently fast at spatial infinity. We cannot do the same thing in the time direction because we would exclude physically interesting histories — specifically the solutions of the classical equations of motion.

The localization of histories on the domain Ω gives us also a localization of elements of the tangent spaces $\mathbf{T}\,\boldsymbol{\mathcal{H}}$, i.e., we can speak about a space $\mathbf{T}\,\boldsymbol{\mathcal{H}}[\Omega]$. We will call tangent vectors *linearized histories*. Tangent spaces at some history h can be represented as vector bundles over the inner manifold or the domain Ω. Therefore we can speak about distributions $(\mathbf{T}_{\mathrm{h}}\,\boldsymbol{\mathcal{H}})'$ and $(\mathbf{T}_{\mathrm{h}}\,\boldsymbol{\mathcal{H}}[\Omega])'$. Let us note that by distributions $(\mathbf{T}_{\mathrm{h}}\,\boldsymbol{\mathcal{H}}[\Omega])'$ we mean distributions in the sense of $(\mathbf{T}_{\mathrm{h}}\,\boldsymbol{\mathcal{H}})'$ with a support on

Ω. See more in appendix A.

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

$$S[\Omega] \;:\; \boldsymbol{\mathcal{H}} \to \mathbb{R} \quad . \tag{1.1}$$

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

The action is local and additive under smooth joining of domains, i.e.

$$\begin{gathered} S[\Omega](\mathrm{h}_1) = S[\Omega](\mathrm{h}_2) \qquad \text{for} \qquad \mathrm{h}_1 = \mathrm{h}_2 \;\text{ on }\; \Omega \qquad \text{and for all }\; \Omega \quad , \\ S[\Omega](\mathrm{h}) = S[(\Omega_1](\mathrm{h}) + S[\Omega_2](\mathrm{h}) \quad , \end{gathered} \tag{1.2}$$

where $\Omega = \Omega_1 \cup \Omega_2$ is a domain and $\Omega_1 \cap \Omega_2$ is a submanifold without boundary which is 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 question.

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

$$\mathrm{d}S[\Omega](\mathrm{h}) = \chi[\Omega]\delta S(\mathrm{h}) - \mathfrak{P}[\partial\Omega](\mathrm{h}) \quad , \tag{1.3}$$

This relation represents a usual "integration by parts" in the variation of the action.

δS represents the variation of the action on the whole inner manifold. It is a form on the space of histories and we require that $\delta S(\mathrm{h})$ contain at most second-order inner space derivatives of the history h and be smooth in the variational argument. Thanks to this smoothness the multiplication by $\chi[\Omega]$ is well defined. $\chi[\Omega]$ is the characteristic function of the domain Ω (eq. (A.12)). The distribution $\chi[\Omega]\delta S(\mathrm{h})$ is not smooth in the variational argument on the whole inner manifold (more precisely as a distribution $(\mathbf{T}_{\mathrm{h}}\,\boldsymbol{\mathcal{H}})'$), but it is a smooth distribution from the space $(\mathbf{T}_{\mathrm{h}}\,\boldsymbol{\mathcal{H}}[\Omega])'$.

$\mathfrak{P}[\partial\Omega]$ is the momentum on the boundary $\partial\Omega$. It is localized on the boundary in both its history dependence and in the variational argument (i.e. as a distribution from $\mathbf{T}_{\mathrm{h}}{}^0_1\,\boldsymbol{\mathcal{H}}'$). 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. I.e., it can be represented as a distribution on boundary values of the linearized histories.

The *classical equations of motion* are given by the condition

$$\delta S(\mathrm{h}) = 0 \quad , \tag{1.4}$$

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

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

$$\overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S}(\mathrm{h}) \bullet \delta\mathrm{h} = 0 \quad , \tag{1.5}$$

where $\delta\mathrm{h}$ is a linearized history (tangent vector to $\boldsymbol{\mathcal{H}}$) at a classical history h and the second variation of the action $\overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S}$,

$$\overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S}(\mathrm{h})^{\top} = \overset{\leftsquigarrow\leftsquigarrow}{\delta^2 S}(\mathrm{h}) = \mathfrak{D}\delta S(\mathrm{h}) \tag{1.6}$$

is a derivative of the form δS using an ultralocal connection $\mathfrak{D}$. It is easy to check that, thanks to (1.4), for a classical history the second variation of the action $\overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S}(\mathrm{h})$ does not depend on a choice of the connection $\mathfrak{D}$. We denote

$$\overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S}[\Omega] = (\chi[\Omega]\delta) \bullet \overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S} \quad , \quad \overset{\leftsquigarrow\leftsquigarrow}{\delta^2 S}[\Omega] = \overset{\rightsquigarrow\rightsquigarrow}{\delta^2 S}[\Omega]^{\top} \quad . \tag{1.7}$$

We assume that the equation of motion has a well-defined boundary problem on the domain Ω — there is a unique solution in $\boldsymbol{\mathcal{S}}$ with a given restriction 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 of the linearized equation of motion for a given linearized value on the boundary or linearized momentum on the boundary. This requires some genericity 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 [1] for some details on this case.

If we work only with the manifold $\boldsymbol{\mathcal{S}}$, we use $_{A}, _{B}, \dots$ for tangent tensors and the dot $\circ$ for the contraction in these spaces.

Boundary phase space

Next we define the *boundary symplectic structure* $\mathrm{d}\mathfrak{P}[\partial\Omega]$ as the external derivative of the $\mathfrak{P}[\partial\Omega]$ form, which turns out to be the Wronskian of the second variation of the action,

$$\mathrm{d}\mathfrak{P}[\partial\Omega] = \overleftrightarrow{\delta^2} S[\Omega] - \overrightarrow{\delta^2} S[\Omega] \quad . \tag{1.8}$$

We say that two histories are canonically equivalent on the boundary if they have the same restriction on the boundary and the same momentum $\mathfrak{P}$. We call the quotient of the space $\boldsymbol{\mathcal{H}}$ with this equivalence the *boundary phase space* $\boldsymbol{\mathcal{B}}[\partial\Omega]$. We use $_{\mathrm{A}}, _{\mathrm{B}}, \dots$ as tensor indices for tensors from the tangent spaces $\mathbf{T}\,\boldsymbol{\mathcal{B}}[\partial\Omega]$ and the dot $\diamond$ for contraction in these spaces.

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

The space $\boldsymbol{\mathcal{S}}$ gives us a submanifold of the space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ which we denote by the same letter.

Lagrangian density

Until now we have developed the formalism on a very general level. For simplicity in the following we restrict to theories with the action given as an integral of the a Lagrangian density ultralocally dependent on "values" and "velocities" of the history.

The formalism developed above is more general — it covers for example the case of the Einstein-Hilbert action for gravity (except for problems with diffeomorphism symmetry) for which the Lagrangian density contains second spacetime derivatives of the metric. But this dependence is degenerate, and it is possible to satisfy the conditions above if a proper boundary term is chosen.

We now require that the action have the form

$$S[\Omega](\mathrm{h}) = \int_{\Omega} \mathfrak{L}(\mathrm{h}, \mathcal{D}\mathrm{h}) \quad , \tag{1.9}$$

where $\mathfrak{L}$ is the *Lagrangian density* — a density on the inner manifold M ultralocally dependent on a value of the history and inner space derivatives[1] (see Notes near the end of the theses) of the history.

The variation of the action and an integration by parts gives us the decomposition in (1.3)

$$\delta S(\mathrm{h}) = \frac{\mathfrak{D}\mathfrak{L}}{\partial \mathrm{h}}(\mathrm{h}, \mathcal{D}\mathrm{h}) - \big(\mathfrak{D}\frac{\partial \mathfrak{L}}{\partial \mathcal{D}\mathrm{h}}\big)(\mathrm{h}, \mathcal{D}\mathrm{h}) \quad , \tag{1.10}$$

$$\mathfrak{P}[\partial\Omega](\mathrm{h}) = \frac{\partial \mathfrak{L}}{\partial \mathcal{D}_{\alpha}\mathrm{h}}(\mathrm{h}, \mathcal{D}\mathrm{h})\, \delta_{\alpha}[\partial\Omega] \quad , \tag{1.11}$$

where $\delta_{\alpha}[\partial\Omega]$ is defined in equation (A.13).

Space of boundary values

We call the restriction of the history to the boundary the *boundary value* of the history, and we denote by $\boldsymbol{\mathcal{V}}[\partial\Omega]$ the *space of all boundary values*. (The boundary values do not include any normal derivatives of the histories.) It can be represented as a fibre bundle with the boundary as the base manifold. We use $\mathsf{x}, \mathsf{y}, \ldots$ as tensor indices for tensors from the tangent spaces $\mathbf{T}\,\boldsymbol{\mathcal{V}}[\partial\Omega]$ and the dot $\cdot$ for contraction in these spaces. It contains, of course, the integration over the boundary.

We denote by $\mathbf{x}[\partial\Omega]$ the projection from $\boldsymbol{\mathcal{H}}$ to $\boldsymbol{\mathcal{V}}[\partial\Omega]$. The conditions on the momentum allow us to represent it as

$$\mathfrak{P}_{\boldsymbol{x}}[\partial\Omega] = \mathbf{p}_{\mathsf{x}}[\partial\Omega]\,\mathrm{D}^{\mathsf{x}}_{\boldsymbol{x}}\mathbf{x}[\partial\Omega] \tag{1.12}$$

with $\mathbf{p}[\partial\Omega](\mathrm{h})$ from the cotangent bundle $\mathbf{T}^{\star}_{\mathbf{x}(\mathrm{h})}\boldsymbol{\mathcal{V}}[\partial\Omega]$. Here $\mathrm{D}\mathbf{x}[\partial\Omega]$ is the differential of the map $\mathbf{x}[\partial\Omega]$. In the following we drop the boundary dependence of $\mathbf{x}$ and $\mathbf{p}$.

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

$$\delta S(\bar{\mathrm{h}}(\mathrm{x})) = 0 \quad \wedge \quad \mathbf{x}(\bar{\mathrm{h}}(\mathrm{x})) = \mathrm{x} \tag{1.13}$$

and the classical action

$$\bar{S}[\Omega](\mathrm{x}) = S[\Omega](\bar{\mathrm{h}}(\mathrm{x})) \quad . \tag{1.14}$$

The space $\boldsymbol{\mathcal{S}}$ can be characterized using the condition

$$\mathbf{p} = -\mathrm{d}\bar{S}(\mathbf{x}) \quad , \tag{1.15}$$

which follows from

$$\begin{aligned} \mathrm{d}_{\mathsf{x}}\bar{S} &= \mathrm{D}^{\boldsymbol{x}}_{\mathsf{x}}\bar{\mathrm{h}}\;\mathrm{d}_{\boldsymbol{x}}(\bar{\mathrm{h}}) = \mathrm{D}^{\boldsymbol{x}}_{\mathsf{x}}\bar{\mathrm{h}}\;\big(\delta S_{\boldsymbol{x}}[\Omega](\bar{\mathrm{h}}) - \mathfrak{P}_{\boldsymbol{x}}[\partial\Omega](\bar{\mathrm{h}})\big) = \\ &= -\mathrm{D}^{\boldsymbol{x}}_{\mathsf{x}}\bar{\mathrm{h}}\;\mathrm{D}^{\mathsf{y}}_{\boldsymbol{x}}\mathbf{x}(\bar{\mathrm{h}})\;\mathbf{p}_{\mathsf{y}}(\bar{\mathrm{h}}) = -\mathbf{p}_{\mathsf{x}}(\bar{\mathrm{h}}) \quad . \end{aligned} \tag{1.16}$$

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

$$\nabla_{\mathsf{A}}\mathbf{p}_{\mathsf{x}} \wedge \mathrm{D}^{\mathsf{x}}_{\mathsf{B}}\mathbf{x} = \mathrm{d}_{\mathsf{A}}(\mathbf{p}_{\mathsf{x}}\mathrm{D}^{\mathsf{x}}_{\mathsf{B}}\mathbf{x}) = \mathrm{d}_{\mathsf{A}}\mathfrak{P}_{\mathsf{B}} \quad . \tag{1.17}$$

The linearization of eq. (1.15) gives

$$\mathrm{D}^{\mathsf{A}}_{\mathsf{x}}\bar{\mathrm{h}} = \frac{\nabla^{\mathsf{A}}_{\mathsf{x}}}{\partial\mathbf{x}} - \big(\nabla_{\mathsf{x}}\mathrm{d}_{\mathsf{y}}\bar{S}\big)\frac{\partial^{\mathsf{A}}}{\partial\mathbf{p}_{\mathsf{y}}} \quad . \tag{1.18}$$

Causal structure

Until now we have not needed any time flow in the underlying inner manifold M. It could be spacetime, but the formalism works in a more general situation. We can use it, for example, for the Euclidian form of the theory. In the following we will assume some additional causal structure which allows us to define concepts such as canonical and covariant phase spaces.

Let assume that the boundary of the domain can be split into two disjunct parts without boundary

$$\begin{gathered} \partial\Omega = \partial\Omega_{\mathrm{f}} \cup \partial\Omega_{\mathrm{i}} = -\Sigma_{\mathrm{f}} \cup \Sigma_{\mathrm{i}} \quad , \\ \partial\Omega_{\mathrm{f}} = -\Sigma_{\mathrm{f}} \quad , \quad \partial\Omega_{\mathrm{i}} = \Sigma_{\mathrm{i}} \quad . \end{gathered} \tag{1.19}$$

Here the minus sign suggests an opposite choice of the orientation of the normal direction for one part of the boundary. Clearly we have in mind two Cauchy hypersurfaces which define a sandwich domain in a globally hyperbolic spacetime. The decomposition in (1.19) allows us to write

$$\begin{aligned} \boldsymbol{\mathcal{V}}[\partial\Omega] &= \boldsymbol{\mathcal{V}}[\Sigma_{\mathrm{f}}] \times \boldsymbol{\mathcal{V}}[\Sigma_{\mathrm{i}}] \quad , \\ \boldsymbol{\mathcal{B}}[\partial\Omega] &= -\boldsymbol{\mathcal{B}}[\Sigma_{\mathrm{f}}] \oplus \boldsymbol{\mathcal{B}}[\Sigma_{\mathrm{i}}] \quad , \\ \mathbf{T}\,\boldsymbol{\mathcal{V}}[\partial\Omega] &= \mathbf{T}\,\boldsymbol{\mathcal{V}}[\Sigma_{\mathrm{f}}] \oplus \mathbf{T}\,\boldsymbol{\mathcal{V}}[\Sigma_{\mathrm{i}}] \quad , \end{aligned} \tag{1.20}$$

and we will use shorthands $\boldsymbol{\mathcal{V}}$, $\boldsymbol{\mathcal{V}}_{\mathrm{f}}$, $\boldsymbol{\mathcal{V}}_{\mathrm{i}}$ and $\boldsymbol{\mathcal{B}}$, $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$, $\boldsymbol{\mathcal{B}}_{\mathrm{i}}$.

We require that both parts contain a full set of boundary data — there should exist a unique classical history for given element from $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$ or $\boldsymbol{\mathcal{B}}_{\mathrm{i}}$.

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

$$\mathrm{d}\mathfrak{P}[\partial\Omega] = -\mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{f}}] + \mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{i}}] \quad . \tag{1.21}$$

$\mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{f}}]$ and $\mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{i}}]$ play the role of the symplectic structure on $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$ and $\boldsymbol{\mathcal{B}}_{\mathrm{i}}$. We will call these spaces *canonical phase spaces*. The minus sign in the relations (1.20) reflects the relation of these spaces as symplectic spaces.

The canonical phase spaces can be again represented as cotangent bundles $\mathbf{T}\,\boldsymbol{\mathcal{V}}_{\mathrm{f}}$ and $\mathbf{T}\,\boldsymbol{\mathcal{V}}_{\mathrm{i}}$ through the maps $\mathbf{x}_{\mathrm{f}}$, $\mathbf{p}_{\mathrm{f}}$ and $\mathbf{x}_{\mathrm{i}}$, $\mathbf{p}_{\mathrm{i}}$. Let us note that $\mathbf{p}_{\mathrm{f}}$ takes in account the opposite orientation of the normal direction to Σ_{f} and $\partial\Omega_{\mathrm{f}}$, so

$$\mathbf{p} = -\mathbf{p}_{\mathrm{f}} \oplus \mathbf{p}_{\mathrm{i}} \quad . \tag{1.22}$$

Covariant phase space

Finally we can give a phase space structure also to the space of classical histories $\boldsymbol{\mathcal{S}}$. First we note that for solutions of linearized equations of motion $\xi_1, \xi_2 \in \mathbf{T}\,\boldsymbol{\mathcal{S}}$

$$\xi_1 \bullet \mathrm{d}\mathfrak{P}[\partial\Omega] \bullet \xi_2 = \xi_1 \bullet (\overleftarrow{\delta^2} S[\Omega] - \overrightarrow{\delta^2} S[\Omega]) \bullet \xi_2 = 0 \quad . \tag{1.23}$$

$\mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{f}}]$ and $\mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{i}}]$ have the same restriction $\overleftrightarrow{\omega}$ on the space $\boldsymbol{\mathcal{S}}$.

$$\xi_1 \circ \overleftrightarrow{\omega} \circ \xi_2 = \xi_1 \bullet \mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{f}}] \bullet \xi_2 = \xi_1 \bullet \mathrm{d}\mathfrak{P}[\Sigma_{\mathrm{i}}] \bullet \xi_2 \quad . \tag{1.24}$$

In the same way we check that the same expression for $\overleftrightarrow{\omega}$ holds for any future oriented Cauchy hypersurface Σ. It means that we have equipped the space of classical histories $\boldsymbol{\mathcal{S}}$ with a symplectic structure. We will call this space the *covariant phase space*. We use indices $\scriptstyle A, B, \ldots$ for tensor indices and the dot $\circ$ for contraction in $\mathbf{T}\,\boldsymbol{\mathcal{S}}$. Clearly the $\boldsymbol{\mathcal{V}}_{\mathrm{f,i}}$ and $\mathbf{T}^{\star}\,\boldsymbol{\mathcal{V}}_{\mathrm{f,i}}$-valued observables $\mathbf{x}_{\mathrm{f,i}}$ and $\mathbf{p}_{\mathrm{f,i}}$ are canonically conjugate on this space, so

$$\overleftrightarrow{\omega}_{AB} = \nabla_{A} \mathbf{p}_{\mathrm{f}\mathbf{x}} \wedge \mathrm{D}^{\mathbf{x}}_{B} \mathbf{x}_{\mathrm{f}} = \nabla_{A} \mathbf{p}_{\mathrm{i}\mathbf{x}} \wedge \mathrm{D}^{\mathbf{x}}_{B} \mathbf{x}_{\mathrm{i}} \quad . \tag{1.25}$$

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

$$\overleftrightarrow{\omega}^{-1} \circ \overleftrightarrow{\omega} = \overleftrightarrow{\omega} \circ \overleftrightarrow{\omega}^{-1} = -\delta_{\boldsymbol{\mathcal{S}}} \quad . \tag{1.26}$$

The tensor tangent to $\boldsymbol{\mathcal{S}}$ as a subspace of the boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ has to be expressible as

$$\overleftrightarrow{\omega}^{-1} = \mathrm{D}\bar{\mathrm{h}} \cdot g_c \cdot \mathrm{D}\bar{\mathrm{h}} \tag{1.27}$$

with an antisymmetric tensor $g_c \in \mathbf{T}^2\,\boldsymbol{\mathcal{V}}[\partial\Omega]$. Using (1.18), (1.26) and (1.25) we get

$$g_c \cdot (\mathrm{d}_{\mathrm{f}} \mathrm{d}_{\mathrm{i}} \bar{S} - \mathrm{d}_{\mathrm{i}} \mathrm{d}_{\mathrm{f}} \bar{S}) = \delta_{\boldsymbol{\mathcal{V}}} \quad . \tag{1.28}$$

This means that

$$
\begin{gathered}
g_c = g_{\mathrm{if}} - g_{\mathrm{fi}} \quad , \quad g_{\mathrm{if}} = g_{\mathrm{fi}}^{\top} \quad , \\
g_{\mathrm{if}} \cdot \mathrm{d}_{\mathrm{f}}\mathrm{d}_{\mathrm{i}}\bar{S} = \delta_{\boldsymbol{\mathcal{V}}_{\mathrm{i}}} \quad , \quad g_{\mathrm{fi}} \cdot \mathrm{d}_{\mathrm{i}}\mathrm{d}_{\mathrm{f}}\bar{S} = \delta_{\boldsymbol{\mathcal{V}}_{\mathrm{f}}} \quad ,
\end{gathered}
\tag{1.29}
$$

and we get

$$
\begin{aligned}
\overset{\leftrightsquigarrow}{\omega}^{\text{-}1} &= \Big(\frac{\nabla_{\mathbf{x}}}{\partial \mathbf{x}} - \frac{\partial}{\partial \mathbf{p}_{\mathbf{u}}}(\nabla_{\mathbf{u}}\mathrm{d}_{\mathbf{x}}\bar{S})\Big)\, g_c^{\mathbf{xy}}\, \Big(\frac{\nabla_{\mathbf{y}}}{\partial \mathbf{x}} - (\nabla_{\mathbf{y}}\mathrm{d}_{\mathbf{v}}\bar{S})\frac{\partial}{\partial \mathbf{p}_{\mathbf{v}}}\Big) = \\
&= \Big(\frac{\partial}{\partial \mathbf{p}_{\mathrm{f}\mathbf{u}}}\frac{\nabla_{\mathbf{u}}}{\partial \mathbf{x}_{\mathrm{f}}} - \frac{\nabla_{\mathbf{u}}}{\partial \mathbf{x}_{\mathrm{f}}}\frac{\partial}{\partial \mathbf{p}_{\mathrm{f}\mathbf{u}}}\Big) + \Big(\frac{\partial}{\partial \mathbf{p}_{\mathrm{i}\mathbf{u}}}\frac{\nabla_{\mathbf{u}}}{\partial \mathbf{x}_{\mathrm{i}}} - \frac{\nabla_{\mathbf{u}}}{\partial \mathbf{x}_{\mathrm{i}}}\frac{\partial}{\partial \mathbf{p}_{\mathrm{i}\mathbf{u}}}\Big) + \\
&\quad + \Big(\frac{\nabla_{\mathbf{x}}}{\partial \mathbf{x}}\, g_c^{\mathbf{xy}}\, \frac{\nabla_{\mathbf{y}}}{\partial \mathbf{x}}\Big) + \\
&\quad + \Bigg(\frac{\partial}{\partial \mathbf{p}_{\mathrm{f}\mathbf{x}}}\Big((\nabla_{\mathrm{f}\mathbf{x}}\mathrm{d}_{\mathrm{f}\mathbf{u}}\bar{S}) g_{\mathrm{fi}}^{\mathbf{uv}} (\nabla_{\mathrm{i}\mathbf{v}}\mathrm{d}_{\mathrm{i}\mathbf{y}}\bar{S}) - \mathrm{d}_{\mathrm{f}\mathbf{x}}\mathrm{d}_{\mathrm{i}\mathbf{y}}\bar{S}\Big)\frac{\partial}{\partial \mathbf{p}_{\mathrm{i}\mathbf{y}}} \\
&\qquad\qquad - \frac{\partial}{\partial \mathbf{p}_{\mathrm{i}\mathbf{x}}}\Big((\nabla_{\mathrm{i}\mathbf{x}}\mathrm{d}_{\mathrm{i}\mathbf{u}}\bar{S}) g_{\mathrm{if}}^{\mathbf{uv}} (\nabla_{\mathrm{f}\mathbf{v}}\mathrm{d}_{\mathrm{f}\mathbf{y}}\bar{S}) - \mathrm{d}_{\mathrm{i}\mathbf{x}}\mathrm{d}_{\mathrm{f}\mathbf{y}}\bar{S}\Big)\frac{\partial}{\partial \mathbf{p}_{\mathrm{f}\mathbf{y}}}\Bigg) + \\
&\quad + \Big(\frac{\nabla_{\mathbf{x}}}{\partial \mathbf{x}_{\mathrm{i}}} g_{\mathrm{if}}^{\mathbf{xy}} (\nabla_{\mathrm{f}\mathbf{y}}\mathrm{d}_{\mathrm{f}\mathbf{u}}\bar{S})\frac{\partial}{\partial \mathbf{p}_{\mathrm{f}\mathbf{u}}} - \frac{\partial}{\partial \mathbf{p}_{\mathrm{f}\mathbf{u}}}(\nabla_{\mathrm{f}\mathbf{u}}\mathrm{d}_{\mathrm{f}\mathbf{y}}\bar{S}) g_{\mathrm{fi}}^{\mathbf{yx}}\frac{\nabla_{\mathbf{x}}}{\partial \mathbf{x}_{\mathrm{i}}}\Big) + \\
&\quad + \Big(\frac{\nabla_{\mathbf{x}}}{\partial \mathbf{x}_{\mathrm{f}}} g_{\mathrm{fi}}^{\mathbf{xy}} (\nabla_{\mathrm{i}\mathbf{y}}\mathrm{d}_{\mathrm{i}\mathbf{u}}\bar{S})\frac{\partial}{\partial \mathbf{p}_{\mathrm{i}\mathbf{u}}} - \frac{\partial}{\partial \mathbf{p}_{\mathrm{i}\mathbf{u}}}(\nabla_{\mathrm{i}\mathbf{u}}\mathrm{d}_{\mathrm{i}\mathbf{y}}\bar{S}) g_{\mathrm{if}}^{\mathbf{yx}}\frac{\nabla_{\mathbf{x}}}{\partial \mathbf{x}_{\mathrm{f}}}\Big) \quad ,
\end{aligned}
\tag{1.30}
$$

where we view $\boldsymbol{\mathcal{S}}$ as the subspace of the boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ (i.e. $\overset{\leftrightsquigarrow}{\omega}^{\text{-}1}$ is a tangent tensor from $\mathbf{T}^2\,\boldsymbol{\mathcal{B}}[\partial\Omega]$).

Or, if we view $\boldsymbol{\mathcal{S}}$ as a subspace of the space of histories $\boldsymbol{\mathcal{H}}$ we can understand $\overset{\leftrightsquigarrow}{\omega}^{\text{-}1}$ as a tangent tensor from $\mathbf{T}^2\,\boldsymbol{\mathcal{H}}$ which satisfies the linear equation of motion in both indices. We call this representation the *causal Green function* G_c

$$
G_c^{\boldsymbol{xy}} = \mathrm{D}^{\boldsymbol{x}}_{\mathbf{x}}\bar{\mathrm{h}}\, g_c^{\mathbf{xy}}\, \mathrm{D}^{\boldsymbol{y}}_{\mathbf{y}}\bar{\mathrm{h}} \quad . \tag{1.31}
$$

In the space $\mathbf{T}\,\boldsymbol{\mathcal{H}}$ equation (1.26) takes the form

$$
G_c \bullet \mathrm{d}\mathfrak{P}[\Sigma] = -D_C[\Sigma] \quad , \tag{1.32}
$$

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

Poisson brackets

The *Poisson brackets* of two observables on a phase space are defined by (B.5). We can compare now Poisson brackets in the sense of different phase spaces. Clearly any observable on $\boldsymbol{\mathcal{H}}$ generates an observable on $\boldsymbol{\mathcal{S}}$, and we can define

$$
\{A,B\}_{\boldsymbol{\mathcal{S}}} = \mathrm{d}_{\boldsymbol{x}}A\, G_c^{\boldsymbol{xy}}\, \mathrm{d}_{\boldsymbol{y}}B \quad \text{on} \quad \boldsymbol{\mathcal{S}} \quad . \tag{1.33}
$$

For observables depending only on the boundary values and momenta — i.e. observables on $\boldsymbol{\mathcal{B}}[\partial\Omega]$ we can define Poisson brackets in the sense of the boundary phase space

$$
\{A,B\}_{\boldsymbol{\mathcal{B}}} = \mathrm{d}_{\mathsf{A}}A\, \mathrm{d}\mathfrak{P}^{\text{-}1\,\mathsf{AB}}\, \mathrm{d}_{\mathsf{B}}B = \frac{\partial A}{\partial \mathbf{x}_{\mathbf{x}}}\frac{\nabla_{\mathbf{x}}B}{\partial \mathbf{x}} - \frac{\nabla_{\mathbf{x}}A}{\partial \mathbf{x}}\frac{\partial B}{\partial \mathbf{x}_{\mathbf{x}}} \quad . \tag{1.34}
$$

The covariant Poisson brackets for such observables are given by

$$
\begin{aligned}
\{A,B\}_{\boldsymbol{\mathcal{S}}} &= \mathrm{d}_{\mathsf{A}}A\, \overset{\leftrightsquigarrow}{\omega}^{\text{-}1\,\mathsf{AB}}\, \mathrm{d}_{\mathsf{B}}B = \\
&= \Big(\frac{\partial A}{\partial \mathbf{p}_{\mathrm{f}\mathbf{u}}}\frac{\nabla_{\mathbf{u}}B}{\partial \mathbf{x}_{\mathrm{f}}} - \frac{\nabla_{\mathbf{u}}A}{\partial \mathbf{x}_{\mathrm{f}}}\frac{\partial A}{\partial \mathbf{p}_{\mathrm{f}\mathbf{u}}}\Big) + \Big(\frac{\partial A}{\partial \mathbf{p}_{\mathrm{i}\mathbf{u}}}\frac{\nabla_{\mathbf{u}}B}{\partial \mathbf{x}_{\mathrm{i}}} - \frac{\nabla_{\mathbf{u}}A}{\partial \mathbf{x}_{\mathrm{i}}}\frac{\partial B}{\partial \mathbf{p}_{\mathrm{i}\mathbf{u}}}\Big) +
\end{aligned}
$$

$$
\begin{aligned}
&+\Big(\frac{\nabla_{\mathbf{x}}A}{\partial\mathbf{x}}\,g_c^{\mathbf{xy}}\,\frac{\nabla_{\mathbf{y}}B}{\partial\mathbf{x}}\Big)+\\
&+\Bigg(\frac{\partial A}{\partial\mathbf{p}_{\mathrm{f}\mathbf{x}}}\Big((\nabla_{\mathrm{f}\mathbf{x}}\mathrm{d}_{\mathrm{f}\mathbf{u}}\bar{S})g_{\mathrm{fi}}^{\mathbf{uv}}(\nabla_{\mathrm{i}\mathbf{v}}\mathrm{d}_{\mathrm{i}\mathbf{y}}\bar{S})-\mathrm{d}_{\mathrm{f}\mathbf{x}}\mathrm{d}_{\mathrm{i}\mathbf{y}}\bar{S}\Big)\frac{\partial B}{\partial\mathbf{p}_{\mathrm{i}\mathbf{y}}}\\
&\qquad-\frac{\partial A}{\partial\mathbf{p}_{\mathrm{i}\mathbf{x}}}\Big((\nabla_{\mathrm{i}\mathbf{x}}\mathrm{d}_{\mathrm{i}\mathbf{u}}\bar{S})g_{\mathrm{if}}^{\mathbf{uv}}(\nabla_{\mathrm{f}\mathbf{v}}\mathrm{d}_{\mathrm{f}\mathbf{y}}\bar{S})-\mathrm{d}_{\mathrm{i}\mathbf{x}}\mathrm{d}_{\mathrm{f}\mathbf{y}}\bar{S}\Big)\frac{\partial B}{\partial\mathbf{p}_{\mathrm{f}\mathbf{y}}}\Bigg)+\\
&+\Big(\frac{\nabla_{\mathbf{x}}A}{\partial\mathbf{x}_{\mathrm{i}}}g_{\mathrm{if}}^{\mathbf{xy}}(\nabla_{\mathrm{f}\mathbf{y}}\mathrm{d}_{\mathrm{f}\mathbf{u}}\bar{S})\frac{\partial B}{\partial\mathbf{p}_{\mathrm{f}\mathbf{u}}}-\frac{\partial A}{\partial\mathbf{p}_{\mathrm{f}\mathbf{u}}}(\nabla_{\mathrm{f}\mathbf{u}}\mathrm{d}_{\mathrm{f}\mathbf{y}}\bar{S})g_{\mathrm{fi}}^{\mathbf{yx}}\frac{\nabla_{\mathbf{x}}B}{\partial\mathbf{x}_{\mathrm{i}}}\Big)+\\
&+\Big(\frac{\nabla_{\mathbf{x}}A}{\partial\mathbf{x}_{\mathrm{f}}}g_{\mathrm{fi}}^{\mathbf{xy}}(\nabla_{\mathrm{i}\mathbf{y}}\mathrm{d}_{\mathrm{i}\mathbf{u}}\bar{S})\frac{\partial B}{\partial\mathbf{p}_{\mathrm{i}\mathbf{u}}}-\frac{\partial A}{\partial\mathbf{p}_{\mathrm{i}\mathbf{u}}}(\nabla_{\mathrm{i}\mathbf{u}}\mathrm{d}_{\mathrm{i}\mathbf{y}}\bar{S})g_{\mathrm{if}}^{\mathbf{yx}}\frac{\nabla_{\mathbf{x}}B}{\partial\mathbf{x}_{\mathrm{f}}}\Big)\quad.
\end{aligned}
\tag{1.35}
$$

Moreover, for observables localized only on Σ_{f} or Σ_{i} we have

$$
\begin{aligned}
\{A_{\mathrm{f}},B_{\mathrm{f}}\}_{\boldsymbol{\mathcal{B}}_{\mathrm{f}}}&=-\{A_{\mathrm{f}},B_{\mathrm{f}}\}_{\boldsymbol{\mathcal{B}}}=\{A_{\mathrm{f}},B_{\mathrm{f}}\}_{\boldsymbol{\mathcal{S}}}\quad,\\
\{A_{\mathrm{i}},B_{\mathrm{i}}\}_{\boldsymbol{\mathcal{B}}_{\mathrm{i}}}&=\{A_{\mathrm{i}},B_{\mathrm{i}}\}_{\boldsymbol{\mathcal{B}}}=\{A_{\mathrm{i}},B_{\mathrm{i}}\}_{\boldsymbol{\mathcal{S}}}\quad.
\end{aligned}
\tag{1.36}
$$

During the quantization of the theory we will be interested in special kind of observables on the boundary phase space (or in general, on any phase space which has the structure of a cotangent bundle). 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 $\boldsymbol{\mathcal{V}}$

$$\mathsf{F}_f=f(\mathbf{x})\quad,\tag{1.37}$$

$$\mathsf{G}_a=a^{\mathbf{x}}(\mathbf{x})\,\mathbf{p}_{\mathbf{x}}\quad.\tag{1.38}$$

The Poisson brackets of these observables are[2]

$$
\begin{aligned}
\{\mathsf{F}_{f_1},\mathsf{F}_{f_2}\}_{\boldsymbol{\mathcal{B}}}&=0\quad,\\
\{\mathsf{F}_{f},\mathsf{G}_{a}\}_{\boldsymbol{\mathcal{B}}}&=-\mathsf{F}_{a\bullet\mathrm{d}f}\quad,\\
\{\mathsf{G}_{a_1},\mathsf{G}_{a_2}\}_{\boldsymbol{\mathcal{B}}}&=\mathsf{G}_{[a_1,a_2]}\quad.
\end{aligned}
\tag{1.39}
$$

In the sense of the covariant phase space we have

$$\{\mathsf{F}_{f_1},\mathsf{F}_{f_2}\}_{\boldsymbol{\mathcal{S}}}=\mathsf{F}_{\mathrm{d}f_1\bullet g_c\bullet\mathrm{d}f_2}\quad\text{on}\quad\boldsymbol{\mathcal{S}}\tag{1.40}$$

and

$$\mathsf{G}_a=\mathsf{F}_{a\bullet\mathrm{d}\bar{S}}\quad\text{on}\quad\boldsymbol{\mathcal{S}}\quad.\tag{1.41}$$

Summary

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

But if we could only use experimental devices localized on the boundary of the investigated domain (i.e. in the case of a sandwich domain in a globally hyperbolic spacetime we could perform experiments only at initial and final moments of time), the space $\boldsymbol{\mathcal{B}}$ would be sufficient for the 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 a special subspace — the physical phase space $\boldsymbol{\mathcal{S}}$ which tell 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 $\boldsymbol{\mathcal{B}}$ represents all possible values of canonical observables at the initial and the final time without knowledge of equations of motion. The subspace $\boldsymbol{\mathcal{S}}$ represents values of canonical observables correlated by dynamical development of the system. An advantage of the $\boldsymbol{\mathcal{B}}$ is that we do not need any causal structure for it. I.e. we can construct it even for the Euclidian theory. And this advantage will be even more appealing in the quantum case.

2 Scalar field theory

Introduction

In the first three parts we will mainly investigate the non-interacting scalar field in a general spacetime. By *non-interacting* we mean a theory without *self-interaction*, i.e. it can interact with an external sources or fields (specifically, with the gravitational field). It can also contain an external potential interaction (spacetime-dependent mass term), which is not counted as a self-interaction. Indeed, such a nonzero potential is needed in order that the Neumann boundary problem be well formulated, as was discussed above. We will call a theory without external sources *free theory*.

In this chapter we will apply the previously developed formalism to the scalar field theory. It will take a much simpler form because of the linearity of the space of histories. We also review the $3+1$ splitting of the spacetime and the scalar field theory.

Space of histories and the action

The space of histories $\boldsymbol{\mathcal{P}}$ is composed of all possible field configurations which can be represented as (smooth) real functions on a spacetime manifold M, i.e $\boldsymbol{\mathcal{P}} = \mathfrak{F}\, M$. The space $\boldsymbol{\mathcal{P}}$ is a linear space, and this simplifies all considerations. The vector indices can be identified with points in the spacetime manifold, and the contraction is essentially the integration over the spacetime. In general we do not have to distinguish between the elements of the space $\boldsymbol{\mathcal{P}}$ and its tangent spaces. We have also a natural linear connection on $\boldsymbol{\mathcal{P}}$. We define a *basic field observable*

$$\Phi^x(\phi) = \phi(x) \tag{2.1}$$

which gives a value of the field at chosen spacetime point. It can be also understood as an identical $\boldsymbol{\mathcal{P}}$-valued observable on $\boldsymbol{\mathcal{P}}$.

The spacetime is equipped with a fixed gravitational field g (a metric on M), a scalar potential V (a function on M) and possibly an external source J (a density on M). We use the indices $\boldsymbol{\alpha}, \boldsymbol{\beta}, \dots$ for tensor indices of the tangent spaces or the dot $\cdot$ for contraction in these spaces. We also use the dot $\bullet$ for integration over spacetime, i.e for the contraction in the space $\boldsymbol{\mathcal{P}}$.

We are interested mainly in globally hyperbolic Lorentzian manifolds, but to a great extent the formalism can be applied also to a Euclidian manifold. In the former case, we will study the theory usually on a sandwich domain $\Omega = \langle \Sigma_{\mathrm{f}}, \Sigma_{\mathrm{i}} \rangle$ between two Cauchy hypersurfaces Σ_{f} and Σ_{i}. In the latter case we will study the theory on a compact domain Ω. Let us note that when we speak about a boundary or its parts we always assume that an orientation of the normal direction is associated with it. For the boundary of a domain we assume an inside-oriented normal direction. We use the Lorentzian convention for all quantities in the sense of appendix D.

The dynamics is given by the action

$$S[\Omega](\phi) = -\frac{1}{2}\, \phi \bullet \mathcal{F}_d[\Omega] \bullet \phi + J[\Omega] \bullet \phi \quad , \tag{2.2}$$

where the *wave operator* (or, more precisely, quadratic form)

$$\mathcal{F}_d[\Omega] = \overset{\leftrightsquigarrow}{\mathrm{d}}_{\boldsymbol{\alpha}} \bullet (\chi[\Omega] g^{-1\,\boldsymbol{\alpha\beta}}\, \mathcal{G}) \bullet \overset{\rightsquigarrow}{\mathrm{d}}_{\boldsymbol{\beta}} + (\chi[\Omega]\, V\, \mathcal{G}) \quad , \tag{2.3}$$

is a symmetric bi-distribution with support on the domain Ω and

$$J[\Omega] = \chi[\Omega] J \quad . \tag{2.4}$$

The bi-distributions $\big(f\mathcal{G}\big)$, $\overset{\leftsquigarrow}{\mathrm{d}}$ and $\overset{\rightsquigarrow}{\mathrm{d}}$ are defined in appendix A (equations (A.6), (A.7)).

The first variation of the action is

$$\mathrm{d}S[\Omega](\phi) = -\mathcal{F}_d[\Omega] \bullet \phi + J[\Omega] = \chi[\Omega]\delta S - \overset{\rightsquigarrow}{d\mathcal{F}}_d[\partial\Omega] \bullet \phi \quad , \tag{2.5}$$

where

$$\delta S(\phi) = -\overset{\rightsquigarrow}{\mathcal{F}} \bullet \phi + J \quad , \tag{2.6}$$

$$\overset{\rightsquigarrow}{\mathcal{F}} = -\overset{\rightsquigarrow}{\mathrm{d}}_{\boldsymbol{\alpha}} \bullet g^{\text{-}1\,\boldsymbol{\alpha\beta}} \mathfrak{g}^{\frac{1}{2}} \overset{\rightsquigarrow}{\mathrm{d}}_{\boldsymbol{\beta}} + (V\mathcal{G}) \quad , \quad \overset{\leftsquigarrow}{\mathcal{F}} = \overset{\rightsquigarrow}{\mathcal{F}}^{\top} \quad , \tag{2.7}$$

$$\overset{\rightsquigarrow}{\mathcal{F}}[\Omega] = \chi[\Omega]\overset{\rightsquigarrow}{\mathcal{F}} \quad , \quad \overset{\leftsquigarrow}{\mathcal{F}}[\Omega] = \overset{\leftsquigarrow}{\mathcal{F}}\chi[\Omega] \quad , \tag{2.8}$$

$$\overset{\rightsquigarrow}{d\mathcal{F}}_d[\partial\Omega] = (-\mathfrak{g}^{\frac{1}{2}}\, \delta_{\boldsymbol{\alpha}}[\partial\Omega]\, g^{\text{-}1\,\boldsymbol{\alpha\beta}} \overset{\rightsquigarrow}{\mathrm{d}}_{\boldsymbol{\beta}}) \quad , \quad \overset{\leftsquigarrow}{d\mathcal{F}}_d[\partial\Omega] = \overset{\rightsquigarrow}{d\mathcal{F}}_d[\partial\Omega]^{\top} \quad , \tag{2.9}$$

$$\mathcal{F}_d[\Omega] = \overset{\rightsquigarrow}{\mathcal{F}}[\Omega] + \overset{\rightsquigarrow}{d\mathcal{F}}_d[\partial\Omega] = \overset{\leftsquigarrow}{\mathcal{F}}[\Omega] + \overset{\leftsquigarrow}{d\mathcal{F}}_d[\partial\Omega] \quad . \tag{2.10}$$

Eq. (2.5) represents a formal integration by parts in the variation of the action, and $\overset{\rightsquigarrow}{d\mathcal{F}}_d[\partial\Omega] \bullet \phi$ is a boundary term representing the momentum. We assume that all fields fall off sufficiently fast at spatial infinity (if the domain Ω is not compact) so we can ignore boundary terms there. δS plays a role of a variation of the action on the full spacetime M. But it is not a gradient of any finite functional (in contrast to $\mathrm{d}S[\Omega]$).

The boundary term $\overset{\rightsquigarrow}{d\mathcal{F}}_d[\Sigma]$ can be generalized for any oriented hypersurface Σ. It is sensitive to the orientation of the hypersurface through the delta-function $\delta_{\boldsymbol{\alpha}}[\Sigma]$. In the Lorentzian spacetime, if the normal direction to Σ is time-like, we can choose a normal vector $\vec{n}$ normalized to -1 oriented in the sense of the hypersurface, and we can write

$$\overset{\rightsquigarrow}{d\mathcal{F}}_d[\Sigma] = (\mathfrak{g}^{\frac{1}{2}}\, \delta_{\vec{n}}[\Sigma]\, \vec{n}^{\boldsymbol{\alpha}} \overset{\rightsquigarrow}{\mathrm{d}}_{\boldsymbol{\alpha}}) \quad , \tag{2.11}$$

where $\delta_{\vec{n}}[\Sigma]$, defined in (A.13). It acts in the following way

$$\varphi \bullet \overset{\rightsquigarrow}{d\mathcal{F}}_d[\Sigma] \bullet \psi = \int\limits_{\Sigma} \varphi \mathfrak{q}^{\frac{1}{2}}\, \vec{n}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \psi \quad . \tag{2.12}$$

Here $\mathfrak{q}^{\frac{1}{2}}$ is the volume element (2.51) of the metric restricted on the submanifold Σ.

Phase spaces

The equation of motion is

$$\delta S(\phi) = 0 \quad . \tag{2.13}$$

We call the space of solutions a *covariant phase space* $\boldsymbol{\mathcal{S}}_J$ and in the case of the free theory $\boldsymbol{\mathcal{S}} = \boldsymbol{\mathcal{S}}_0$. Its tangent space $\mathbf{T}\,\boldsymbol{\mathcal{S}}_J$ is formed by solutions of the linearized equation of motion

$$\overset{\rightsquigarrow}{\mathcal{F}} \bullet \psi = 0 \quad . \tag{2.14}$$

The space $\boldsymbol{\mathcal{S}}_J$ is generally nonlinear because of the source term. Thanks to the linearity of the space of histories we can identify the tangent vectors with the space of histories itself. Clearly, the solution of the linearized equation of motion (2.14), i.e. vectors from tangent vector spaces $\mathbf{T}\,\boldsymbol{\mathcal{S}}_J$, all lie in the same vector space $\boldsymbol{\mathcal{S}}$ in this identification. The dot $\circ$ will represent contraction in this space[3].

The boundary symplectic form (1.8) reduces to the Klein-Gordon form $\partial\mathcal{F}[\partial\Omega]$

$$\begin{aligned} \mathrm{d}\mathfrak{P} &= \partial\mathcal{F}[\partial\Omega] \stackrel{\text{def}}{=} \overrightarrow{\mathcal{F}}[\Omega] - \overleftarrow{\mathcal{F}}[\Omega] = \overleftarrow{d\mathcal{F}}_d[\partial\Omega] - \overrightarrow{d\mathcal{F}}_d[\partial\Omega] = \\ &= \overleftarrow{\mathrm{d}}_{\boldsymbol{\alpha}}(-g^{-1\,\boldsymbol{\alpha\beta}}\mathfrak{g}^{\frac{1}{2}}\delta_{\boldsymbol{\beta}}[\partial\Omega]) - (-\mathfrak{g}^{\frac{1}{2}}\delta_{\boldsymbol{\alpha}}[\partial\Omega]\,g^{-1\,\boldsymbol{\alpha\beta}})\overrightarrow{\mathrm{d}}_{\boldsymbol{\beta}} \quad . \end{aligned} \tag{2.15}$$

From the definition we immediately get

$$\phi_1 \bullet \partial\mathcal{F}[\partial\Omega] \bullet \phi_2 = 0 \quad \text{for} \quad \phi_1,\, \phi_2 \in \boldsymbol{\mathcal{S}} \quad . \tag{2.16}$$

The boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ is defined as the space of classes of field configurations with the same value and normal derivative on the boundary $\partial\Omega$. The Klein-Gordon form plays the role of the symplectic structure on this space.

In the case of the sandwich domain $\Omega = \langle\Sigma_{\mathrm{f}}, \Sigma_{\mathrm{i}}\rangle$ in a globally hyperbolic manifold we can split the Klein-Gordon form to two pieces localized on the initial and final hypersurfaces

$$\partial\mathcal{F}[\partial\Omega] = -\partial\mathcal{F}[\Sigma_{\mathrm{f}}] + \partial\mathcal{F}[\Sigma_{\mathrm{i}}] \quad , \tag{2.17}$$

where we assume an oposite orientation of the normal for the final hypersurface Σ_{f} and the boundary $\partial\Omega$. As discussed in the previous chapter, $\partial\mathcal{F}[\Sigma_{\mathrm{f}}]$ and $\partial\mathcal{F}[\Sigma_{\mathrm{i}}]$ are symplectic structures on the canonical phase spaces $\boldsymbol{\mathcal{B}}[\Sigma_{\mathrm{f}}]$ and $\boldsymbol{\mathcal{B}}[\Sigma_{\mathrm{i}}]$.

In general, we can define a phase space $\boldsymbol{\mathcal{B}}[\Sigma]$ on any oriented hypersurface Σ. We use the dot $\diamond$ for the contraction in these spaces. We also define the natural projection $\underline{\partial\Phi}[\Sigma]$ from $\boldsymbol{\mathcal{P}}$ to $\boldsymbol{\mathcal{B}}[\Sigma]$ and the identical *basic observable* $\partial\Phi[\Sigma]$ on $\boldsymbol{\mathcal{B}}[\Sigma]$, similar to Φ on $\boldsymbol{\mathcal{P}}$.

The Poisson brackets of two observables are

$$\{A, B\}_{\boldsymbol{\mathcal{B}}} = \mathrm{d}\,A \diamond G_c \diamond \mathrm{d}\,B \quad . \tag{2.18}$$

Applied to the basic variable $\partial\Phi$ we get

$$\{\Phi, \Phi\}_{\boldsymbol{\mathcal{B}}} = \partial\mathcal{F}[\Sigma]^{-1} \quad . \tag{2.19}$$

Moreover the forms $\partial\mathcal{F}[\Sigma]$ generate a symplectic form $\overleftrightarrow{\omega}$ on the space $\boldsymbol{\mathcal{S}}$ independent of the choice of the hypersurface. Its action is given by well-known Klein-Gordon product

$$\phi_1 \circ \overleftrightarrow{\omega} \circ \phi_2 = \phi_1 \bullet \partial\mathcal{F}[\Sigma] \bullet \phi_2 = \int\limits_{\Sigma} \big((\vec{n}^{\boldsymbol{\alpha}}\mathrm{d}_{\boldsymbol{\alpha}}\phi_1)\phi_2 - \phi_1(\vec{n}^{\boldsymbol{\alpha}}\mathrm{d}_{\boldsymbol{\alpha}}\phi_2)\big)\mathfrak{q}^{\frac{1}{2}} \quad . \tag{2.20}$$

computed on any Cauchy hypersurface Σ with the future oriented normalized normal vector $\vec{n}$.

We can define its inversion — causal Green function —

$$\begin{aligned} G_c \in \boldsymbol{\mathcal{S}}^2 \quad &, \quad G_c^{\top} = -G_c \quad , \\ G_c \circ \overleftrightarrow{\omega} = \overleftrightarrow{\omega} \circ G_c &= -\delta_{\boldsymbol{\mathcal{S}}} \quad , \end{aligned} \tag{2.21}$$

or, formulated in the space of histories $\boldsymbol{\mathcal{P}}$,

$$\begin{aligned} G_c \in \boldsymbol{\mathcal{P}}^2 \quad , \quad \overrightarrow{\mathcal{F}} \bullet G_c = G_c \bullet \overleftarrow{\mathcal{F}} = 0 \quad , \quad G_c^{\top} = -G_c \quad , \\ G_c \bullet \partial\mathcal{F}[\Sigma] = \partial\mathcal{F}[\Sigma] \bullet G_c = -D_C[\Sigma] \quad . \end{aligned} \tag{2.22}$$

Here $D_C[\Sigma]$ propagates Cauchy data on a hypersurface Σ to a solution of the linearized equation of motion (2.14). It is a projection from $\boldsymbol{\mathcal{P}}$ to $\boldsymbol{\mathcal{S}}$ using the Cauchy data on Σ.

The Poisson bracket of two observables $A, B \in \mathfrak{F}\boldsymbol{\mathcal{S}}$ is given by

$$\{A, B\}_{\boldsymbol{\mathcal{S}}} = \mathrm{d}\, A \circ G_c \circ \mathrm{d}\, B \quad . \tag{2.23}$$

Applied to the basic variable $\Phi^{\boldsymbol{x}}$ we get

$$\{\Phi^{\boldsymbol{x}}, \Phi^{\boldsymbol{y}}\}_{\boldsymbol{\mathcal{S}}} = G_c^{\boldsymbol{xy}} \quad , \tag{2.24}$$

or, if we define a linear observable on $\boldsymbol{\mathcal{S}}$ labeled by an element $\phi \in \boldsymbol{\mathcal{S}}$

$$\mathsf{L}_\phi = \phi \circ \overleftrightarrow{\omega} \circ \Phi \tag{2.25}$$

(any linear observable on $\boldsymbol{\mathcal{S}}$ can be written in this way thanks to non-degeneracy of the symplectic form $\overleftrightarrow{\omega}$), the Poisson brackets of such observables are

$$\{\mathsf{L}_{\phi_1}, \mathsf{L}_{\phi_2}\}_{\boldsymbol{\mathcal{S}}} = \phi_1 \circ \overleftrightarrow{\omega} \circ \phi_2 \quad . \tag{2.26}$$

Green functions

G_c is called the causal Green function. We can introduce also other natural Green functions. For a smooth source J on the domain $\Omega = \langle \Sigma_\mathrm{f}, \Sigma_\mathrm{i} \rangle$ (i.e. with support in Ω and smooth up to the boundary) we define retarded and advanced solutions of the equation of motion

$$\begin{aligned} \overrightarrow{\mathcal{F}} \bullet \bar{\phi}_\mathrm{adv}(J) = J \quad &, \quad D_C[\Sigma_\mathrm{f}] \bullet \bar{\phi}_\mathrm{adv}(J) = 0 \quad , \\ \overrightarrow{\mathcal{F}} \bullet \bar{\phi}_\mathrm{ret}(J) = J \quad &, \quad D_C[\Sigma_\mathrm{i}] \bullet \bar{\phi}_\mathrm{ret}(J) = 0 \quad , \end{aligned} \tag{2.27}$$

$$\bar{\phi}_\mathrm{sym}(J) = \frac{1}{2}(\bar{\phi}_\mathrm{adv}(J) + \bar{\phi}_\mathrm{ret}(J)) \quad , \tag{2.28}$$

and coresponding Green functions — bi-forms on smooth sources —

$$\bar{\phi}_\mathrm{adv}(J) = G_\mathrm{adv} \bullet J \quad , \quad \bar{\phi}_\mathrm{ret}(J) = G_\mathrm{ret} \bullet J \quad , \quad \bar{\phi}_\mathrm{sym}(J) = G_\mathrm{sym} \bullet J \quad , \tag{2.29}$$

$$G_\mathrm{sym} = \frac{1}{2}(G_\mathrm{ret} + G_\mathrm{adv}) \quad . \tag{2.30}$$

Let us note that the solutions given by (2.29) satisfy the relations (2.28) only for the source with support in the domain Ω.

If we denote

$$\phi_c(J) = G_c \bullet J \quad , \tag{2.31}$$

we find

$$\begin{aligned} &\overrightarrow{\mathcal{F}} \bullet \big(\bar{\phi}_\mathrm{adv}(J) + \phi_c(J)\big) = J \quad , \\ D_C[\Sigma_\mathrm{i}] \bullet \big(\bar{\phi}_\mathrm{adv}(J) + \phi_c(J)\big) &= -G_c \bullet \partial\mathcal{F}[\Sigma_\mathrm{f}] \bullet \big(\bar{\phi}_\mathrm{adv}(J) + \phi_c(J)\big) = \\ &= -G_c \bullet \partial\mathcal{F}[\Sigma_\mathrm{f}] \bullet \big(\bar{\phi}_\mathrm{adv}(J) + \phi_c(J)\big) - G_c \bullet \big(\overrightarrow{\mathcal{F}}[\Omega] - \overleftarrow{\mathcal{F}}[\Omega]\big) \bullet \big(\bar{\phi}_\mathrm{adv}(J) + \phi_c(J)\big) = \\ &= D_C[\Sigma_\mathrm{f}] \bullet G_c \bullet J - G_c \bullet J = 0 \quad . \end{aligned} \tag{2.32}$$

This means

$$\begin{aligned} \phi_c(J) &= \bar{\phi}_\mathrm{ret}(J) - \bar{\phi}_\mathrm{adv}(J) \quad , \\ G_c &= G_\mathrm{ret} - G_\mathrm{adv} \quad . \end{aligned} \tag{2.33}$$

Space of boundary values

For any hypersurface Σ we can define a space of boundary values $\boldsymbol{\mathcal{V}}[\Sigma]$. A boundary value of the field can be represented as a function on Σ, i.e $\boldsymbol{\mathcal{V}}[\Sigma] = \mathfrak{F}\,\Sigma$. We denote by $\tilde{\boldsymbol{\mathcal{V}}}[\Sigma] = \tilde{\mathfrak{F}}\,\Sigma$ the space of densities on Σ. We use the dot $\cdot$ for contraction between an element in $\boldsymbol{\mathcal{V}}[\Sigma]$ and an element in $\tilde{\boldsymbol{\mathcal{V}}}[\Sigma]$ (integration over boundary). We define $\boldsymbol{\mathcal{V}}[\Sigma]$ and $\tilde{\boldsymbol{\mathcal{V}}}[\Sigma]$-valued observables $\varphi[\Sigma]$ and $\pi[\Sigma]$ on the space of histories called value and momentum as

$$\varphi[\Sigma](\phi) = \phi|_\Sigma \quad , \quad \pi[\Sigma](\phi) = -\mathfrak{q}^{\frac{1}{2}}\, n_{\boldsymbol{\alpha}}\, g^{-1\,\boldsymbol{\alpha\beta}}\, \mathrm{d}_{\boldsymbol{\beta}}\phi|_\Sigma \quad . \tag{2.34}$$

Here n is the normalized normal form on Σ with the same orientation as the hypersurface and $\mathfrak{q}^{\frac{1}{2}}$ is the volume element of the restricted metric on the Σ (see (2.50) and (2.51)). The momentum observable depends on the orientation of the normal vector. Both observables are linear and can be generated by $\boldsymbol{\mathcal{V}}[\Sigma]$ and $\tilde{\boldsymbol{\mathcal{V}}}[\Sigma]$-valued forms $\underline{\varphi}[\Sigma]$ and $\underline{\pi}[\Sigma]$ on the space $\boldsymbol{\mathcal{P}}$

$$\varphi[\Sigma](\phi) = \underline{\varphi}[\Sigma] \bullet \phi \quad , \quad \pi[\Sigma](\phi) = \underline{\pi}[\Sigma] \bullet \phi \quad . \tag{2.35}$$

The momentum observable satisfies

$$\overset{\leadsto}{d\mathcal{F}}_d[\Sigma] = \underline{\varphi}[\Sigma] \cdot \underline{\pi}[\Sigma] \quad , \tag{2.36}$$

and therefore we get

$$\partial\mathcal{F}[\Sigma] = \underline{\pi}[\Sigma] \cdot \underline{\varphi}[\Sigma] - \underline{\varphi}[\Sigma] \cdot \underline{\pi}[\Sigma] \quad , \tag{2.37}$$

$$\tag{2.38}$$

We can pull back the value and momentum observables on the boundary phase space localized on the hypersurface Σ, and equations (2.37) tells us that they are canonically conjugate in the sense of the symplectic structure $\partial\mathcal{F}[\Sigma]$.

Now let us investigate the value and momentum on the boundary of the domain Ω. As in the general case discussed in the previous chapter, we restrict ourselves only to the case when either value or momentum on the whole boundary represents sufficient boundary data. Therefore we can express the momentum of a solution of the homogenous field equation (2.14) in terms its boundary value. We define a quadratic form $\gamma[\partial\Omega]$ on $\boldsymbol{\mathcal{V}}[\partial\Omega]$ as

$$\underline{\pi}[\partial\Omega] \bullet \phi = \gamma[\partial\Omega] \cdot \underline{\varphi}[\partial\Omega] \bullet \phi \quad \text{for} \quad \phi \in \boldsymbol{\mathcal{S}} \quad . \tag{2.39}$$

Using (2.37) and (2.16) we find that $\gamma[\partial\Omega]$ is symmetric

$$\gamma[\partial\Omega]^\top = \gamma[\partial\Omega] \quad . \tag{2.40}$$

Next we define an "inversion" $\underline{D}[\Omega]$ of the form $\underline{\varphi}[\partial\Omega]$ in $\boldsymbol{\mathcal{S}}$,

$$\underline{D}[\partial\Omega] : \boldsymbol{\mathcal{V}}[\partial\Omega] \to \boldsymbol{\mathcal{S}} \qquad , \qquad \underline{\varphi}[\partial\Omega] \bullet \underline{D}[\partial\Omega] = \delta_{\boldsymbol{\mathcal{V}}[\partial\Omega]} \quad , \tag{2.41}$$

which creates a solution of the homogenous field equation with given the value on the boundary,

$$\overset{\leadsto}{\mathcal{F}} \bullet \phi = 0 \quad \wedge \quad \underline{\varphi}[\partial\Omega] \bullet \phi = \varphi \qquad \Leftrightarrow \qquad \phi = \underline{D}[\partial\Omega] \cdot \varphi \quad . \tag{2.42}$$

We also define the projectors $D_D[\partial\Omega]$ and $D_N[\partial\Omega]$ from $\boldsymbol{\mathcal{P}}$ to $\boldsymbol{\mathcal{S}}$ which map a field to the solution with the same value or momentum on the boundary $\partial\Omega$

$$\begin{aligned} D_D[\partial\Omega] &= \underline{D}[\partial\Omega] \cdot \underline{\varphi}[\partial\Omega] \quad , \\ D_N[\partial\Omega] &= \underline{D}[\partial\Omega] \cdot \gamma[\partial\Omega]^{-1} \cdot \underline{\pi}[\partial\Omega] \quad . \end{aligned} \tag{2.43}$$

We can also define a *generator of the phase space* $\underline{\vartheta}[\partial\Omega]$

$$\begin{aligned}\underline{\vartheta}[\partial\Omega] &: \boldsymbol{\mathcal{P}} \to \tilde{\boldsymbol{\mathcal{V}}}[\partial\Omega] \quad , \\ \underline{\vartheta}[\partial\Omega] = -\underline{D}[\partial\Omega] \bullet \partial\mathcal{F}[\partial\Omega] &= \underline{\pi}[\partial\Omega] - \gamma[\partial\Omega] \cdot \underline{\varphi}[\partial\Omega] \quad .\end{aligned} \tag{2.44}$$

It is easy to check that

$$\underline{\vartheta}[\partial\Omega] \bullet \phi[\partial\Omega] = 0 \quad \Leftrightarrow \quad \phi \in \boldsymbol{\mathcal{S}} \quad , \tag{2.45}$$

$$\partial\mathcal{F}[\partial\Omega] = \underline{\vartheta}[\partial\Omega] \cdot \underline{\varphi}[\partial\Omega] - \underline{\varphi}[\partial\Omega] \cdot \underline{\vartheta}[\partial\Omega] \quad . \tag{2.46}$$

Finally we define the restriction of a smooth source J to the boundary

$$\vartheta[\Omega] : \tilde{\boldsymbol{\mathcal{P}}}[\Omega] \to \tilde{\boldsymbol{\mathcal{V}}}[\partial\Omega] \qquad , \qquad \vartheta[\Omega](J) = -J \bullet \underline{D}[\partial\Omega] \quad . \tag{2.47}$$

3 + 1 splitting

Let us assume we are working in a globally hyperbolic spacetime. A $3+1$ splitting of a spacetime [2] is defined using a time coordinate t and a time flow vector $\vec{t}^{\boldsymbol{\alpha}} \in \mathfrak{T}M$ consistent with the time coordinate:

$$\vec{t}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} t = 1 \quad . \tag{2.48}$$

"Space at moment t" is a hypersurface Σ_t of constant time t. We assume it is a Cauchy hypersurface. The time flow vector gives us a diffeomorphism between these hypersurfaces. All "spacetime" quantities can be expressed using "space" quantities in the standard way:

$$\vec{t}^{\boldsymbol{\alpha}} = N\vec{n}^{\boldsymbol{\alpha}} + \vec{N}^{\boldsymbol{\alpha}} \quad , \quad N\,\mathrm{d}_{\boldsymbol{\alpha}} t = n_{\boldsymbol{\alpha}} \quad , \tag{2.49}$$

$$\vec{n}^{\boldsymbol{\alpha}}\, g_{\boldsymbol{\alpha\beta}}\, \vec{n}^{\boldsymbol{\beta}} = -1 \quad , \quad \vec{n}^{\boldsymbol{\alpha}} n_{\boldsymbol{\alpha}} = 1 \quad , \quad q_{\boldsymbol{\alpha\beta}} = (g|_\Sigma)_{\boldsymbol{\alpha\beta}} \quad , \tag{2.50}$$

$$\mathfrak{g}^{\frac12} = N\,dt\,\mathfrak{q}^{\frac12} \quad , \quad \mathfrak{q}^{\frac12} = (\mathrm{Det}\, q_{\boldsymbol{\alpha\beta}})^{\frac12} \quad , \tag{2.51}$$

$$\mathsf{j} = J\mathfrak{q}^{\frac12}/\mathfrak{g}^{\frac12} \quad , \quad \tilde{\mathsf{j}} = N\mathsf{j} \quad . \tag{2.52}$$

Here $q_{\boldsymbol{\alpha\beta}}$ is the space part of the metric $g_{\boldsymbol{\alpha\beta}}$, the normal vector $\vec{n}$ and the hypersurface Σ_t are future oriented, and N and $\vec{N}^{\boldsymbol{\alpha}}$ are the lapse and the shift[4].

For each hypersurface Σ_t we can construct the boundary value space $\boldsymbol{\mathcal{V}}[\Sigma_t]$ and define the value observable $\varphi[\Sigma_t]$. For simplicity of the notation we we drop the hypersurface dependence in the rest of this section. The diffeomorphism between hypersurfaces allows us to define the *time derivative*

$$\varphi' = (\vec{t}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}}\, \Phi)|_{\Sigma_t} = N(\vec{n}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \Phi)|_{\Sigma_t} + \vec{N}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \varphi \quad . \tag{2.53}$$

The action can be written using the Lagrangian

$$S[\langle \Sigma_{t_\mathrm{f}} | \Sigma_{t_\mathrm{i}} \rangle] = \int_{t_\mathrm{i}}^{t_\mathrm{f}} L(\varphi, \varphi')\, dt \quad , \tag{2.54}$$

$$\begin{aligned} L(\varphi,\varphi') = \int_{\Sigma_t} \Big(\Big[\, & \frac12 \frac1N \varphi'^{\,2} - \varphi' \vec{N}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \varphi \\ - \; & \frac12 N \Big((\mathrm{d}_{\boldsymbol{\alpha}}\varphi)(q^{-1\,\boldsymbol{\alpha\beta}} - \vec{N}^{\boldsymbol{\alpha}} \frac{1}{N^2} \vec{N}^{\boldsymbol{\beta}})(\mathrm{d}_{\boldsymbol{\beta}}\varphi) + V\varphi^2 \Big) \Big] \mathfrak{q}^{\frac12} + N\mathsf{j}\varphi \Big) \quad . \end{aligned} \tag{2.55}$$

As we expect the momentum observable defined in the Hamiltonian formalism coincides with the definition (2.34) above:

$$\begin{aligned} \pi &= \frac{\partial L}{\partial \varphi'} = \mathfrak{q}^{\frac12} \frac1N (\varphi' - \vec{N}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \varphi) = \mathfrak{q}^{\frac12} (\vec{n}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \Phi)|_{\Sigma_t} \quad , \\ \varphi' &= N\mathfrak{q}^{\frac12 - \frac12} \pi + \vec{N}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \varphi = \tilde{\mathsf{q}}^{-1} \cdot \pi + \mathsf{p} \cdot \varphi \quad . \end{aligned} \tag{2.56}$$

The Hamiltonian is

$$
\begin{aligned}
H[\Sigma_t,\vec{t}] = H(\varphi,\pi) = \int\limits_{\Sigma_t} N\Big[\frac{1}{2}\pi^2 \mathsf{q}^{\frac{1}{2}^{-\frac{1}{2}}} + \pi \vec{N}^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}}\varphi \\
+ \frac{1}{2}\Big((\mathrm{d}_{\boldsymbol{\alpha}}\varphi)(q^{-1\,\boldsymbol{\alpha\beta}} - \vec{N}^{\boldsymbol{\alpha}} \frac{1}{N^2} \vec{N}^{\boldsymbol{\beta}})(\mathrm{d}_{\boldsymbol{\beta}}\varphi) + V\varphi^2 \Big) \mathsf{q}^{\frac{1}{2}} - \mathsf{j}\varphi \Big] = \\
= \frac{1}{2}\Big(\, \pi \cdot \tilde{\mathsf{q}}^{-1} \cdot \pi + \pi \cdot \mathsf{p} \cdot \varphi + \varphi \cdot \mathsf{p} \cdot \pi + \varphi \cdot \mathsf{v} \cdot \varphi \,\Big) - \tilde{\mathsf{j}} \cdot \varphi \quad ,
\end{aligned}
\tag{2.57}
$$

where[5]

$$
\begin{aligned}
\tilde{\mathsf{q}} = (\frac{1}{N}\mathsf{q}^{\frac{1}{2}}\delta) = \frac{1}{N}\mathsf{q} \quad , \quad \mathsf{p} = \vec{N}^{\boldsymbol{\alpha}} \overleftrightarrow{\mathrm{d}}_{\boldsymbol{\alpha}} \quad , \\
\mathsf{v} = \overleftrightarrow{\mathrm{d}}_{\boldsymbol{\alpha}} \cdot (N q^{-1\,\boldsymbol{\alpha\beta}} - \frac{1}{N}\vec{N}^{\boldsymbol{\alpha}}\vec{N}^{\boldsymbol{\beta}})\mathsf{q} \cdot \overleftrightarrow{\mathrm{d}}_{\boldsymbol{\beta}} + NV\mathsf{q} \quad .
\end{aligned}
\tag{2.58}
$$

The Hamiltonian $H[\Sigma,\vec{t}]$ as an observable on the space $\boldsymbol{\mathcal{P}}$ can be defined for any hypersurface Σ equipped with a non-tangential non-degenerate vector field $\vec{t}$. It is a quadratic observable (in the sense of $\boldsymbol{\mathcal{P}}$), and it has support on the hypersurface Σ. It can be written as

$$
H[\Sigma,\vec{t}](\phi) = \frac{1}{2}\,\phi \bullet \mathcal{H}[\Sigma,\vec{t}] \bullet \phi - \mathcal{J}[\Sigma,\vec{t}] \bullet \phi \quad , \tag{2.59}
$$

where

$$
\mathcal{H} = \underline{\pi} \cdot \tilde{\mathsf{q}}^{-1} \cdot \underline{\pi} + \underline{\pi} \cdot \mathsf{p} \cdot \underline{\varphi} + \underline{\varphi} \cdot \mathsf{p} \cdot \underline{\pi} + \underline{\varphi} \cdot \mathsf{v} \cdot \underline{\varphi} \quad , \tag{2.60}
$$

$$
\mathcal{J} = J\delta_{\vec{t}}[\Sigma] = \tilde{\mathsf{j}} \cdot \underline{\varphi} \quad . \tag{2.61}
$$

This is also a well-defined observable on the boundary phase space $\boldsymbol{\mathcal{B}}[\Sigma]$.

3 Boundary conditions and extensions of Laplace-like operators

Generalized boundary value

In this chapter we will investigate the question of boundary conditions. In the previous chapter we have seen that the phase space can also be parametrized using values of the field on the boundary $\partial\Omega$ of the spacetime domain Ω. Now we would like to introduce a more general notion of the boundary values.

Most objects introduced in this chapter should carry an argument with the specification of the spacetime domain Ω (e.g. $\overleftrightarrow{\mathcal{F}}[\Omega]$) or the boundary $\partial\Omega$ (e.g. $\partial\mathcal{F}[\partial\Omega]$). Because we will work with one fixed domain Ω, we will drop the domain argument here to simplify the notation.

We can characterize a *generalized boundary value* by fixing a complementary vector space $\boldsymbol{\mathcal{P}}_B$ to the space $\boldsymbol{\mathcal{S}}$ in the space of all histories $\boldsymbol{\mathcal{P}}$, i.e. the space which satisfies

$$\boldsymbol{\mathcal{P}} = \boldsymbol{\mathcal{P}}_B \oplus \boldsymbol{\mathcal{S}} \quad , \quad \boldsymbol{\mathcal{P}}_B \cap \boldsymbol{\mathcal{S}} = \{0\} \quad . \tag{3.1}$$

Let D_B and Δ_B be projectors onto $\boldsymbol{\mathcal{S}}$ and $\boldsymbol{\mathcal{P}}_B$

$$\begin{gathered} D_B \bullet \phi = \phi \;\Leftrightarrow\; \phi \in \boldsymbol{\mathcal{S}} \quad , \quad \Delta_B \bullet \phi = \phi \;\Leftrightarrow\; \phi \in \boldsymbol{\mathcal{P}}_B \\ D_B \bullet D_B = D_B \quad , \quad \Delta_B \bullet \Delta_B = \Delta_B \\ D_B \bullet \Delta_B = \Delta_B \bullet D_B = 0 \quad , \quad D_B + \Delta_B = \delta_{\boldsymbol{\mathcal{P}}} \quad . \end{gathered} \tag{3.2}$$

Using the definition of $\boldsymbol{\mathcal{S}}$ and (2.16) we get

$$\overleftrightarrow{\mathcal{F}} \bullet D_B = 0 \quad , \tag{3.3}$$

$$D_B \bullet \partial\mathcal{F} \bullet D_B = 0 \tag{3.4}$$

The space $\boldsymbol{\mathcal{P}}_B$ can be interpreted as a space of histories with zero *generalized* B*-value*. The projector D_B is an operator which acting on a history gives a solution of the free equation of motion with "the same B-value".

The reason for the necessity to investigate boundary conditions is that the field operator $\overleftrightarrow{\mathcal{F}}$ is degenerate and non-symmetric on the space $\boldsymbol{\mathcal{P}}$. We choose a space $\boldsymbol{\mathcal{P}}_B$ in such way that it is the maximal space of smooth field configurations on which the operator $\overleftrightarrow{\mathcal{F}}$ is non-degenerate. The *maximality* is expressed by condition (3.1). Of course, the choice of the space $\boldsymbol{\mathcal{P}}_B$ is not unique — we can have different boundary conditions.

It could seem that there are more unique choices of a subspace of $\boldsymbol{\mathcal{P}}$ on which the operator $\overleftrightarrow{\mathcal{F}}$ is non-degenerate — for example the space $\boldsymbol{\mathcal{P}}_o$ of all histories with support in the interior of the domain Ω. But such a space is too small. In general, there is no solution in $\boldsymbol{\mathcal{P}}_o$ of equation (2.13) with a non-zero source J. On the other hand, the operator $\mathcal{F}_o$ (the restriction of $\overleftrightarrow{\mathcal{F}}$ on $\boldsymbol{\mathcal{P}}_o$) is symmetric on $\boldsymbol{\mathcal{P}}_o$. We would like to impose the same condition on the space $\boldsymbol{\mathcal{P}}_B$. In other words, we are looking for a self-adjoint extension of the operator $\mathcal{F}_o$ which coincides with $\overset{\leftrightarrow}{\mathcal{F}}$ on the space $\boldsymbol{\mathcal{P}}_B$. The symmetry condition

$$\phi_1, \phi_2 \in \boldsymbol{\mathcal{P}}_B \quad \Rightarrow \quad \phi_1 \bullet \overset{\leftrightarrow}{\mathcal{F}} \bullet \phi_2 = \phi_2 \bullet \overset{\leftrightarrow}{\mathcal{F}} \bullet \phi_1 \tag{3.5}$$

can be formulated in terms of a projector Δ_B

$$\Delta_B \bullet \partial\mathcal{F} \bullet \Delta_B = 0 \quad . \tag{3.6}$$

To conclude the definition of generalized boundary value we need to add a condition of localization on the boundary $\partial\Omega$. If we view the projector $D_B{}^{\boldsymbol{x}}_{\boldsymbol{y}}$ as a bi-distribution (with one functional and one density argument), we will require that it has support on $\partial\Omega$ in the density argument. More precisely, any distribution obtained by smoothing D_B with a smooth source $j \in \tilde{\boldsymbol{\mathcal{P}}}$ has a support in $\partial\Omega$

$$\operatorname{supp}\big(j \bullet D_B\big) \subset \partial\Omega \quad . \tag{3.7}$$

Finally we pick up two special cases. We use the indices D and N for Dirichlet and Neumann boundary conditions. It means that $\boldsymbol{\mathcal{P}}_D$ is the space of fields with zero value on the boundary and $\boldsymbol{\mathcal{P}}_N$ is the space of fields with zero momentum.

Space of boundary values

The conditions on the projectors D_B and Δ_B restrict the character of the generalized boundary value. We will prove that the generalized boundary value depends only on the value and momentum on the boundary.

First we introduce a notion similar to the form $\underline{\varphi}$ for the generalized boundary value. We use again the fact that the value of the solution of the homogenous field equation on the whole boundary is sufficient to determine the solution. Therefore we can define the *form of generalized boundary value* $\underline{\varphi}_B$ which assigns to a field ϕ the boundary value of the solution from $\boldsymbol{\mathcal{S}}$ with the same B-value, i.e.

$$\underline{\varphi}_B : \boldsymbol{\mathcal{P}} \to \boldsymbol{\mathcal{V}} \qquad , \qquad \underline{\varphi}_B = \underline{\varphi} \bullet D_B \quad . \tag{3.8}$$

Clearly

$$\underline{\varphi}_B \bullet \phi = 0 \;\Leftrightarrow\; \phi \in \boldsymbol{\mathcal{P}}_B \quad , \quad \underline{\varphi}_B = \underline{\varphi}_B \bullet D_B \quad , \tag{3.9}$$

$$\underline{\varphi}_B \cdot \underline{D} = \delta_{\boldsymbol{\mathcal{V}}} \quad , \quad D_B = \underline{D} \cdot \underline{\varphi}_B \tag{3.10}$$

and

$$\overset{\leftrightarrow}{\mathcal{F}} \bullet \phi = 0 \quad \wedge \quad \underline{\varphi}_B \bullet \phi = \varphi \qquad \Leftrightarrow \qquad \phi = \underline{D} \cdot \varphi \quad . \tag{3.11}$$

Using the localization condition (3.7) we know that D_B and therefore also $\underline{\varphi}_B$ can be sensitive only to the value and (multiple) normal derivatives on the boundary. If we denote by $\underline{\varphi}^{(k)}$ the form which gives the k-th normal derivative on the boundary, we can write

$$\underline{\varphi}_B = \gamma^{-1} \cdot \lambda_B \cdot \underline{\varphi} + \kappa_B \cdot \underline{\pi} + \sum_{k=2,3,\dots} \epsilon^k_B \cdot \underline{\varphi}^{(k)} \quad , \tag{3.12}$$

where λ_B, κ_B and ϵ^k_B are linear coefficients (bi-density, bi-vector and operators on $\boldsymbol{\mathcal{V}}$). We have used $\underline{\varphi}$ and $\underline{\pi}$ instead of $\underline{\varphi}^{(0)}$ and $\underline{\varphi}^{(1)}$, and we have scaled the zero-th coefficient by the quadratic form γ defined in (2.39) for convenience.

The condition (3.6) together with (3.4) is equivalent to

$$\partial\mathcal{F} = \partial\mathcal{F} \bullet D_B + D_B \bullet \partial\mathcal{F} \quad . \tag{3.13}$$

Substituting expressions (2.37), (2.39), (3.8) and (3.12) and comparing coefficients of terms with the same order of normal derivatives, we get conditions

$$\kappa_B^\top = \kappa_B \quad , \quad \lambda_B^\top = \lambda_B \quad , \tag{3.14}$$

$$\kappa_B \cdot \gamma + \gamma^{-1} \cdot \lambda_B = \delta_{\boldsymbol{\mathcal{V}}} \quad , \tag{3.15}$$

$$\epsilon_B^k = 0 \quad \text{for} \quad n = 2, 3, \dots \quad . \tag{3.16}$$

It is straightforward to check that other conditions on D_B do not provide additional conditions on the coefficients λ_B and κ_B. We see that the choice of the boundary conditions can be characterized by the choice of a quadratic form κ_B on $\tilde{\boldsymbol{\mathcal{V}}}$

$$D_B = \underline{D} \cdot (\gamma^{-1} \cdot \lambda_B \cdot \underline{\varphi} + \kappa_B \cdot \underline{\pi}) \quad , \tag{3.17}$$

where λ_B is given by normalization (3.15). It means that a field with a zero B-value (i.e. from the space $\boldsymbol{\mathcal{P}}_B$) has a value proportional to a momentum on the boundary with coefficients given by κ_B and λ_B. Similarly to (2.46) we also have

$$\partial\mathcal{F} = \underline{\vartheta} \cdot \underline{\varphi}_B - \underline{\varphi}_B \cdot \underline{\vartheta} \quad . \tag{3.18}$$

The fact that it is possible to characterize the generalized boundary conditions we are interested in by using the value and the momentum on the boundary allows us to restrict to the boundary phase space $\boldsymbol{\mathcal{B}}$. The boundary phase space inherits structures from the space of all field configurations $\boldsymbol{\mathcal{P}}$. We can define an equivalent of the phase space $\boldsymbol{\mathcal{S}}$ (we use the same letter $\boldsymbol{\mathcal{S}}$ to denote it) and spaces $\boldsymbol{\mathcal{B}}_B$ as an equivalent of spaces $\boldsymbol{\mathcal{P}}_B$. They are linear subspaces of the space $\boldsymbol{\mathcal{B}}$. We can also project objects D_B, Δ_B, $\partial\mathcal{F}$ and $\underline{\varphi}$, $\underline{\pi}$, $\underline{\vartheta}$, $\underline{\varphi}_B$, $\underline{\pi}_B$ on the space $\boldsymbol{\mathcal{P}}$ to the space $\boldsymbol{\mathcal{B}}$ using $\underline{\partial\Phi}$ and we use the same letter for them. The subspace $\boldsymbol{\mathcal{S}}$ of the space $\boldsymbol{\mathcal{B}}$ is characterized by the condition

$$\phi \in \boldsymbol{\mathcal{S}} \quad \Leftrightarrow \quad \underline{\vartheta} \diamond \phi = (\underline{\pi} - \gamma \cdot \underline{\varphi}) \diamond \phi = 0 \quad . \tag{3.19}$$

Similarly

$$\phi \in \boldsymbol{\mathcal{B}}_B \quad \Leftrightarrow \quad \underline{\varphi}_B \diamond \phi = (\kappa_B \cdot \underline{\pi} + \gamma^{-1} \cdot \lambda_B \cdot \underline{\varphi}) \diamond \phi = 0 \quad . \tag{3.20}$$

Thanks to (3.18) we see that observables generated by forms $\underline{\varphi}$, $\underline{\vartheta}$ or $\underline{\varphi}_B$, $\underline{\vartheta}$ are canonically conjugate in the sense of the boundary phase space. A generalization of the momentum $\underline{\pi}$ which is canonically conjugate to a generalized boundary value $\underline{\varphi}_B$ will be introduced later.

Spaces of sources

The space of smooth sources $\tilde{\boldsymbol{\mathcal{P}}}$ is the space of smooth densities on Ω. It is clearly a subspace of the distributional sources $\tilde{\boldsymbol{\mathcal{P}}}' = \boldsymbol{\mathcal{P}}^\star$.

In the previous section we have imposed the condition that the support of the projector D_B in the density argument is localized on the boundary $\partial\Omega$. It suggests that we should work with a class of sources broader than the smooth sources $\tilde{\boldsymbol{\mathcal{P}}}$. We should include sources with support on the boundary. For our purposes a sufficiently wide set of sources is the class of sources which are sensitive to some kind of B-value localized on the boundary. We have seen that such sources can be sensitive only to a value and a normal derivative of the field on the boundary. Therefore these sources can be defined as following

$$\partial\tilde{\boldsymbol{\mathcal{J}}} = \{\, J : \exists\, \phi \in \boldsymbol{\mathcal{P}} \quad J = \partial\mathcal{F} \bullet \phi \,\} \quad . \tag{3.21}$$

By $\tilde{\boldsymbol{\mathcal{J}}}$ we denote the class of all generalized sources

$$\tilde{\boldsymbol{\mathcal{J}}} = \partial\tilde{\boldsymbol{\mathcal{J}}} \oplus \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{3.22}$$

It will be useful to introduce subsets of these spaces

$$\begin{aligned}
\tilde{\boldsymbol{\mathcal{I}}} &= \{\, J : \exists\, \phi \in \boldsymbol{\mathcal{P}} \quad J = \phi \bullet \overset{\leadsto}{\mathcal{F}} \,\} \quad , && (3.23)\\
\partial\tilde{\boldsymbol{\mathcal{I}}} &= \{\, J : \exists\, \phi \in \boldsymbol{\mathcal{S}} \quad J = \partial\mathcal{F} \bullet \phi \,\} = \\
&= \{\, J : J \in \partial\tilde{\boldsymbol{\mathcal{J}}} \,\wedge\, \forall\, \phi \in \boldsymbol{\mathcal{S}} \quad J \bullet \phi = 0 \,\} = && (3.24)\\
&= \partial\tilde{\boldsymbol{\mathcal{J}}} \cap \tilde{\boldsymbol{\mathcal{I}}} \quad .
\end{aligned}$$

The class $\tilde{\boldsymbol{\mathcal{J}}}$ is the set of all generalized sources sensitive to any generalized value. Next we introduce the sets of sources connected with fixed choice of the boundary value. The space of all distributional sources $\partial\tilde{\boldsymbol{\mathcal{J}}}_{B}$ which are localized on Ω and sensitive only to the B-value is

$$\begin{aligned}
\partial\tilde{\boldsymbol{\mathcal{J}}}_{B} &= \{\, J : J \in \partial\tilde{\boldsymbol{\mathcal{J}}} \,\wedge\, \forall\, \phi \in \boldsymbol{\mathcal{P}}_{B} \quad J \bullet \phi = 0 \,\} = \\
&= \{\, J : \exists\, j \in \tilde{\boldsymbol{\mathcal{P}}} \quad J = j \bullet D_{B} \,\} \quad .
\end{aligned} \tag{3.25}$$

Similarly we define the space

$$\begin{aligned}
\tilde{\boldsymbol{\mathcal{I}}}_{B} &= \{\, J : \exists\, \phi \in \boldsymbol{\mathcal{P}}_{B} \quad J = \phi \bullet \overset{\leadsto}{\mathcal{F}} \,\} = \\
&= \{\, J : \exists\, j \in \tilde{\boldsymbol{\mathcal{P}}} \quad J = j \bullet \Delta_{B} \,\}
\end{aligned} \tag{3.26}$$

and

$$\tilde{\boldsymbol{\mathcal{J}}}_{B} = \partial\tilde{\boldsymbol{\mathcal{J}}}_{B} \oplus \tilde{\boldsymbol{\mathcal{P}}} = \partial\tilde{\boldsymbol{\mathcal{J}}}_{B} \oplus \tilde{\boldsymbol{\mathcal{I}}}_{B} \quad . \tag{3.27}$$

Feynman Green function

We define $\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ as a projection of $\overset{\leadsto}{\mathcal{F}}$ on $\boldsymbol{\mathcal{P}}_{B}$, i.e.

$$\overset{\vee\vee\vee}{\mathcal{F}}_{B} = \Delta_{B} \bullet \overset{\leadsto}{\mathcal{F}} = \overset{\leftsquigarrow}{\mathcal{F}} \bullet \Delta_{B} \quad . \tag{3.28}$$

Using this definition and the relations above we immediately get

$$\overset{\vee\vee\vee}{\mathcal{F}}_{B} = \overset{\leadsto}{\mathcal{F}} - D_{B} \bullet \partial\mathcal{F} = \overset{\leadsto}{\mathcal{F}} + \underline{\varphi}_{B} \cdot \underline{\vartheta} \quad . \tag{3.29}$$

$\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ is a degenerate symmetric quadratic form on $\boldsymbol{\mathcal{P}}$ which coincides with $\overset{\leadsto}{\mathcal{F}}$ on $\boldsymbol{\mathcal{P}}_{B}$ in the sense of quadratic forms

$$\phi_1 \bullet \overset{\vee\vee\vee}{\mathcal{F}}_{B} \bullet \phi_2 = \phi_1 \bullet \overset{\leadsto}{\mathcal{F}} \bullet \phi_2 = \phi_1 \bullet \overset{\leftsquigarrow}{\mathcal{F}} \bullet \phi_2 \quad \text{for} \quad \phi_1, \phi_2 \in \boldsymbol{\mathcal{P}}_{B} \quad , \tag{3.30}$$

$$\overset{\vee\vee\vee}{\mathcal{F}}_{B} \bullet \phi = 0 \quad \Leftrightarrow \quad \phi \in \boldsymbol{\mathcal{S}} \quad . \tag{3.31}$$

We can understand $\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ also as an operator from the space $\boldsymbol{\mathcal{P}}$ to the space of generalized sources $\tilde{\boldsymbol{\mathcal{J}}}$. Using the definitions (3.26) and (3.28), we see that the range of such an operator is

$$\tilde{\boldsymbol{\mathcal{I}}}_{B} = \{\, J : \exists\, \phi \in \boldsymbol{\mathcal{P}} \quad J = \phi \bullet \overset{\vee\vee\vee}{\mathcal{F}}_{B} \,\} \quad . \tag{3.32}$$

The smallest space of sources which contains all smooth sources and sources generated by $\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ is the space $\tilde{\boldsymbol{\mathcal{J}}}_{B}$.

We can define an inverse $\overset{\vee\vee\vee}{G}_{B}$ of the quadratic form $\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ as a bi-form on $\tilde{\boldsymbol{\mathcal{J}}}_{B}$. More precisely $\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ is non-degenerate on $\boldsymbol{\mathcal{P}}_{B}$ and zero on $\boldsymbol{\mathcal{S}}$. $\overset{\vee\vee\vee}{G}_{B}$ is the inverse of the non-degenerate part of $\overset{\vee\vee\vee}{\mathcal{F}}_{B}$ and is annihilated by the projection on $\boldsymbol{\mathcal{S}}$.

$$\overset{\vee\vee\vee}{G}_{B} \bullet \overset{\vee\vee\vee}{\mathcal{F}}_{B} = \Delta_{B} \quad , \quad D_{B} \bullet \overset{\vee\vee\vee}{G}_{B} = 0 \quad , \quad \overset{\vee\vee\vee}{G}{}_{B}^{\top} = \overset{\vee\vee\vee}{G}_{B} \quad . \tag{3.33}$$

Finally, we call the Feynman Green function G^F_B the restriction of $\overset{\smile\smile\smile}{G}_B$ to the space of smooth sources $\tilde{\boldsymbol{\mathcal{P}}}$

$$G^F_B = \overset{\smile\smile\smile}{G}_B|_{\tilde{\boldsymbol{\mathcal{P}}}\times\tilde{\boldsymbol{\mathcal{P}}}} \quad . \tag{3.34}$$

It can be also viewed as an operator from the space of smooth sources $\tilde{\boldsymbol{\mathcal{P}}}$ to the distributions. It is well known that the range of such an operator lies in the space of smooth fields $\boldsymbol{\mathcal{P}}$. Therefore we can give meaning to expressions such as $J \bullet (G^F_B \bullet j)$ with $j \in \tilde{\boldsymbol{\mathcal{P}}}$ and general $J \in \tilde{\boldsymbol{\mathcal{J}}}$. For example we have

$$D_B \bullet (G^F_B \bullet j) = D_B \bullet \overset{\smile\smile\smile}{G}_B \bullet j = 0 \quad \text{for} \quad j \in \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{3.35}$$

This means that $G^F_B \bullet j \in \boldsymbol{\mathcal{P}}_B$ for $j \in \tilde{\boldsymbol{\mathcal{P}}}$. In the next chapter we will evaluate an action of other sources localized on the boundary on the smoothed Feynman Green function, and we discuss why we cannot consistently extend the Feynman Green function to the whole space $\tilde{\boldsymbol{\mathcal{J}}}$ in both arguments. Let us note that this is the place where we have to be more careful about associativity and domain dependence.

Let us look for a smooth solution with zero B-value $\phi \in \boldsymbol{\mathcal{P}}_B$ of the equation

$$\overset{\smile\smile\smile}{\mathcal{F}}_B \bullet \phi = \overset{\smile\smile\smile}{J}_B \quad , \tag{3.36}$$

where $\overset{\smile\smile\smile}{J}_B \in \tilde{\boldsymbol{\mathcal{I}}}_B$ and therefore has the form

$$\overset{\smile\smile\smile}{J}_B = J \bullet \Delta_B \quad \text{for some} \quad J \in \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{3.37}$$

Using $\overset{\smile\smile\smile}{G}_B$ we can write the solution explicitly as

$$\phi = \overset{\smile\smile\smile}{G}_B \bullet \overset{\smile\smile\smile}{J}_B = \overset{\smile\smile\smile}{G}_B \bullet J = \bar{\phi}_B(J) \quad , \tag{3.38}$$

where

$$\bar{\phi}_B(J) = G^F_B \bullet J \quad \text{for} \quad J \in \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{3.39}$$

Now, equation (3.36) is possible to rewrite, using (3.29) and (2.47), as

$$\overset{\smile\rightarrow}{\mathcal{F}} \bullet \bar{\phi}_B(J) - J = \underline{\varphi}_B \cdot \big(\vartheta(J) - \underline{\vartheta} \bullet \bar{\phi}_B(J)\big) \quad . \tag{3.40}$$

The left side of this equation is a smooth density, and the right side is a source with support localized on the boundary. Therefore both sides have to vanish separately.

$$\overset{\smile\rightarrow}{\mathcal{F}} \bullet \bar{\phi}_B(J) = J \quad , \tag{3.41}$$

$$\underline{\vartheta} \bullet \bar{\phi}_B(J) = \vartheta(J) \quad . \tag{3.42}$$

This means that $\bar{\phi}_B(J)$ is the solution of the equation of motion with zero B-value on the boundary. It is easy to check that (3.42) is a consequence of (3.41), and it represents the "restriction" of the equation of motion to the observables on the boundary.

We can also write down a solution of the equation of motion with given non-zero B-value on the boundary

$$\begin{matrix} \overset{\smile\rightarrow}{\mathcal{F}} \bullet \phi = J \\ \underline{\varphi}_B \bullet \phi = \varphi \end{matrix} \quad \text{where} \quad J \in \tilde{\boldsymbol{\mathcal{P}}},\ \varphi \in \boldsymbol{\mathcal{V}} \qquad \Leftrightarrow \qquad \phi = \bar{\phi}_B(J,\varphi) \overset{\text{def}}{=} G^F_B \bullet J + \underline{D} \cdot \varphi \quad . \tag{3.43}$$

Extension of the field operator on the space $\boldsymbol{\mathcal{P}}$

The quadratic form $\overset{\smile\smile}{\mathcal{F}}_{B}$ is non-degenerate on $\boldsymbol{\mathcal{P}}_{B}$, and it represents the "wave operator" for field configurations with zero B-value on the boundary. Now we would like to find a generalization of the quadratic form $\mathcal{F}_d$ from the action for a general boundary conditions. Such form has to be non-degenerate on all smooth histories, even on histories from the phase space $\boldsymbol{\mathcal{S}}$. Therefore we need to investigate a further extension of $\overset{\smile\smile}{\mathcal{F}}_{B}$ to a quadratic form $\mathcal{F}_b$ non-degenerate on the whole space $\boldsymbol{\mathcal{P}}$. It will be necessary to introduce an additional structure which, as we will see later, corresponds in the quantum case to the fixing of relative phases for some quantum states.

We will assume that $\mathcal{F}_b$ preserves the decomposition $\boldsymbol{\mathcal{P}} = \boldsymbol{\mathcal{P}}_{B} \oplus \boldsymbol{\mathcal{S}}$, and we change the form $\overset{\smile\smile}{\mathcal{F}}_{B}$ only on the phase space $\boldsymbol{\mathcal{S}}$. I.e. we define

$$\mathcal{F}_b = \overset{\smile\smile}{\mathcal{F}}_{B} + \bar{\mathcal{F}}_b \quad , \tag{3.44}$$

where

$$\bar{\mathcal{F}}_b^{\top} = \bar{\mathcal{F}}_b \quad , \quad \Delta_{B} \bullet \bar{\mathcal{F}}_b = 0 \quad , \quad D_{B} \bullet \bar{\mathcal{F}}_b = \bar{\mathcal{F}}_b \quad . \tag{3.45}$$

The index b "includes" the index B and information about an additional structure. $\bar{\mathcal{F}}_b$ is the quadratic form of the classical action — it gives a value of the action on classical solutions of the equation of motion. We assume that $\bar{\mathcal{F}}_b$ is non-degenerate on $\boldsymbol{\mathcal{S}}$.

Next we describe a specific construction of the quadratic forms $\mathcal{F}_b$ and $\bar{\mathcal{F}}_b$ which will be useful in the quantum theory. We show that $\mathcal{F}_b$ is possible to fix by a choice of generalized momentum canonically conjugate with the generalized boundary value.

The *generalized B'-momentum* can be characterized in the same way as a B-value by projectors $D_{B'}$ and $\Delta_{B'}$ on spaces $\boldsymbol{\mathcal{P}}_{B'}$ and $\boldsymbol{\mathcal{S}}$ which satisfy the same conditions listed in the section above. The spaces $\boldsymbol{\mathcal{P}}_{B}$ and $\boldsymbol{\mathcal{P}}_{B'}$ have to be *canonically conjugate*, i.e. it has to be possible to write the symplectic form $\partial\mathcal{F}$ as

$$\partial\mathcal{F} = \overleftarrow{d\mathcal{F}}_{BB'} - \overrightarrow{d\mathcal{F}}_{BB'} \quad , \tag{3.46}$$

where

$$\begin{gathered}
\overrightarrow{d\mathcal{F}}_{BB'} = D_{B} \bullet \overrightarrow{d\mathcal{F}}_{BB'} = \overrightarrow{d\mathcal{F}}_{BB'} \bullet D_{B'} \quad , \\
\Delta_{B} \bullet \overrightarrow{d\mathcal{F}}_{BB'} = 0 \quad , \quad \overrightarrow{d\mathcal{F}}_{BB'} \bullet \Delta_{B'} = 0 \quad , \\
\overleftarrow{d\mathcal{F}}_{BB'} = \overrightarrow{d\mathcal{F}}_{BB'}^{\top} \quad .
\end{gathered} \tag{3.47}$$

Clearly

$$\overrightarrow{d\mathcal{F}}_{BB'} + \overleftarrow{d\mathcal{F}}_{B'B} = 0 \quad . \tag{3.48}$$

For simplicity we will use a cumulative index b for an ordered pair of indices which characterize generalized value and momentum (we write e.g. $b = BB'$). We use the notation $\sim b = B_2B_1$ if $b = B_1B_2$. If some quantity is characterized by a single index of a generalized value but carries a cumulative index, it is sensitive to the first index in the pair (i.e. $\underline{\wp}_b = \underline{\wp}_{B_1}$ if $b = B_1B_2$). Also the b-value means the B_1-value and the b-momentum means the B_2-momentum for $b = B_1B_2$. We fix the meaning of indices d and n as

$$d = DN \quad , \quad n = ND \quad , \quad d = \sim n \quad . \tag{3.49}$$

The meaning of the canonically conjugate spaces will be more clear if we introduce a *form of generalized momentum* — a mapping from $\boldsymbol{\mathcal{P}}$ onto the space $\tilde{\boldsymbol{\mathcal{V}}}$ of densities on the boundary

$$\underline{\pi}_{BB'} : \boldsymbol{\mathcal{P}} \to \tilde{\boldsymbol{\mathcal{V}}} \quad , \quad \underline{\pi}_{BB'} = \underline{D} \bullet \overrightarrow{d\mathcal{F}}_{BB'} \quad . \tag{3.50}$$

We have

$$\underline{\pi}_b \bullet D_{\sim b} = \underline{\pi}_b \quad , \quad \underline{\pi}_b \bullet \Delta_{\sim b} = 0 \quad , \tag{3.51}$$

so $\underline{\pi}_b$ is equivalent to the map $\underline{\varphi}_{\sim b}$ for the $\sim b$-value, except it maps to the space of densities. From (3.46) and (3.10) follows

$$\partial\mathcal{F} = \underline{\pi}_b \cdot \underline{\varphi}_b - \underline{\varphi}_b \cdot \underline{\pi}_b \quad , \tag{3.52}$$

$$\overset{\rightsquigarrow}{d\mathcal{F}}_b = \underline{\varphi}_b \cdot \underline{\pi}_b \quad , \quad \overset{\leftsquigarrow}{d\mathcal{F}}_b = \underline{\pi}_b \cdot \underline{\varphi}_b \quad , \tag{3.53}$$

i.e. linear observables generated by $\underline{\varphi}_b$ and $\underline{\pi}_b$ are canonically conjugate in the sense of the boundary phase space $\boldsymbol{\mathcal{B}}$.

We can classify all possible momenta canonically conjugate with a generalized B-value. Similar to $\underline{\varphi}_b$ we know that $\underline{\pi}_b$ has to be a linear combination of the forms $\underline{\varphi}$ and $\underline{\pi}$ and therefore also a linear combination of $\underline{\varphi}_b$ and $\underline{\vartheta}$, so we can write

$$\underline{\pi}_b = \gamma_b \cdot \underline{\varphi}_b + \underline{\vartheta} = \gamma_b \cdot \left(\gamma^{-1} \cdot (\lambda_b - \gamma \cdot \gamma_b^{-1} \cdot \gamma) \cdot \underline{\varphi} + (\kappa_b + \gamma_b^{-1}) \cdot \underline{\pi}\right) \quad , \tag{3.54}$$

with a non-degenerate symmetric quadratic form γ_b as a coefficient. The symmetry of γ_b and the choice of the trivial coefficient in front of $\underline{\vartheta}$ follows from the conditions (3.52) and (3.18), and non-degeneracy follows from the condition (3.1) for the momentum space $\boldsymbol{\mathcal{P}}_{\sim b}$. It means that all generalized B'-momentum canonically conjugate with a generalized B-value can be characterized by a choice of a quadratic form $\gamma_{BB'}$ on the space $\boldsymbol{\mathcal{V}}$.

We said that the form $\underline{\pi}_b$ plays the role of the form $\underline{\varphi}_{\sim b}$ except for the normalization. The right normalization is given by (3.15), so we obtain

$$\underline{\varphi}_{\sim b} = \underline{\varphi}_b + \gamma_b^{-1} \cdot \underline{\vartheta} = \gamma^{-1} \cdot (\lambda_b - \gamma \cdot \gamma_b^{-1} \cdot \gamma) \cdot \underline{\varphi} + (\kappa_b + \gamma_b^{-1}) \cdot \underline{\pi} \quad , \tag{3.55}$$

i.e.

$$\kappa_{\sim b} = \kappa_b + \gamma_b^{-1} \quad , \quad \lambda_{\sim b} = \lambda_b - \gamma \cdot \gamma_b^{-1} \cdot \gamma \quad . \tag{3.56}$$

We also see that

$$\underline{\pi}_b = \gamma_b \cdot \underline{\varphi}_{\sim b} \quad , \quad \underline{\pi}_b \cdot \underline{D} = \gamma_b \tag{3.57}$$

and

$$\gamma_b + \gamma_{\sim b} = 0 \quad . \tag{3.58}$$

Finally we can define the quadratic form $\bar{\mathcal{F}}_b$

$$\bar{\mathcal{F}}_b = \overset{\rightsquigarrow}{d\mathcal{F}}_b \bullet D_b = D_b \bullet \overset{\leftsquigarrow}{d\mathcal{F}}_b \quad . \tag{3.59}$$

The definition is consistent thanks to equations (3.4) and (3.46). I.e. the form $\bar{\mathcal{F}}_b$ is symmetric. We can also express $\bar{\mathcal{F}}_b$ using quantities on the space $\boldsymbol{\mathcal{V}}$. Using (3.53), (3.54), (3.10) and (3.57) we get

$$\bar{\mathcal{F}}_b = \underline{\varphi}_b \cdot \gamma_b \cdot \underline{\varphi}_b \quad . \tag{3.60}$$

As we expected, it is clear from this expression that the quadratic form $\bar{\mathcal{F}}_b$ is degenerate on $\boldsymbol{\mathcal{P}}_b$ and non-degenerate on $\boldsymbol{\mathcal{S}}$.

From the definition of $\mathcal{F}_b$ follows that

$$\mathcal{F}_b = \overset{\smile\smile\smile}{\mathcal{F}}_b + \bar{\mathcal{F}}_b = \overset{\rightsquigarrow}{\mathcal{F}} + \overset{\rightsquigarrow}{d\mathcal{F}}_b = \overset{\leftsquigarrow}{\mathcal{F}} + \overset{\leftsquigarrow}{d\mathcal{F}}_b \quad . \tag{3.61}$$

Green functions

Now we will introduce new Green functions connected with the structure discussed in the previous chapter. Similar to $\overset{\smile\smile\smile}{G}_B$ we can define inverses of the quadratic forms $\mathcal{F}_b$ and $\bar{\mathcal{F}}_b$ by

$$\bar{G}_b \bullet \bar{\mathcal{F}}_b = D_b \quad , \quad \bar{G}_b^\top = \bar{G}_b \quad , \quad \Delta_b \bullet \bar{G}_b = 0 \quad , \tag{3.62}$$

$$G_b \bullet \mathcal{F}_b = \delta \quad , \quad G_b^\top = G_b \quad , \quad G_b = \overset{\smile\smile\smile}{G}_b + \bar{G}_b \quad . \tag{3.63}$$

Here G_b, $\bar{G}_b$ and $\overset{\smile\smile\smile}{G}_b$ can be viewed as quadratic forms on the space of sources $\tilde{\boldsymbol{\mathcal{J}}}_b$ or as bi-vectors on the space $\boldsymbol{\mathcal{P}}$ or as operators from $\tilde{\boldsymbol{\mathcal{J}}}_b$ to $\boldsymbol{\mathcal{P}}$.

Because $\bar{G}_b$ as the inverse of $\bar{\mathcal{F}}_b$ on $\boldsymbol{\mathcal{S}}$ is a solution of the homogenous equation of motion in both arguments, we can write it as

$$\bar{G}_b = \underline{D} \cdot \gamma_b^{-1} \cdot \underline{D} \quad . \tag{3.64}$$

From this follows

$$\begin{aligned} &\underline{\varphi}_b \bullet \bar{G}_b \bullet \underline{\varphi}_b = \gamma_b^{-1} \quad , \quad \underline{\varphi}_b \bullet \bar{G}_b \bullet \underline{\pi}_b = \delta_{\boldsymbol{\mathcal{V}}} \quad , \quad \underline{\pi}_b \bullet \bar{G}_b \bullet \underline{\pi}_b = \gamma_b \quad , \\ &\bar{G}_b \bullet \overleftarrow{d\mathcal{F}}_b = D_b \quad , \quad \bar{G}_b \bullet \overleftarrow{d\mathcal{F}}_{\sim b} = -D_{\sim b} \quad , \quad \bar{G}_b \bullet \partial\mathcal{F} = D_b - D_{\sim b} \quad . \end{aligned} \tag{3.65}$$

For a smooth source $J \in \tilde{\boldsymbol{\mathcal{P}}}$ we have

$$\underline{\pi}_{\sim b} \bullet G_b \bullet J = -\underline{D} \bullet J = \vartheta(J) \tag{3.66}$$

and

$$\begin{aligned} \underline{\pi}_b \bullet G_b \bullet J &= (\gamma_b \cdot \underline{\varphi}_b + \underline{\vartheta}) \bullet \overset{\smile\smile\smile}{G}_b \bullet J + \underline{\pi}_b \bullet \bar{G}_b \bullet J = \\ &= \underline{\vartheta} \bullet \overset{\smile\smile\smile}{G}_b \bullet J + \underline{D} \bullet J = \underline{\vartheta} \bullet \bar{\phi}_b(J) - \vartheta(J) = 0 \quad . \end{aligned} \tag{3.67}$$

This means that

$$G_{BB'} \bullet J \in \boldsymbol{\mathcal{P}}_{B'} \quad \text{for} \quad J \in \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{3.68}$$

Further,

$$\overrightarrow{\mathcal{F}} \bullet G_b \bullet J = -\overrightarrow{d\mathcal{F}}_b \bullet G_b \bullet J + \mathcal{F}_b \bullet G_b \bullet J = J \quad . \tag{3.69}$$

Comparing with (3.41) we see that

$$\bar{\phi}_{\sim b}(J) = G_b \bullet J \quad \text{for} \quad J \in \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{3.70}$$

This also means that $G_{\sim b}$ acting on smooth sources coincides with the Feynman Green function G_b^F

$$G_b^F = G_{\sim b}|_{\tilde{\boldsymbol{\mathcal{P}}} \times \tilde{\boldsymbol{\mathcal{P}}}} \quad . \tag{3.71}$$

We have different extensions $\overset{\smile\smile\smile}{G}_B$ and $G_{B'B}$ of the Feynman Green function G_B^F on the spaces $\tilde{\boldsymbol{\mathcal{J}}}_B$ and $\tilde{\boldsymbol{\mathcal{J}}}_{B'}$ which allow us to compute the action of sources localized on the boundary which have a form $j \cdot \underline{\varphi}_B$ or $j \cdot \underline{\varphi}_{B'}$ with $j \in \tilde{\boldsymbol{\mathcal{V}}}$ on the smoothed Feynman Green function. For $J \in \tilde{\boldsymbol{\mathcal{P}}}$ we have

$$\begin{aligned} (j \cdot \underline{\varphi}_B) \bullet (G_B^F \bullet J) &= j \cdot \underline{\varphi}_B \bullet \overset{\smile\smile\smile}{G}_B \bullet J = 0 \quad , \\ (j \cdot \underline{\varphi}_{B'}) \bullet (G_B^F \bullet J) &= j \cdot \underline{\varphi}_{B'} \bullet G_{B'B} \bullet J = -j \cdot \gamma_{B'B}^{-1} \cdot \vartheta(J) \quad . \end{aligned} \tag{3.72}$$

But we cannot consistently define an action of the Feynman Green function on the sources localized on the boundary in both arguments because of problems with an associativity

$$\begin{aligned} \underline{\varphi}_B \bullet (G_B^F \bullet \underline{\varphi}_{B'}) &\overset{\text{def}}{\approx} \underline{\varphi}_B \bullet G_{B'B} \bullet \underline{\varphi}_{B'} = \gamma_{B'B}^{-1} \quad , \\ (\underline{\varphi}_B \bullet G_B^F) \bullet \underline{\varphi}_{B'} &\overset{\text{def}}{\approx} \underline{\varphi}_B \bullet \overset{\smile\smile\smile}{G}_B \bullet \underline{\varphi}_{B'} = 0 \quad . \end{aligned} \tag{3.73}$$

We can give a sense only to the action of the Feynman Green function on the special sources both from the space $\partial\tilde{\boldsymbol{\mathcal{J}}}_B$ or both from the space $\partial\tilde{\boldsymbol{\mathcal{J}}}_{B'}$. Such sources can be written as $j \cdot \underline{\varphi}_B$ or $j \cdot \underline{\varphi}_{B'}$ with $j \in \tilde{\boldsymbol{\mathcal{V}}}$. We can write

$$\begin{aligned} (j_1 \cdot \underline{\varphi}_B) \bullet G_B^F \bullet (\underline{\varphi}_B \cdot j_2) &\overset{\text{def}}{=} (j_1 \cdot \underline{\varphi}_B) \bullet \overset{\smile\smile\smile}{G}_B \bullet (\underline{\varphi}_B \cdot j_2) = 0 \quad , \\ (j_1 \cdot \underline{\varphi}_{B'}) \bullet G_B^F \bullet (\underline{\varphi}_{B'} \cdot j_2) &\overset{\text{def}}{=} (j_1 \cdot \underline{\varphi}_{B'}) \bullet G_{B'B} \bullet (\underline{\varphi}_{B'} \cdot j_2) = j_1 \cdot \gamma_{B'B}^{-1} \cdot j_2 \quad . \end{aligned} \tag{3.74}$$

Specifically, we write down the following applications

$$J \bullet G_b^F \bullet \partial\mathcal{F} = J \bullet G_b^F \bullet \overleftarrow{d\mathcal{F}}_b = -J \bullet D_b \quad , \quad J \bullet G_b^F \bullet \overrightarrow{d\mathcal{F}}_b = 0 \quad , \tag{3.75}$$

$$\overrightarrow{d\mathcal{F}}_b \bullet G_b^F \bullet \overleftarrow{d\mathcal{F}}_b = -\bar{\mathcal{F}}_b \quad , \quad \overleftarrow{d\mathcal{F}}_b \bullet G_b^F \bullet \overrightarrow{d\mathcal{F}}_b = 0 \quad . \tag{3.76}$$

The structure of the boundary phase space

It can be instructive to investigate the projection of the introduced objects on the boundary phase space $\boldsymbol{\mathcal{B}}$. For objects which depends only on the generalized boundary values, as $\bar{\mathcal{F}}_b$, $\underline{\varphi}_b$ or $\underline{\pi}_b$, we do not lose any information, and it is possible to reconstruct fully the original objects on $\boldsymbol{\mathcal{P}}$ from their equivalents on $\boldsymbol{\mathcal{B}}$.

Let $\boldsymbol{\mathcal{P}}_B$ and $\boldsymbol{\mathcal{P}}_{B'}$ be canonically conjugate subspaces of $\boldsymbol{\mathcal{P}}$ and let $\boldsymbol{\mathcal{B}}_B$ and $\boldsymbol{\mathcal{B}}_{B'}$ be their projections on $\boldsymbol{\mathcal{B}}$. We can write

$$\boldsymbol{\mathcal{B}} = \boldsymbol{\mathcal{B}}_B \oplus \boldsymbol{\mathcal{B}}_{B'} \quad . \tag{3.77}$$

Let $\mathsf{P}^-_{BB'}$, $\mathsf{P}^+_{BB'}$ be projectors on $\boldsymbol{\mathcal{B}}_B$, and $\boldsymbol{\mathcal{B}}_{B'}$. It is straightforward to check that

$$\begin{aligned} \mathsf{P}^+_b \diamond \Delta_b = 0 \quad , \quad \mathsf{P}^+_b \diamond D_b = \mathsf{P}^+_b \quad , \\ \mathsf{P}^-_b \diamond \Delta_{\sim b} = 0 \quad , \quad \mathsf{P}^-_b \diamond D_{\sim b} = \mathsf{P}^-_b \quad , \end{aligned} \tag{3.78}$$

$$\overleftarrow{d\mathcal{F}}_b = \mathsf{P}^-_b \diamond \partial\mathcal{F} \diamond \mathsf{P}^+_b \quad , \quad \overrightarrow{d\mathcal{F}}_b = -\mathsf{P}^+_b \diamond \partial\mathcal{F} \diamond \mathsf{P}^-_b \quad , \tag{3.79}$$

$$\partial\mathcal{F} = \mathsf{P}^+_b \diamond \partial\mathcal{F} \diamond \mathsf{P}^-_b + \mathsf{P}^-_b \diamond \partial\mathcal{F} \diamond \mathsf{P}^+_b \quad . \tag{3.80}$$

Projectors $\mathsf{P}^\pm_b$ can be represented as

$$\begin{aligned} \mathsf{P}^+_b = \underline{\mathsf{P}}_b \cdot \underline{\varphi}_b \quad & \text{where} \quad \underline{\varphi}_b \cdot \underline{\mathsf{P}}_b = \delta_{\boldsymbol{\mathcal{V}}} \quad , \quad \underline{\pi}_b \cdot \underline{\mathsf{P}}_b = 0 \quad , \\ \mathsf{P}^-_b = \underline{\tilde{\mathsf{P}}}_b \cdot \underline{\pi}_b \quad & \text{where} \quad \underline{\pi}_b \cdot \underline{\tilde{\mathsf{P}}}_b = \delta_{\boldsymbol{\mathcal{V}}} \quad , \quad \underline{\varphi}_b \cdot \underline{\tilde{\mathsf{P}}}_b = 0 \quad . \end{aligned} \tag{3.81}$$

It is straightforward to check that

$$\begin{aligned} \underline{\mathsf{P}}_b = (\underline{\mathsf{P}} \cdot \kappa_{\sim b} - \underline{\tilde{\mathsf{P}}} \cdot \lambda_{\sim b} \cdot \gamma^{-1}) \cdot \gamma_b \quad , \\ \underline{\tilde{\mathsf{P}}}_b = \underline{\mathsf{P}} \cdot \kappa_b - \underline{\tilde{\mathsf{P}}} \cdot \lambda_b \cdot \gamma^{-1} \quad , \end{aligned} \tag{3.82}$$

where

$$\underline{\mathsf{P}} = \underline{\mathsf{P}}_d \quad , \quad \underline{\tilde{\mathsf{P}}} = \underline{\tilde{\mathsf{P}}}_d \tag{3.83}$$

are generators of elements of $\boldsymbol{\mathcal{B}}$ with given value and zero momentum and vice versa.

The pair of spaces $\boldsymbol{\mathcal{B}}_B$ and $\boldsymbol{\mathcal{B}}_{B'}$ can be characterized by a choice of a square root of the *unity operator*,

$$\mathsf{I}_{BB'} = \mathsf{P}^+_{BB'} - \mathsf{P}^-_{BB'} \quad . \tag{3.84}$$

Such an operator satisfies the conditions

$$\mathsf{I}_b \diamond \mathsf{I}_b = \delta_{\boldsymbol{\mathcal{B}}} \quad , \quad \mathsf{I}_b \diamond \partial\mathcal{F} \diamond \mathsf{I}_b = -\partial\mathcal{F} \quad . \tag{3.85}$$

We can define

$$i\Delta\mathcal{F}_b = \partial\mathcal{F} \diamond \mathsf{I}_b \quad , \tag{3.86}$$

and it is easy to check that

$$i\Delta\mathcal{F}_b = \overleftarrow{d\mathcal{F}}_b + \overrightarrow{d\mathcal{F}}_b = \overrightarrow{d\mathcal{F}}_b - \overrightarrow{d\mathcal{F}}_{\sim b} = \mathcal{F}_b - \mathcal{F}_{\sim b} \quad . \tag{3.87}$$

So the quadratic form $\Delta\mathcal{F}_b$ is defined also on $\boldsymbol{\mathcal{P}}$, and we see that

$$\mathcal{F}_b = \overleftrightarrow{\mathcal{F}} + \frac{1}{2} i\Delta\mathcal{F}_b \quad , \quad \mathcal{F}_{\sim b} = \overleftrightarrow{\mathcal{F}} - \frac{1}{2} i\Delta\mathcal{F}_b \quad , \tag{3.88}$$

where

$$\overleftrightarrow{\mathcal{F}} = \frac{1}{2}(\overleftarrow{\mathcal{F}} + \overrightarrow{\mathcal{F}}) = \frac{1}{2}(\mathcal{F}_b + \mathcal{F}_{\sim b}) \quad . \tag{3.89}$$

4 Complex boundary conditions and complex structure

Complex structure on a linear phase space

In the previous sections we have studied a wide class of boundary conditions of a Laplace-like operator. They can be characterized by subspaces $\boldsymbol{\mathcal{P}}_B$ in the boundary phase space $\boldsymbol{\mathcal{P}}$. Thanks to the linearity of this space we can introduce a *complex variant of the boundary condition* described by subspaces in the complexified space $\boldsymbol{\mathcal{P}}^{\mathbb{C}}$.

The complex boundary conditions will play a key role in the definition of Fock quantization of the scalar field. They provide us with a general *positive-negative frequency splitting*. Because the frequency splitting and the Fock quantization is not necessarily connected with the scalar field, we define these notions for a general linear symplectic space. We will return to the realization on the boundary phase space in the next sections.

To define a general positive-negative frequency splitting we use a complex analog of the objects described in the previous section. We introduce the *complex structure* J_p and projectors $\mathsf{P}_p^{\pm}$ as an equivalent of the unity operator I_b and the projectors $\mathsf{P}_b^{\pm}$. We will look at this analogy in more detail later.

So, let us assume that we have a vector space $\boldsymbol{\mathcal{G}}$ with a symplectic structure $\overleftrightarrow{\omega}$. We denote by $\circ$ the contraction over vector indices. (In the next chapters $(\boldsymbol{\mathcal{G}}, \overleftrightarrow{\omega}, \circ)$ will be realized as both the boundary phase space $(\boldsymbol{\mathcal{B}}, \partial\mathcal{F}, \diamond)$ and the covariant phase space $(\boldsymbol{\mathcal{S}}, \overleftrightarrow{\omega}, \circ)$.) First we turn the space $\boldsymbol{\mathcal{G}}$ to a complex space. It will be the same as the real vector space but we define additionally a multiplication $\star$ by a complex number inside of $\boldsymbol{\mathcal{G}}$

$$i \star \phi = \mathsf{J}_p \circ \phi \quad . \tag{4.1}$$

Here J_p is an operator on $\boldsymbol{\mathcal{G}}$ which satisfies

$$\mathsf{J}_p \circ \mathsf{J}_p = -\delta_{\boldsymbol{\mathcal{G}}} \quad . \tag{4.2}$$

Such operator is called a complex structure on the vector space $\boldsymbol{\mathcal{G}}$. There exist a lot of different complex structures on $\boldsymbol{\mathcal{G}}$, and we will discuss their relation in chapter 8. At this moment we pick up one and we use the index p for all quantities which depend on this complex structure. If we want to stress the additional complex structure of the phase space we denote it as $\boldsymbol{\mathcal{G}}_p$.

Next we define a positive definite product on $\boldsymbol{\mathcal{G}}_p$. This is possible to do if we assume that J_p possesses the following properties:

$$\mathsf{J}_p \circ \overleftrightarrow{\omega} \circ \mathsf{J}_p = \overleftrightarrow{\omega} \quad \text{or} \quad \mathsf{J}_p \circ \overleftrightarrow{\omega} = -\overleftrightarrow{\omega} \circ \mathsf{J}_p \quad , \tag{4.3}$$

$$\bar{\omega}_p = \mathsf{J}_p \circ \overleftrightarrow{\omega} \quad \text{is positive definite} \quad . \tag{4.4}$$

The first property is called compatibility of J_p with the symplectic structure $\overleftrightarrow{\omega}$. Let's note that if J_p is compatible with $\overleftrightarrow{\omega}$, the bi-form $\bar{\omega}_p$ is automatically symmetric

$$\bar{\omega}_p = \bar{\omega}_p^{\top} \quad . \tag{4.5}$$

Let assume that J_p satisfies both conditions (4.3) and (4.4). Now we can define a *scalar product on* $\boldsymbol{\mathcal{G}}$ by

$$\langle \phi_1, \phi_2 \rangle_p = \phi_1 \circ \frac{1}{2}(\bar{\omega}_p - i \overset{\leftrightsquigarrow}{\omega}) \circ \phi_2 \quad . \tag{4.6}$$

It is linear in the second argument, antilinear in the first argument, and positive definite.

$$\langle i \star \phi_1, \phi_2 \rangle_p = -i \langle \phi_1, \phi_2 \rangle_p \quad , \quad \langle \phi_1, i \star \phi_2 \rangle_p = i \langle \phi_1, \phi_2 \rangle_p \quad , \tag{4.7}$$

$$\langle \phi, \phi \rangle_p = \frac{1}{2} \phi \circ \bar{\omega}_p \circ \phi > 0 \quad \text{for} \quad \phi \neq 0 \quad . \tag{4.8}$$

The introduced complex structure allows us to define a *positive-negative frequency splitting* of an element from $\boldsymbol{\mathcal{G}}$. J_p as the operator on $\boldsymbol{\mathcal{G}}$ does not have eigenvectors in $\boldsymbol{\mathcal{G}}$, but it has eigenvectors in the complexification $\boldsymbol{\mathcal{G}}^{\mathbb{C}} = \mathbb{C} \otimes \boldsymbol{\mathcal{G}}$ of the phase space. Its eigenvalues are $\pm i$ (because squares of them have to be -1), and we can explicitly write projectors on subspaces $\boldsymbol{\mathcal{G}}_p^{\pm}$ of $\boldsymbol{\mathcal{G}}^{\mathbb{C}}$ with these eigenvalues

$$\mathsf{P}_p^{\pm} = \frac{1}{2}(\delta_{\boldsymbol{\mathcal{G}}} \mp i \mathsf{J}_p) \quad . \tag{4.9}$$

They have the properties

$$\begin{gathered} \mathsf{J}_p \circ \mathsf{P}_p^{+} = i \mathsf{P}_p^{+} \quad , \quad \mathsf{J}_p \circ \mathsf{P}_p^{-} = -i \mathsf{P}_p^{-} \quad , \\ \mathsf{P}_p^{\pm} \circ \mathsf{P}_p^{\pm} = \mathsf{P}_p^{\pm} \quad , \quad \mathsf{P}_p^{\pm} \circ \mathsf{P}_p^{\mp} = 0 \quad , \quad \mathsf{P}_p^{\pm *} = \mathsf{P}_p^{\mp} \quad , \\ \mathsf{P}_p^{+} + \mathsf{P}_p^{-} = \delta_{\boldsymbol{\mathcal{G}}} \quad , \quad i(\mathsf{P}_p^{+} - \mathsf{P}_p^{-}) = \mathsf{J}_p \quad . \end{gathered} \tag{4.10}$$

The compatibility (4.3) of J_p and $\overset{\leftrightsquigarrow}{\omega}$ is possible to reformulate as

$$\mathsf{P}_p^{\pm} \circ \overset{\leftrightsquigarrow}{\omega} = \overset{\leftrightsquigarrow}{\omega} \circ \mathsf{P}_p^{\mp} \tag{4.11}$$

or

$$\mathsf{P}_p^{\pm} \circ \overset{\leftrightsquigarrow}{\omega} \circ \mathsf{P}_p^{\pm} = 0 \quad , \quad \overset{\leftrightsquigarrow}{\omega} = \mathsf{P}_p^{-} \circ \overset{\leftrightsquigarrow}{\omega} \circ \mathsf{P}_p^{+} + \mathsf{P}_p^{+} \circ \overset{\leftrightsquigarrow}{\omega} \circ \mathsf{P}_p^{-} \quad . \tag{4.12}$$

Similarly

$$\mathsf{P}_p^{\pm} \circ \bar{\omega}_p \circ \mathsf{P}_p^{\pm} = 0 \quad , \quad \bar{\omega}_p = \mathsf{P}_p^{-} \circ \bar{\omega}_p \circ \mathsf{P}_p^{+} + \mathsf{P}_p^{+} \circ \bar{\omega}_p \circ \mathsf{P}_p^{-} \quad , \tag{4.13}$$

We will call the *positive* or *negative frequency part*, respectively, of the element ϕ of the phase space $\boldsymbol{\mathcal{G}}$ the complex vector ϕ_p^{+} or ϕ_p^{-} defined by

$$\phi_p^{\pm} = \mathsf{P}_p^{\pm} \circ \phi \quad . \tag{4.14}$$

We have

$$\phi = \phi_p^{+} + \phi_p^{-} \quad , \quad \mathsf{J}_p \circ \phi = i(\phi_p^{+} - \phi_p^{-}) \quad , \quad \phi_p^{\pm *} = \phi_p^{\mp} \quad . \tag{4.15}$$

The scalar product is possible to write as

$$\langle \phi_1, \phi_2 \rangle_p = {\phi_1}_p^{-} \circ \bar{\omega}_p \circ {\phi_2}_p^{+} = -i \, {\phi_1}_p^{-} \circ \overset{\leftrightsquigarrow}{\omega} \circ {\phi_2}_p^{+} \tag{4.16}$$

Note that not all linear operators on $\boldsymbol{\mathcal{G}}$ are also p-linear on $\boldsymbol{\mathcal{G}}_p$. *$p$-linearity* of an operator L means that L is linear with respect of multiplication $\star$. Therefore it has to commute with multiplication by the imaginary unity which is given by the action of the complex structure J_p, i.e.

$$L \circ \mathsf{J}_p = \mathsf{J}_p \circ L \tag{4.17}$$

or equivalently

$$L \circ \mathsf{P}_p^{\pm} = \mathsf{P}_p^{\pm} \circ L \quad \Leftrightarrow \quad L = \mathsf{P}_p^{-} \circ L \circ \mathsf{P}_p^{-} + \mathsf{P}_p^{+} \circ L \circ \mathsf{P}_p^{+} \quad . \tag{4.18}$$

Similarly p-*antilinearity* of an operator A is equivalent to

$$A \circ \mathsf{J}_p = -\mathsf{J}_p \circ A \tag{4.19}$$

or

$$A \circ \mathsf{P}_p^{\pm} = \mathsf{P}_p^{\mp} \circ A \quad \Leftrightarrow \quad A = \mathsf{P}_p^{-} \circ A \circ \mathsf{P}_p^{+} + \mathsf{P}_p^{-} \circ A \circ \mathsf{P}_p^{+} \quad . \tag{4.20}$$

We introduce the hermitian conjugation $L^{\langle\dagger\rangle}$ of a p-linear operator L defined by

$$\langle \phi_1 \circ L^{\langle\dagger\rangle}, \phi_2 \rangle_p = \langle \phi_1, L \circ \phi_2 \rangle_p \quad . \tag{4.21}$$

It can be written explicitly as (remember $\overset{\leftrightsquigarrow}{\omega}^{-1} \circ \overset{\leftrightsquigarrow}{\omega} = -\delta_{\boldsymbol{\mathcal{G}}}$)

$$L^{\langle\dagger\rangle} = -\overset{\leftrightsquigarrow}{\omega}^{-1} \circ L \circ \overset{\leftrightsquigarrow}{\omega} \quad , \tag{4.22}$$

and we see that it depends on the choice of J_p only through the p-linearity condition on L. Similarly we can define the transposition $A^{\langle\top\rangle}$ for a p-antilinear operator A by

$$\langle \phi_1 \circ A^{\langle\top\rangle}, \phi_2 \rangle_p^* = \langle \phi_1, A \circ \phi_2 \rangle_p \tag{4.23}$$

or

$$A^{\langle\top\rangle} = \overset{\leftrightsquigarrow}{\omega}^{-1} \circ A \circ \overset{\leftrightsquigarrow}{\omega} \quad . \tag{4.24}$$

Both these operator are particular cases of the transposition O^{T_p} of any operator O on $\boldsymbol{\mathcal{G}}$ defined using the bi-form $\bar{\omega}_p$:

$$O^{\mathrm{T}_p} = \bar{\omega}_p^{-1} \circ O \circ \bar{\omega}_p \quad , \tag{4.25}$$

$$\begin{aligned} L^{\langle\dagger\rangle} &= L^{\mathrm{T}_p} \quad \text{for} \quad L \quad p\text{-linear} \quad , \\ A^{\langle\top\rangle} &= A^{\mathrm{T}_p} \quad \text{for} \quad A \quad p\text{-antilinear} \quad . \end{aligned} \tag{4.26}$$

This operation depends on the choice of J_p explicitly.

Let us note that we can choose a p-orthonormal $\mathbb{C}$-base $\mathbf{u} = \{u_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$ in $\boldsymbol{\mathcal{G}}_p$ where k is an index from some, for simplicity discrete, set $\mathcal{I}$. p-orthonormality means

$$\langle u_{\mathrm{k}}, u_{\mathrm{l}} \rangle_p = \delta_{\mathrm{kl}} \quad . \tag{4.27}$$

The $\mathbb{C}$-base is a set $\mathbf{u}$ that is complete in the Hilbert space $\boldsymbol{\mathcal{G}}_p$, i.e. in the vector space with multiplication $\star$. The set $\{u_{\mathrm{k}}{}_p^{+}, u_{\mathrm{k}}{}_p^{-}; \mathrm{k} \in \mathcal{I}\}$ of positive and negative frequency parts of vectors u_{k} forms a complete set in $\boldsymbol{\mathcal{G}}^{\mathbb{C}}$ with the properties

$$\begin{gathered} u_{\mathrm{k}}{}_p^{\pm} \circ \overset{\leftrightsquigarrow}{\omega} \circ u_{\mathrm{l}}{}_p^{\pm} = 0 \quad , \quad -i u_{\mathrm{k}}{}_p^{-} \circ \overset{\leftrightsquigarrow}{\omega} \circ u_{\mathrm{l}}{}_p^{+} = \delta_{\mathrm{kl}} \quad , \\ u_{\mathrm{k}}{}_p^{\pm *} = u_{\mathrm{l}}{}_p^{\mp} \quad . \end{gathered} \tag{4.28}$$

Characterization using value and momentum

Let us assume that we have defined a value and a momentum in our phase space $\boldsymbol{\mathcal{G}}$ — i.e we have a canonically conjugate pair of subspaces $\boldsymbol{\mathcal{G}}_{\scriptscriptstyle D}$, $\boldsymbol{\mathcal{G}}_{\scriptscriptstyle N}$ generated by a $\boldsymbol{\mathcal{V}}$-valued form $\underline{\varphi}$ and a $\tilde{\boldsymbol{\mathcal{V}}}$-valued form $\underline{\pi}$ which satisfy

$$\overset{\leftrightsquigarrow}{\omega} = \underline{\pi} \cdot \underline{\varphi} - \underline{\varphi} \cdot \underline{\pi} \quad . \tag{4.29}$$

As before we can define the generator $\underline{\mathsf{P}}$ of vectors with given value and zero momentum and the generator $\underline{\tilde{\mathsf{P}}}$ of vectors with given momentum and zero value (see (3.83)). We can decompose the complex structure to objects acting on the value space $\boldsymbol{\mathcal{V}}$. Using properties (4.2) and (4.3) we get

$$\mathsf{J}_p = \underline{\mathsf{P}} \cdot \mathcal{A}_p \cdot \underline{\varphi} - \underline{\mathsf{P}} \cdot \mathcal{B}_p \cdot \underline{\pi} + \underline{\tilde{\mathsf{P}}} \cdot \mathcal{C}_p \cdot \underline{\varphi} - \underline{\tilde{\mathsf{P}}} \cdot \mathcal{A}_p \cdot \underline{\pi} \quad , \tag{4.30}$$

where $\mathcal{A}_p$ is an operator on $\boldsymbol{\mathcal{V}}$, $\mathcal{B}_p$ and $\mathcal{C}_p$ are non-degenerate symmetric quadratic forms on $\tilde{\boldsymbol{\mathcal{V}}}$ and $\boldsymbol{\mathcal{V}}$ which satisfy

$$\begin{gathered}\mathcal{B}_p = \mathcal{B}_p^\top \quad , \quad \mathcal{C}_p = \mathcal{C}_p^\top \quad , \\ \mathcal{A}_p \cdot \mathcal{B}_p = \mathcal{B}_p \cdot \mathcal{A}_p \quad , \quad \mathcal{A}_p \cdot \mathcal{C}_p = \mathcal{C}_p \cdot \mathcal{A}_p \quad , \\ \mathcal{B}_p \cdot \mathcal{C}_p = \mathcal{C}_p \cdot \mathcal{B}_p = \delta_{\boldsymbol{\mathcal{V}}} + \mathcal{A}_p \cdot \mathcal{A}_p \quad .\end{gathered} \tag{4.31}$$

Now we can get

$$\begin{aligned}\tilde{\tilde{\omega}} &= i\underline{\psi}_p^- \cdot 2\mathcal{B}_p^{-1} \cdot \underline{\psi}_p^+ - i\underline{\psi}_p^+ \cdot 2\mathcal{B}_p^{-1} \cdot \underline{\psi}_p^- \quad , \\ \bar{\omega}_p &= \underline{\varphi} \cdot \mathcal{C}_p \cdot \underline{\varphi} - \underline{\pi} \cdot \mathcal{A}_p \cdot \underline{\varphi} - \underline{\varphi} \cdot \mathcal{A}_p \cdot \underline{\pi} + \underline{\pi} \cdot \mathcal{B}_p \cdot \underline{\pi} = \\ &= \underline{\psi}_p^- \cdot 2\mathcal{B}_p^{-1} \cdot \underline{\psi}_p^+ + \underline{\psi}_p^+ \cdot 2\mathcal{B}_p^{-1} \cdot \underline{\psi}_p^- \quad ,\end{aligned} \tag{4.32}$$

$$\mathsf{P}_p^+ = \frac{1}{2}(\underline{\mathsf{P}} + i\underline{\tilde{\mathsf{P}}} \cdot \theta_p)^* \cdot \mathcal{B}_p \cdot (\theta_p \cdot \underline{\varphi} + i\underline{\pi}) = (\underline{\mathsf{P}} + i\underline{\tilde{\mathsf{P}}} \cdot \theta_p)^* \cdot \underline{\psi}_p^+ \quad , \tag{4.33}$$

$$\frac{1}{2}(\bar{\omega} - i\tilde{\tilde{\omega}}) = \frac{1}{2}(\underline{\varphi} \cdot \theta_p + i\underline{\pi})^* \cdot \mathcal{B}_p \cdot (\theta_p \cdot \underline{\varphi} + i\underline{\pi}) = \underline{\psi}_p^- \cdot 2\mathcal{B}_p^{-1} \cdot \underline{\psi}_p^+ \quad , \tag{4.34}$$

where θ_p is a complex symmetric non-degenerate quadratic form on $\boldsymbol{\mathcal{V}}$ defined as

$$\theta_p = \mathcal{B}_p^{-1} \cdot (\delta_{\boldsymbol{\mathcal{V}}} - i\mathcal{A}_p) = \mathcal{C}_p \cdot (\delta_{\boldsymbol{\mathcal{V}}} + i\mathcal{A}_p)^{-1} \tag{4.35}$$

and

$$\begin{aligned}\underline{\psi}_p^+ &= \underline{\varphi} \circ \mathsf{P}_p^+ = \frac{1}{2}\mathcal{B}_p \cdot (\theta_p \cdot \underline{\varphi} + i\underline{\pi}) \quad , \\ \underline{\psi}_p^- &= \underline{\varphi} \circ \mathsf{P}_p^- = \frac{1}{2}\mathcal{B}_p \cdot (\theta_p^* \cdot \underline{\varphi} - i\underline{\pi}) \quad .\end{aligned} \tag{4.36}$$

The forms $\underline{\psi}_p^+$ and $\underline{\psi}_p^-$ gives the value of the positive and negative frequency parts. We can also write conditions on the spaces $\boldsymbol{\mathcal{G}}_p^+$, $\boldsymbol{\mathcal{G}}_p^-$ in terms of the value and momentum

$$\begin{aligned}\phi \in \boldsymbol{\mathcal{G}}_p^- \quad &\Leftrightarrow \quad (\theta_p \cdot \underline{\varphi} + i\underline{\pi}) \circ \phi = 0 \quad , \\ \phi \in \boldsymbol{\mathcal{G}}_p^+ \quad &\Leftrightarrow \quad (\theta_p^* \cdot \underline{\varphi} - i\underline{\pi}) \circ \phi = 0 \quad ,\end{aligned} \tag{4.37}$$

which can be interpreted in the case of the covariant phase space $\boldsymbol{\mathcal{S}}$ as complex boundary conditions for positive and negative frequency solutions.

Complex boundary conditions

Now we apply the formalism of positive-negative frequency splitting in the case of the boundary phase space $\boldsymbol{\mathcal{B}}$. There the complex structure J_p defines complex subspaces $\boldsymbol{\mathcal{B}}_p^+$, $\boldsymbol{\mathcal{B}}_p^-$ of $\boldsymbol{\mathcal{B}}^{\mathbb{C}}$ with projectors P_p^+, P_p^-. These can be also characterized using quantities on the value space $\boldsymbol{\mathcal{V}}$.

We have mentioned that the complex structure J_p is an analog of the unity operator I_b. We can define such an operator for p-boundary conditions

$$i\mathsf{I}_p = \mathsf{J}_p \quad . \tag{4.38}$$

So we can speak about subspaces of zero p-value or zero p-momentum which turn out to be exactly subspaces of negative or positive frequency parts, i.e. $\boldsymbol{\mathcal{B}}_p^- = \boldsymbol{\mathcal{B}}_p$ and $\boldsymbol{\mathcal{B}}_p^+ = \boldsymbol{\mathcal{B}}_{\sim p}$. The difference is that now the spaces $\boldsymbol{\mathcal{B}}_p$ and $\boldsymbol{\mathcal{B}}_{\sim p}$ are subspaces of the complexification $\boldsymbol{\mathcal{B}}^{\mathbb{C}}$ and they are not chosen independently — they are complex conjugate. We have compensated the expansion to $\boldsymbol{\mathcal{B}}^{\mathbb{C}}$ by imposing the reality condition which can be expressed as

$$\mathsf{J}_p^* = \mathsf{J}_p \quad \text{or} \quad \mathsf{I}_p^* = -\mathsf{I}_p \quad \text{or} \quad \mathsf{P}_p^{+*} = \mathsf{P}_p^- \quad . \tag{4.39}$$

In the boundary phase space $\boldsymbol{\mathcal{B}}$ we have additionally the subspace of physical solutions $\boldsymbol{\mathcal{S}}$ characterized, for example, by the quadratic form γ via (3.19). We can check that $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$ and $\boldsymbol{\mathcal{B}}_p^+$ or $\boldsymbol{\mathcal{B}}_p^-$ do not have common elements. For example an element of $\boldsymbol{\mathcal{B}}_p^-$ has the form $\phi = (\underline{\mathsf{P}} + i\underline{\tilde{\mathsf{P}}} \bullet \theta_p) \bullet \psi$ for some $\psi \in \boldsymbol{\mathcal{V}}$ (see (4.33)) and therefore

$$\underline{\vartheta} \diamond \phi = (i\mathcal{B}_p^{-1} + \mathcal{B}_p^{-1} \bullet \mathcal{A}_p - \gamma) \bullet \psi \neq 0 \quad , \tag{4.40}$$

thanks to the non-degeneracy of $\mathcal{B}_p$. So we can define projectors $\Delta_p = \Delta_p^-$, $D_p = D_p^-$ on subspaces $\boldsymbol{\mathcal{B}}_p = \boldsymbol{\mathcal{B}}_p^-$, $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$ and $\Delta_{\sim p} = \Delta_p^+$, $D_{\sim p} = D_p^+$ on subspaces $\boldsymbol{\mathcal{B}}_{\sim p} = \boldsymbol{\mathcal{B}}_p^+$ and lift their action to the complexified space of field configurations $\boldsymbol{\mathcal{P}}^{\mathbb{C}}$.

One thus defines canonically conjugate subspaces $\boldsymbol{\mathcal{P}}_p = \boldsymbol{\mathcal{P}}_p^-$ and $\boldsymbol{\mathcal{P}}_{\sim p} = \boldsymbol{\mathcal{P}}_p^+$ in $\boldsymbol{\mathcal{P}}^{\mathbb{C}}$, and all objects we have introduced for canonically conjugate pair of real subspaces $\boldsymbol{\mathcal{P}}_b$, $\boldsymbol{\mathcal{P}}_{\sim b}$ can be also defined for the pair of complex subspaces $\boldsymbol{\mathcal{P}}_p$, $\boldsymbol{\mathcal{P}}_{\sim p}$. Specifically we define $\overrightarrow{d\mathcal{F}}_p$, $\overleftarrow{d\mathcal{F}}_p$, $\Delta\mathcal{F}_p$, $\bar{\mathcal{F}}_p$, $\breve{\mathcal{F}}_p$, $\mathcal{F}_p$ and $\breve{G}_p$, $\bar{G}_p$, G_p^F and $\underline{\varphi}_p$, λ_p, κ_p, γ_p.

In the case of the boundary phase space we use the brackets $(\,,)$ for the scalar product (4.6), and we define a similar operation for the real b-boundary condition (but it is not a scalar product on $\boldsymbol{\mathcal{G}}$ in the real case):

$$(\phi_1, \phi_2)_m = -i\phi_1 \diamond \overleftrightarrow{d\mathcal{F}}_m \diamond \phi_2 = \phi_1 \diamond \frac{1}{2}(\mathsf{J}_m \diamond \partial\mathcal{F} - i\partial\mathcal{F}) \diamond \phi_2 \quad , \tag{4.41}$$

where m can be a b or p-like index.

Let us note that the spaces $\boldsymbol{\mathcal{P}}_p^\pm$ contain histories with positive or negative frequency parts *on the boundary* — we have defined the complex structure J_p in the boundary phase space.

Only properties of objects dependent on real or complex boundary conditions which can differ are properties based on the complex conjugation. The main differences can be found in the following list.

$$\begin{array}{ll}
b\text{-conditions} & p\text{-conditions} \\
\mathsf{J}_b^* = -\mathsf{J}_b \quad , \quad \mathsf{I}_b^* = \mathsf{I}_b & \mathsf{J}_p^* = \mathsf{J}_p \quad , \quad \mathsf{I}_p^* = -\mathsf{I}_p = \mathsf{I}_{\sim p} \\
\mathsf{P}_b^{\pm *} = \mathsf{P}_b^\pm & \mathsf{P}_p^{\pm *} = \mathsf{P}_p^\mp = \mathsf{P}_{\sim p}^\pm \\
\overrightarrow{d\mathcal{F}}_b{}^* = \overrightarrow{d\mathcal{F}}_b \quad , \quad \overleftarrow{d\mathcal{F}}_b{}^* = \overleftarrow{d\mathcal{F}}_b & \overrightarrow{d\mathcal{F}}_p{}^* = -\overleftarrow{d\mathcal{F}}_p = \overrightarrow{d\mathcal{F}}_{\sim p} \\
\Delta\mathcal{F}_b^* = -\Delta\mathcal{F}_b & \Delta\mathcal{F}_p^* = \Delta\mathcal{F}_p = -\Delta\mathcal{F}_{\sim p} \\
\mathcal{F}_b^* = \mathcal{F}_b & \mathcal{F}_p^* = \mathcal{F}_{\sim p} \\
 & \operatorname{Re}\mathcal{F}_p = \overleftrightarrow{\mathcal{F}} \quad , \quad \operatorname{Im}\mathcal{F}_p = \frac{1}{2}\Delta\mathcal{F}_p = \frac{1}{2}\mathsf{J}_p \diamond \partial\mathcal{F} \\
\bar{\mathcal{F}}_b{}^* = \bar{\mathcal{F}}_b \quad , \quad \breve{\mathcal{F}}_b{}^* = \breve{\mathcal{F}}_b & \bar{\mathcal{F}}_p{}^* = \bar{\mathcal{F}}_{\sim p} \quad , \quad \breve{\mathcal{F}}_p{}^* = \breve{\mathcal{F}}_{\sim p} \\
(\phi_2, \phi_1)_b = -(\phi_2, \phi_1)_b^* = (\phi_1, \phi_2)_{\sim b}^* & (\phi_2, \phi_1)_p = (\phi_1, \phi_2)_p^* = -(\phi_2, \phi_1)_{\sim p}^*
\end{array} \tag{4.42}$$

Finally, we express the coefficients λ_p, κ_p using the complex structure. Clearly the forms $\underline{\psi}_p^+$ and $\underline{\psi}_p^-$ are operator-proportional to $\underline{\varphi}_p$ and $\underline{\varphi}_{\sim p}$. The right normalization given by (3.15) implies

$$\begin{aligned}
\kappa_p &= (\gamma - i\theta_p)^{-1} \quad , \quad \lambda_p = (\gamma^{-1} + i\theta_p^{-1})^{-1} \quad , \\
\kappa_{\sim p} &= (\gamma + i\theta_p^*)^{-1} \quad , \quad \lambda_{\sim p} = (\gamma^{-1} - i\theta_p^{*-1})^{-1}
\end{aligned} \tag{4.43}$$

and the relation (3.56) gives

$$\begin{aligned}
\gamma_p = -\gamma_{\sim p} &= \frac{1}{2} i \,(\mathcal{C}_p + \gamma \bullet \mathcal{B}_p \bullet \gamma - \gamma \bullet \mathcal{A}_p - \mathcal{A}_p \bullet \gamma) = \\
&= \frac{1}{2} i \,(\gamma + i\theta_p^*) \bullet \mathcal{B}_p \bullet (\gamma - i\theta_p) \quad .
\end{aligned} \tag{4.44}$$

Dependence on the orientation of the hypersurface

Now we will investigate a dependence on the orientation of the boundary. Or more generally, let's assume we are working on a phase space $\boldsymbol{\mathcal{B}}[\Sigma]$ over some oriented hypersurface (not necessary a whole boundary), and we choose a complex structure J_p consistent with the symplectic structure $\partial\mathcal{F}[\Sigma]$. If we change the orientation of the hypersurface, the complex structure J_p is not consistent with $\partial\mathcal{F}[\Sigma]$ any more because of the non-positivity of $\mathsf{J}_p \diamond \partial\mathcal{F}[\Sigma]$. But clearly the complex structure

$$\mathsf{J}_{\sim p} = -\mathsf{J}_p \quad , \tag{4.45}$$

which we already have used above, is consistent with $\partial\mathcal{F}[-\Sigma]$.

Moreover, we define $\underline{\varphi}[\Sigma]$, $\underline{\pi}[\Sigma]$, and we find

$$\begin{gathered}\underline{\pi}[-\Sigma] = -\underline{\pi}[\Sigma] \quad , \\ \mathcal{A}_{\sim p}[-\Sigma] = -\mathcal{A}_p[\Sigma] \quad , \quad \mathcal{B}_{\sim p}[-\Sigma] = \mathcal{B}_p[\Sigma] \quad , \quad \mathcal{C}_{\sim p}[-\Sigma] = \mathcal{C}_p[\Sigma] \quad , \\ \theta_{\sim p}[-\Sigma] = \mathcal{C}_p[\Sigma]^* \quad , \quad \underline{\psi}^{\pm}_{\sim p}[-\Sigma] = \underline{\psi}^{\mp}_{p}[\Sigma]^* \quad .\end{gathered} \tag{4.46}$$

In the case where the domain on which we are working is a sandwich-like region of a globally hyperbolic spacetime, we can represent the boundary phase space as a direct sum of initial and final canonical phase spaces $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$ and $\boldsymbol{\mathcal{B}}_{\mathrm{i}}$ with symplectic structures $\partial\mathcal{F}_{\mathrm{f}}$ and $\partial\mathcal{F}_{\mathrm{i}}$. We will be mainly interested in the complex structures J_p which do not mix these subspaces. I.e., we can write such a complex structure as

$$\mathsf{J}_p = -\mathsf{J}_{p_{\mathrm{f}}} + \mathsf{J}_{p_{\mathrm{i}}} \quad , \tag{4.47}$$

with $\mathsf{J}_{p_{\mathrm{f}}}$ an operator on $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$, and $\mathsf{J}_{p_{\mathrm{i}}}$ an operator on $\boldsymbol{\mathcal{B}}_{\mathrm{i}}$. The minus sign in front of $\mathsf{J}_{p_{\mathrm{f}}}$ is necessary due to the different choices of the orientation of the final hypersurface in the case of final canonical phase space $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$ and in the case of the boundary phase space $\boldsymbol{\mathcal{B}}$.

Therefore the notion of the positive frequency part in the boundary phase space is equivalent to the notion of the positive frequency part on the initial hypersurface and the negative frequency part on the final hypersurface. This explains also a possible confusion that the space of complex solutions $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$ and the space of positive frequency parts (in the sense of the boundary phase space) do not have common elements.

Part II

QFT — Canonical Quantization

5 Configuration quantization

Ideas of quantization

Quantization is a heuristic procedure of a construction of a quantum theory for a given classical theory. Let us have a classical system described by a phase space $\boldsymbol{\mathcal{G}}$ and symplectic structure $\overset{\leftrightarrow}{\omega}$. Observables are functions on $\boldsymbol{\mathcal{G}}$, and the Poisson brackets are given by (B.5). Quantization tells us 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 which 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 $\hat{\mathrm{A}}, \hat{\mathrm{B}}, \hat{\mathrm{C}}$, they should be related by

$$[\hat{\mathrm{A}}, \hat{\mathrm{B}}] \overset{\text{def}}{=} \hat{\mathrm{A}}\hat{\mathrm{B}} - \hat{\mathrm{B}}\hat{\mathrm{A}} = -i\hat{\mathrm{C}} \quad . \tag{5.1}$$

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 some specific class of classical observables and construct the 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 demonstrate quantization for a general example of a classical theory given on a phase space $\boldsymbol{\mathcal{G}}$ which has a cotangent bundle structure $\mathbf{T}^\star\, \boldsymbol{\mathcal{V}}$ as we discussed in chapter 1. The mathematical structure of such a phase space is reviewed in appendix C. Afterwards we apply this method briefly to scalar field theory. But we do not attempt to solve the dynamics of the theory here. We will leave this question for the following chapters.

Let us note that the procedure described below has a well-defined sense for a finite-dimensional configuration space $\boldsymbol{\mathcal{V}}$. Of course, this is not the case for the scalar field, where the configuration space is $\boldsymbol{\mathcal{V}}[\Sigma]$ as defined in chapter 2 — the space of functions on the manifold Σ. The technical problems with generalization to infinite dimensional spaces is one of the reasons why we will not primarily use this type of quantization for a scalar field. But we will apply the formalism to a scalar field, which is, with some effort, possible to do, thanks mainly to linearity of the configuration space $\boldsymbol{\mathcal{V}}$. But it leads to problems with the definition of a “constant measure” on infinite-dimensional spaces which we do not want to investigate.

Algebra of observables

At the end of chapter 1 we have introduced special kinds of observables on the phase space with a cotangent bundle structure. We have defined the observables F_f depending only on “position” (eq. (1.37)) and the observables G_a linear in momentum (eq. (1.38)). Their Poisson brackets are given in (1.39). 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 $\hat{\mathsf{F}}$ and $\hat{\mathsf{G}}$ from the test functions and test vector fields on the configuration space $\boldsymbol{\mathcal{V}}$ to the space of quantum observables $\mathcal{O}$

$$\begin{aligned} \hat{\mathsf{F}}_f \in \mathcal{O} \qquad & \text{for} \quad f \in \mathfrak{F}\boldsymbol{\mathcal{V}} \quad , \\ \hat{\mathsf{G}}_a \in \mathcal{O} \qquad & \text{for} \quad a \in \mathfrak{T}\boldsymbol{\mathcal{V}} \quad , \end{aligned} \tag{5.2}$$

which should be hermitian (for real f and a)

$$\hat{\mathsf{F}}_f^\dagger = \hat{\mathsf{F}}_f \quad , \quad \hat{\mathsf{G}}_a^\dagger = \hat{\mathsf{G}}_a \quad , \tag{5.3}$$

and should satisfy commutation relations motivated by Poisson brackets (1.39)

$$[\hat{\mathsf{F}}_{f_1}, \hat{\mathsf{F}}_{f_2}] = 0 \quad , \tag{5.4}$$

$$[\hat{\mathsf{F}}_f, \hat{\mathsf{G}}_a] = i\hat{\mathsf{F}}_{a\cdot \mathrm{d}f} \quad , \tag{5.5}$$

$$[\hat{\mathsf{G}}_{a_1}, \hat{\mathsf{G}}_{a_2}] = -i\hat{\mathsf{G}}_{[a_1,a_2]} \quad . \tag{5.6}$$

Next we have to formulate the condition that the quantum observables satisfy “the same algebraic relations as the classical ones”. For the observables $\hat{\mathsf{F}}_f$ it is straightforward because they commute — we require that we can take out any algebraic operation g in the argument to the same operation on the observable

$$\hat{\mathsf{F}}_{g(f_1,f_2,\dots)} = g(\hat{\mathsf{F}}_{f_1}, \hat{\mathsf{F}}_{f_2}, \dots) \quad . \tag{5.7}$$

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

$$\hat{\mathsf{G}}_{a_1+\alpha a_2} = \hat{\mathsf{G}}_{a_1} + \alpha\hat{\mathsf{G}}_{a_2} \quad \text{for} \quad \alpha \in \mathbb{R} \quad , \tag{5.8}$$

$$\hat{\mathsf{G}}_{fa} = \hat{\mathsf{F}}_{f^{\frac{1}{2}-i\gamma}}\hat{\mathsf{G}}_a\hat{\mathsf{F}}_{f^{\frac{1}{2}+i\gamma}} \quad \text{for} \quad \gamma \in \mathbb{R} \quad . \tag{5.9}$$

The last condition is an equivalent of the classical expression $\mathsf{G}_{fa} = \mathsf{F}_f\mathsf{G}_a$, but it specifies the ordering of the quantum theory. We have chosen the exponent of the f function in the special form $(\frac{1}{2} - i\gamma)$ and $(\frac{1}{2} + i\gamma)$ to satisfy the hermiticity condition (5.3) with a real constant γ. The ordering condition can be rewritten as

$$\hat{\mathsf{G}}_{fa} = (\frac{1}{2} - i\gamma)\,\hat{\mathsf{F}}_f\hat{\mathsf{G}}_a + (\frac{1}{2} + i\gamma)\,\hat{\mathsf{G}}_a\hat{\mathsf{F}}_f = \frac{1}{2}(\hat{\mathsf{F}}_f\hat{\mathsf{G}}_a + \hat{\mathsf{G}}_a\hat{\mathsf{F}}_f) + \gamma\,\hat{\mathsf{F}}_{a\cdot \mathrm{d}f} \quad . \tag{5.10}$$

Finally we require that the position observables $\hat{\mathsf{F}}_f$ form a complete set of commuting observables

$$\forall f \quad [\hat{\mathsf{F}}_f, \hat{\mathrm{A}}] = 0 \qquad \Rightarrow \qquad \exists g \quad \hat{\mathrm{A}} = \hat{\mathsf{F}}_g \quad . \tag{5.11}$$

Let us note that from these conditions follows

$$\hat{\mathsf{F}}_\alpha = \alpha\hat{\mathbb{1}} \quad \text{for} \quad \alpha \in \mathbb{R} \quad , \tag{5.12}$$

$$\forall f, a \quad [\hat{\mathsf{F}}_f, \hat{\mathrm{A}}] = 0 \quad [\hat{\mathsf{G}}_a, \hat{\mathrm{A}}] = 0 \qquad \Rightarrow \qquad \exists\, \alpha \in \mathbb{R} \quad \hat{\mathrm{A}} = \alpha\hat{\mathbb{1}} \quad . \tag{5.13}$$

Position representation

Next we construct a *position base* in $\mathcal{H}$ on which the action of the operators $\hat{\mathsf{F}}_f$ and $\hat{\mathsf{G}}_a$ is very simple. Or, in other words, we find a realization of the operators $\hat{\mathsf{F}}_f$ and $\hat{\mathsf{G}}_a$, which satisfy the conditions formulated above, as operators on a space of densities on the configuration manifold $\boldsymbol{\mathcal{V}}$.

We have, of course, immediately a candidate for such base. The observables $\hat{\mathsf{F}}_f$ form a complete set of commuting observables, so there exists a base of eigenvectors labeled by position in the configuration space $\boldsymbol{\mathcal{V}}$ such that

$$\hat{\mathsf{F}}_f|pos:\mathrm{x}\rangle = f(\mathrm{x})|pos:\mathrm{x}\rangle \quad . \tag{5.14}$$

Strictly speaking, $|pos:\mathrm{x}\rangle$ are not vectors from the Hilbert space $\mathcal{H}$ but generalized vectors which can be defined, for example, by the conditions that the projectors on them form an operator-valued density on the configuration space. It will be convenient later to give a character of a density of some weight[6] $\alpha \in \mathbb{C}$ to this vectors. I.e., we assume

$$|pos:\mathrm{x}\rangle \in \mathcal{H} \otimes \tilde{\mathbb{C}}^{\alpha}_{\mathrm{x}}\, \boldsymbol{\mathcal{V}} \quad . \tag{5.15}$$

The base of eigenvectors is orthogonal, but to write down a normalization condition we need to be careful. 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 μ on the value space. With such a volume element we can write the orthonormality relation[6]

$$\langle pos:\mathrm{x}|pos:\mathrm{y}\rangle = (\mu^{2\,\mathrm{Re}\,\alpha-1}\delta)(\mathrm{x}|\mathrm{y}) \quad . \tag{5.16}$$

The completeness relation is

$$\hat{\mathbb{1}} = \int_{\boldsymbol{\mathcal{V}}} |pos:.\rangle\langle pos:.|\;\mu^{1-2\,\mathrm{Re}\,\alpha} \quad . \tag{5.17}$$

Let us note that conditions above do not fix the base $|pos:\mathrm{x}\rangle$ uniquely — they fix the base up to an x-dependent phase factor. We will deal with this ambiguity below.

For any vector $|state\rangle \in \mathcal{H}$ we can define a *wave function* — a density of the weight α^* on the configuration space $\boldsymbol{\mathcal{V}}$

$$\Psi_{|state\rangle}(\mathrm{x}) = \langle pos:\mathrm{x}|state\rangle \quad . \tag{5.18}$$

The density μ defines the scalar product on this space which is an isomorphism to the product on the quantum space

$$\langle st1|st2\rangle = (\Psi_{|st1\rangle}, \Psi_{|st2\rangle})_\mu = \int_{\boldsymbol{\mathcal{V}}} \Psi^*_{|st1\rangle}\Psi_{|st2\rangle}\;\mu^{1-2\,\mathrm{Re}\,\alpha} \quad , \tag{5.19}$$

and it induces the hermitian conjugation on operators of densities of weight α

$$(A^\ddagger\psi_1, \psi_2)_\mu = (\psi_1, A\psi_2)_\mu \quad . \tag{5.20}$$

We define the *position representation* of a quantum observable $\hat{\mathrm{A}}$ as an operator $\check{A}$ on wave functions

$$\check{A}\,\Psi_{|state\rangle} = \Psi_{\hat{\mathrm{A}}|state\rangle} \quad . \tag{5.21}$$

Clearly

$$\check{\mathsf{F}}_f = f\delta \quad , \tag{5.22}$$

which can be also written as

$$\hat{\mathsf{F}}_f = \int_{\boldsymbol{\mathcal{V}}} f\,|pos:.\rangle\langle pos:.|\;\mu^{1-2\,\mathrm{Re}\,\alpha} \quad . \tag{5.23}$$

Phase fixing

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

$$\check{\mathsf{G}}_a = -i\overrightarrow{\mathcal{L}}_a \quad , \tag{5.24}$$

where $\overrightarrow{\mathcal{L}}_a$ is 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 $\boldsymbol{\mathcal{V}}$ as

$$\hat{\mathsf{U}}_a(\epsilon) = \exp(-i\epsilon\hat{\mathsf{G}}_a) \quad . \tag{5.25}$$

The commutation relation (5.5) gives us

$$\hat{\mathsf{U}}_a\hat{\mathsf{F}}_f\hat{\mathsf{U}}_a^{-1} = \hat{\mathsf{F}}_{\mathbf{u}_a^\star f} \quad . \tag{5.26}$$

Here $\mathbf{u}_a(\epsilon)$ is a diffeomorphism on $\boldsymbol{\mathcal{V}}$ induced by the vector field a

$$\frac{d}{d\epsilon}\mathbf{u}_a = a \quad , \quad \mathbf{u}_a(\epsilon_1+\epsilon_2) = \mathbf{u}_a(\epsilon_1)\,\mathbf{u}_a(\epsilon_2) \quad , \tag{5.27}$$

and $\mathbf{u}_a^\star$ is a map induced by the diffeomorphism on objects defined on the configuration space. The equation (5.26) gives us

$$\begin{aligned} \hat{\mathsf{F}}_f\,\hat{\mathsf{U}}_a|pos:\mathrm{x}\rangle = \hat{\mathsf{U}}_a\hat{\mathsf{F}}_{\mathbf{u}_a^{\star\,-1}f}|pos:\mathrm{x}\rangle = f(\mathbf{u}_a\mathrm{x})\,\hat{\mathsf{U}}_a|pos:\mathrm{x}\rangle \qquad \Rightarrow \\ \Rightarrow \qquad \hat{\mathsf{U}}_a|pos:\mathrm{x}\rangle \quad \text{is proportional to} \quad |pos:\mathbf{u}_a\mathrm{x}\rangle \quad . \end{aligned} \tag{5.28}$$

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

$$\mathbf{u}_a^\star\Big(\hat{\mathsf{U}}_a\Psi_a(\mathrm{x})|pos:\mathrm{x}\rangle\Big) = \Psi_a(\mathbf{u}_a\mathrm{x})|pos:\mathbf{u}_a\mathrm{x}\rangle \quad , \tag{5.29}$$

where Ψ_a is a function or density on $\boldsymbol{\mathcal{V}}$ which is defined up to a function or density invariant under the action of the diffeomorphism $\mathbf{u}_a$.

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

$$\Psi_a = \mu^{\frac{1}{2}-\alpha}\exp(-i\phi_a) \quad , \tag{5.30}$$

where ϕ_a is a real function on $\boldsymbol{\mathcal{V}}$ defined up to a function constant on the orbits of $\mathbf{u}_a$.

Thanks to the freedom in the choice of Ψ_a, we can write it as a density of the weight $(\frac{1}{2} - \alpha)$ in the form

$$\Psi_a = \mu^{\frac{1}{2}-\alpha}\rho_a\exp(-i\phi_a) \quad , \tag{5.31}$$

with ρ_a, ϕ_a real functions. The differential form of equation (5.29) gives

$$\hat{\mathsf{G}}_a\Big(\mu^{\frac{1}{2}-\alpha}\rho_a\exp(-i\phi_a)|pos:.\rangle\Big) = i\mathcal{L}_a\Big(\mu^{\frac{1}{2}-\alpha}\rho_a\exp(-i\phi_a)|pos:.\rangle\Big) \quad . \tag{5.32}$$

From this follows the position representation of the $\hat{\mathsf{G}}_a$ observables:

$$\check{\mathsf{G}}_a = -i\overrightarrow{\mathcal{L}}_a - i\Big((\frac{1}{2}-\alpha^*)\frac{1}{\mu}\mathcal{L}_a\mu + \frac{1}{\rho_a}\mathcal{L}_a\rho_a + ia\cdot\mathrm{d}\phi_a\Big)\delta \quad . \tag{5.33}$$

The definition (5.20) gives us

$$\overrightarrow{\mathcal{L}}_a^{\,\ddagger} = -\overrightarrow{\mathcal{L}}_a + (2\,\mathrm{Re}\,\alpha - 1)\frac{1}{\mu}(\mathcal{L}_a\mu)\delta \quad . \tag{5.34}$$

The hermiticity (5.3) implies $\check{\mathsf{G}}_a = \check{\mathsf{G}}_a^\ddagger$. Substituting to this condition we obtain

$$\frac{1}{\rho_a}\mathcal{L}_a\rho_a = 0 \quad , \tag{5.35}$$

which means we can choose $\rho_a = 1$, and we have proved statement (5.30).

Finally we show that the function ϕ_a in equation (5.30) has the form

$$\begin{gathered} \phi_a = \varphi + \tilde{\phi}_a \quad , \\ \tilde{\phi}_a(\mathbf{u}_a(\epsilon)\mathrm{x}) - \tilde{\phi}_a(\mathrm{x}) = \gamma\int_0^\epsilon \frac{1}{\mu}(\mathcal{L}_a\mu)d\epsilon \quad , \end{gathered} \tag{5.36}$$

for a real function φ independent of the vector field a.

Let us define a function

$$\lambda_a = a \cdot \mathrm{d}\phi_a - \gamma\frac{1}{\mu}\mathcal{L}_a\mu \quad . \tag{5.37}$$

This allows us to write $\check{\mathsf{G}}_a$ as

$$\check{\mathsf{G}}_a = \check{\mathsf{G}}'_a + \lambda_a\delta \quad , \tag{5.38}$$

$$\check{\mathsf{G}}'_a = -i\overleftrightarrow{\mathcal{L}}_a - i(\frac{1}{2} + i\gamma - \alpha^*)\frac{1}{\mu}(\mathcal{L}_a\mu)\delta \quad . \tag{5.39}$$

It is easy to check that the operators $\check{\mathsf{G}}'_a$ have the same properties as the operators $\check{\mathsf{G}}_a$. Using the consequences of the properties (5.8), (5.9) and (5.6), we get conditions on λ_a:

$$\begin{gathered} \lambda_{a_1+fa_2} = \lambda_{a_1} + f\lambda_{a_2} \quad , \\ \lambda_{[a_1,a_2]} = a \cdot \mathrm{d}\lambda_{a_2} - a_2 \cdot \mathrm{d}\lambda_{a_1} \quad . \end{gathered} \tag{5.40}$$

The first condition implies that $\lambda_a = a \cdot \lambda$ for some form λ on the configuration space $\boldsymbol{\mathcal{V}}$, and the second condition implies that this form is closed: $\mathrm{d}\lambda = 0$. So, if we ignore topological problems (see some comments below), we can rewrite (5.37) as

$$a \cdot \mathrm{d}\phi_a = a \cdot \mathrm{d}\varphi + \gamma\frac{1}{\mu}\mathcal{L}_a\mu \tag{5.41}$$

for some real function φ. Integrating along orbits of $\mathbf{u}_a$, we get the desired (5.36).

If we redefine our position base by the phase factor $\exp(-i\varphi)$, we obtain the position representation for the momentum observables $\check{\mathsf{G}}_a$ in the form (5.39). We see that if we choose the density weight of our position base as

$$\alpha = \frac{1}{2} - i\gamma \quad , \tag{5.42}$$

the position representation reduces to the simple form (5.24). This also allows us to write the action of $\hat{\mathsf{G}}_a$ in the position base:

$$\hat{\mathsf{G}}_a|pos:.\rangle = i\mathcal{L}_a|pos:.\rangle \quad . \tag{5.43}$$

Let us note that for this choice of α we do not need any volume element on $\boldsymbol{\mathcal{V}}$ because the normalization and completeness conditions (5.16) and (5.17) reduce to

$$\langle pos:\mathrm{x}|pos:\mathrm{y}\rangle = \delta(\mathrm{x}|\mathrm{y}) \quad , \quad \hat{\mathbb{1}} = \int_{\boldsymbol{\mathcal{V}}} |pos:.\rangle\langle pos:.| \quad . \tag{5.44}$$

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 assume we have two quantum versions of the basic observables $\hat{\mathsf{F}}_f$, $\hat{\mathsf{G}}_a$ and $\hat{\mathsf{F}}'_f$, $\hat{\mathsf{G}}'_a$ which both satisfy all the conditions formulated above. Clearly we can construct the unitary operator which maps 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 $\hat{\mathsf{G}}_a$ and $\hat{\mathsf{G}}'_a$ which both, together with common position observables $\hat{\mathsf{F}}_f$, satisfy all the conditions above. The commutation relation (5.5) together with completness (5.11) gives

$$\hat{\mathsf{G}}'_a - \hat{\mathsf{G}}_a = \hat{\mathsf{F}}_{\lambda_a} \tag{5.45}$$

for some a-dependent real function λ_a. The linearity (5.8) and the ordering condition (5.9) together with (5.7) gives

$$\lambda_{a_1+fa_2} = \lambda_{a_1} + f\lambda_{a_2} \qquad \Rightarrow \qquad \lambda_a = \lambda \cdot a \tag{5.46}$$

for some form λ on $\boldsymbol{\mathcal{V}}$. The commutation relation (5.6) implies

$$[a_1, a_2] \cdot \lambda = a_1 \cdot \mathrm{d}(a_2 \cdot \lambda) - a_2 \cdot \mathrm{d}(a_1 \cdot \lambda) \qquad \Rightarrow \qquad \mathrm{d}\lambda = 0 \quad . \tag{5.47}$$

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

$$\hat{\mathsf{G}}'_a = \exp(-i\hat{\mathsf{F}}_\varphi)\hat{\mathsf{G}}_a \exp(i\hat{\mathsf{F}}_\varphi) \quad , \tag{5.48}$$

and we see that $\hat{\mathsf{G}}'_a$ and $\hat{\mathsf{G}}_a$ 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 have ignored this possibility in the construction of the position base, and we will not investigate it further here.

Relation between different orderings

Here we will investigate a relation of two different ordering of the momentum observables. Let us assume that ${}^{\gamma_1}\hat{\mathsf{G}}$ and ${}^{\gamma_2}\hat{\mathsf{G}}$ together with position observables $\hat{\mathsf{F}}_f$ satisfy the conditions above with parameter γ_1 or γ_2 in the ordering condition (5.9). Similar to the previous discussion we get

$${}^{\gamma_1}\hat{\mathsf{G}}_a - {}^{\gamma_2}\hat{\mathsf{G}}_a = \hat{\mathsf{F}}_{\tilde{\lambda}_a} \quad , \tag{5.49}$$

$$\tilde{\lambda}_{a_1+\alpha a_2} = \tilde{\lambda}_{a_1} + \alpha\tilde{\lambda}_{a_2} \quad \text{for} \quad \alpha \in \mathbb{R} \quad , \tag{5.50}$$

$$\tilde{\lambda}_{fa} = f\tilde{\lambda}_a + (\gamma_1 - \gamma_2) a \cdot \mathrm{d}f \quad . \tag{5.51}$$

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

$$\tilde{\lambda}_a = (\gamma_1 - \gamma_2)\frac{1}{\mu}\mathcal{L}_a\mu + \lambda_a \quad , \tag{5.52}$$

we find that λ_a satisfies 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. So we have found that different orderings of the momentum observable can be written in the form

$${}^{\gamma}\hat{\mathsf{G}}_a = {}^{0}\hat{\mathsf{G}}_a + \gamma\,\hat{\mathsf{F}}_{\mu^{-1}\mathcal{L}_a\mu} \quad . \tag{5.53}$$

It is easy to check that the μ dependence for fixed γ is of the form discussed in the previous section.

Observables quadratic in momentum

Until now we have discussed only the quantization of observables independent of momentum and linear in momentum. We have seen that these observables are 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 question of the quantization of such observables. I.e., we want to quantize classical observables of the form

$$\mathsf{K}_k(\mathrm{x},\mathrm{p}) = \mathrm{p} \cdot k^{-1}(\mathrm{x}) \cdot \mathrm{p} \quad , \tag{5.54}$$

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

We can formulate the conditions similar to those above for $\hat{\mathsf{F}}_f$ and $\hat{\mathsf{G}}_a$. With a suitable choice of a requirement 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 $\check{\mathsf{K}}_k$ of the quadratic observable is

$$\check{\mathsf{K}}_k = \mathrm{L}_k + \xi \mathcal{R}_k \quad , \tag{5.55}$$

where L_k and $\mathcal{R}_k$ are the Laplace operator and scalar curvature of the metric k. But we will not need this in our work, and therefore we will not discuss it in more detail here.

Scalar field theory

In the case of the scalar field theory we want to apply the previously developed formalism to the quantization of the phase space $\boldsymbol{\mathcal{B}}[\Sigma]$ with Σ a Cauchy hypersurface or the whole boundary of a domain Ω. The space $\boldsymbol{\mathcal{B}}[\Sigma]$ has the structure of a cotangent bundle $\mathbf{T}^\star\, \boldsymbol{\mathcal{V}}[\Sigma]$. This brings good and bad news. The value space $\boldsymbol{\mathcal{V}}[\Sigma]$ is linear, but it is infinite-dimensional. Let's ignore the infinite dimension and do some formal manipulation first.

Linearity allows us to define observables of value and momentum $\hat{\varphi}$ and $\hat{\pi}$ (roughly speaking operators $\hat{\mathrm{x}}$ and $\hat{\mathrm{p}}$ in the previous notations). These are, of course, not well defined objects in the general case but in the case of a linear space $\boldsymbol{\mathcal{V}}$ it is possible to define them as objects from the spaces $\boldsymbol{\mathcal{V}} \otimes \mathcal{O}$ and $\tilde{\boldsymbol{\mathcal{V}}} \otimes \mathcal{O}$. They are connected with general observables $\hat{\mathsf{F}}_f$, $\hat{\mathsf{G}}_a$ from the previous chapters as

$$\begin{gathered} \hat{\mathsf{F}}_f = f(\hat{\varphi}) \quad , \\ \hat{\mathsf{G}}_a = (\frac{1}{2} - i\gamma)\, a(\hat{\varphi}) \cdot \hat{\pi} \;+\; (\frac{1}{2} + i\gamma)\, \hat{\pi} \cdot a(\hat{\varphi}) \quad , \end{gathered} \tag{5.56}$$

where we have used a natural identification of the tangent spaces $\mathbf{T}\,\boldsymbol{\mathcal{V}}$ with $\boldsymbol{\mathcal{V}}$ itself. The value and momentum observables satisfy the canonical commutation relations

$$[\hat{\varphi}, \hat{\pi}] = i\delta_{\boldsymbol{\mathcal{V}}} \hat{\mathbb{1}} \quad . \tag{5.57}$$

We can construct the *value base* normalized to a "constant measure" $\mathfrak{Q}$ on the configuration space $\boldsymbol{\mathcal{V}}$

$$\begin{gathered} \hat{\varphi}|val:\varphi\rangle = \varphi|val:\varphi\rangle \quad \text{for} \quad \varphi \in \boldsymbol{\mathcal{V}} \quad , \\ \hat{\pi}|val:\varphi\rangle = i\,\mathrm{d}|val:\varphi\rangle \quad , \\ \langle val:\varphi_1|val:\varphi_2\rangle = (\mathfrak{Q}^{-1}\delta)(\varphi_1|\varphi_2) \quad , \\ \hat{\mathbb{1}} = \int\limits_{\varphi\in\boldsymbol{\mathcal{V}}} \mathfrak{Q}\, |val:\varphi\rangle\langle val:\varphi| \quad . \end{gathered} \tag{5.58}$$

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

$$\Psi_{|state\rangle}(\varphi) = \langle val:\varphi|state\rangle \quad , \tag{5.59}$$

the scalar product on wave functions is

$$\langle st1|st2\rangle = \int_{\boldsymbol{\mathcal{V}}} \Psi^*_{|st1\rangle}\Psi_{|st2\rangle}\, \mathfrak{Q} \quad , \tag{5.60}$$

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

$$\begin{aligned} \check{\varphi}\, \Psi_{|state\rangle}(\varphi) &= \varphi\Psi_{|state\rangle}(\varphi) \quad , \\ \check{\pi}\, \Psi_{|state\rangle}(\varphi) &= -i\, \mathrm{d}\Psi_{|state\rangle}(\varphi) \quad . \end{aligned} \tag{5.61}$$

The problem is that there is no such thing as a "constant measure" $\mathfrak{Q}$ on the space $\boldsymbol{\mathcal{V}}$, and we do not have a Hilbert space generated by a scalar product on wave functions. The solution of these technical difficulties lies in a restriction of the possible wave functions to those which are sufficiently falling off so the functional integral (5.60) has a sense even if the measure $\mathfrak{Q}$ itself does not have. We will see in the next chapter that it is possible to construct such wave functions — they will be suppressed by a Gaussian exponent — so the integral (5.60) turns into a Gaussian integration which is well defined even for infinite-dimensional spaces.

We stop at this point with the study of the value representation, and we turn to a slightly different way of quantizing the scalar field. We will return to the quantization discussed in this chapter in the beginning of the next part and in the discussion of the quantum mechanics on the boundary for the scalar field.

6 Particle representation

Quantization of the covariant phase space

In this chapter we will quantize the free non-interacting scalar field theory based on the covariant phase formulation. Most of the formalism can be applied to any linear phase space, and we will use this fact in the next part.

But at this moment we want to find a quantum equivalent of observables on the covariant phase space $\boldsymbol{\mathcal{S}}$ — the subspace of the space of all field configurations $\boldsymbol{\mathcal{P}}$ which contains solutions of the free equations of motion (see 2). The situation is simplified by the fact that the space $\boldsymbol{\mathcal{S}}$ is linear. It allows one, similarly to the previous chapter, to quantize first a special kind of observables — observables linear on the space $\boldsymbol{\mathcal{S}}$. It is equivalent to quantization of the basic scalar field observable Φ which can be viewed as a trivial $\boldsymbol{\mathcal{S}}$-valued (or $\boldsymbol{\mathcal{P}}$-valued) function. The quantum version $\hat{\Phi}$ of this observable belongs to the space $\boldsymbol{\mathcal{S}} \otimes \mathcal{O}$. We require it to satisfy the quantum variant of the Poisson brackets (2.24)

$$[\hat{\Phi}, \hat{\Phi}] = -iG_c\hat{\mathbb{1}} \quad , \tag{6.1}$$

where we have used the fact that the causal Green function is constant on the covariant phase space $\boldsymbol{\mathcal{S}}$, so its quantum version is proportional to the unity operator, and we do not have to face any ordering problem yet. The same is true for the quantum versions of the linear observables L_ϕ defined in (2.25)

$$\hat{\mathsf{L}}_\phi = \phi \circ \overleftrightarrow{\omega} \circ \hat{\Phi} \quad , \tag{6.2}$$

$$[\hat{\mathsf{L}}_{\phi_1}, \hat{\mathsf{L}}_{\phi_2}] = -i\phi_1 \circ \overleftrightarrow{\omega} \circ \phi_2 \, \hat{\mathbb{1}} \quad . \tag{6.3}$$

If we realize the space $\boldsymbol{\mathcal{S}}$ as a subspace of the space $\boldsymbol{\mathcal{P}}$, we have additionally the condition

$$\overleftrightarrow{\mathcal{F}} \bullet \hat{\Phi} = 0 \quad . \tag{6.4}$$

Let us note that the quantum variable $\hat{\Phi}$ is not a simple operator-valued solution of the equation of motion (as an element of $\boldsymbol{\mathcal{S}} \otimes \mathcal{O}$) but is rather a distributional object which could be defined, for example, by its smoothed version (6.2).

For quadratic observables

$$A(\Phi) = \frac{1}{2}\, \Phi \circ a \circ \Phi \quad , \tag{6.5}$$

with a a quadratic form on $\boldsymbol{\mathcal{S}}$, we have an ambiguity in the ordering of two $\hat{\Phi}$ observables. However, because the commutator of two observables $\hat{\Phi}$ is proportional to the unit operator, any quantum version of $A(\Phi)$ can be written as

$$\hat{\mathrm{A}} = \frac{1}{2}\, \hat{\Phi} \circ a \circ \hat{\Phi} + \alpha\hat{\mathbb{1}} \quad , \tag{6.6}$$

where the number factor α (maybe infinite) is given by a particular choice of an operator ordering.

Infinite dimensional phase space

Next we want to realize the quantum observables $\hat{\Phi}$ (or more precisely $\hat{\mathsf{L}}_\phi$) defined by the properties above as operators on a space $\mathcal{H}$ which we would ideally like to be a Hilbert space. But first we make a comment about the infinite dimension of the covariant phase space of the scalar field and consequences for the quantum theory. For a finite dimensional phase space a realization of the algebra of linear observables described above would be unique up to unitary equivalence. But there exist unitarily inequivalent representations of the quantum algebra on $\mathcal{H}$ in the case of an infinite dimensional phase space $\boldsymbol{\mathcal{S}}$, and so $\mathcal{H}$ cannot be a Hilbert space.

We will not try to be technically precise in dealing with inequivalent representations, and we will adopt the following intuitive point of view. We will look on $\mathcal{H}$ as a vector space which includes all pure states (i.e. all states from different representations of algebra of observable), with a “scalar product” between any two states (vectors). There exist sets of these states that each forms a Hilbert space, but there are no well-defined unitary operators in the entire space $\mathcal{H}$ which relates one set to another set. We will use formal expressions between states from different sets, but such expressions may not have a well-defined mathematical meaning (e.g., an infinite sum can be divergent).

A mathematically precise approach to this question is algebraic quantization. In this approach the space of states (not necessarily only pure states) is realized as a suitable restriction of the dual of the appropriate algebra of quantum observables. This space contains all possible states and cannot be wholly realized as density matrices on a Hilbert space on which the algebra of observables would be also represented. But we can identify subspaces (called folia) which can be represented as density matrices on a Hilbert space. Pure states from such a folium correspond to the set with well-defined scalar product discussed in the previous paragraph. The difference between different folia means essentially that some states are “too different” to be in the same Hilbert space.

However it is useful keep formally all pure states together in one quantum space $\mathcal{H}$. But we have to be beware of the possibility that some expressions can give ill-defined results — e.g. some expectation values can be infinite. Intuitively, the sets mentioned above represent different “phases” of the same physical system. Physically, for example, a vacuum of one phase contains an infinite mean number of particles of another phase.

For a complete discussion of inequivalent representation see [3,4].

Particles and field

Now we want to find out more about the structure of the space $\mathcal{H}$. To motivate the following construction of the quantum space we will mention a couple of words about the notion of particles.

For the interpretation of a theory we usually need to pick up quantities which are measurable in a physical experiment. This means one needs to find quantities to which a realistic detector coupled to the field is sensitive. But we need even more for understanding a theory. We would like to have an intuitive picture, a more descriptive way how to speak about our quantum system.

A very useful way to describe a quantum field is the language of particles. It is possible to construct special states representing “definite numbers of quanta of field”, and the structure of the theory becomes often much simpler when it is expressed in terms of these states. Particle states do not have to be always straightforwardly measurable quantities — only in special situations it is possible to construct a simple detector sensitive exactly to some particle states. But even in situations when it is not simple to prepare the system in a particle state, it can be useful to use such states for a description of physical processes.

First we have to define what particles are. Here is a short list of some elementary properties of particles:

- discrete nature of particles
- particles as quanta of energy
- definiteness of position or momenta of particles

- measurability by a detector
- a connection with quantization of a relativistic particle

The first property is the property we will use the most in this part. Particles can be counted; they have a piece-like character. We speak about photons because we are able to detect discrete hits on a screen when we illuminate it by a weak electromagnetic field. We speak about quanta of energy in the case of a hydrogen atom because the atom can emit the energy in discrete pieces.

A discrete nature is only one of many properties of classical particles. But we are not speaking about classical particles. We want to construct a useful notion of particles for quantum field theory. And the notion of discrete pieces gives us the weakest sense of the word particle. Or, maybe, it would be better to speak about quanta of the field.

Of course, we can be more restrictive about the notion of particles. As the second item in our list suggests, we could require that particles are quanta of energy - i.e. that some particle states are eigenstates of a Hamiltonian of our system. We will discuss this condition later. Let us only say that this condition picks up a unique notion of particles but, unfortunately, in a general situation we do not have a unique notion of energy.

Similarly, it is difficult to give a well defined sense to the position or momentum of a particle in a general spacetime. Only in the case when our spacetime is sufficiently special we can introduce some generalized momentum operator or find a simple detector sensitive exactly to some kind of particles [5,6]. Localizability is an even more subtle issue.

There exists a completely different way how to construct quantum field theory [7,8] which we will investigate in the last part. It is possible to quantize a relativistic particle using a sum over-histories-approach and to find that transition amplitudes calculated in this way are exactly the same as amplitudes between some particle states of the scalar field theory. This gives us another interesting meaning to particle states.

But in the following construction we will use the notion of particles in the weakest sense of discrete pieces. It is, essentially, only a particular way of construction of a realization of the $\mathcal{H}$ based on a special base which we will call a *particle base*. However, the only formal meaning of this name is that it has the structure of a Fock base.

Fock structure of the quantum space $\mathcal{H}$

Let us concentrate on the basic particle property — the discrete nature of particles. We would like to speak about a state with no particles, about states with one particle, two particles and so on. The representation of this structure in quantum mechanics is well known. We want to find a Fock structure in our quantum space $\mathcal{H}$ which divides $\mathcal{H}$ into subspaces with a vacuum state, one, two and more particle states. As known, the Fock structure can be generated by creation and annihilation operators $\hat{\mathrm{a}}_{\mathrm{k}}^{\dagger}$ and $\hat{\mathrm{a}}_{\mathrm{k}}$ which satisfy the commutation relations

$$[\hat{\mathrm{a}}_{\mathrm{k}}, \hat{\mathrm{a}}_{\mathrm{l}}] = 0 \quad , \quad [\hat{\mathrm{a}}_{\mathrm{k}}^{\dagger}, \hat{\mathrm{a}}_{\mathrm{k}}^{\dagger}] = 0 \quad , \quad [\hat{\mathrm{a}}_{\mathrm{k}}, \hat{\mathrm{a}}_{\mathrm{l}}^{\dagger}] = \alpha_{\mathrm{kl}}\, \hat{\mathbb{1}} \quad , \tag{6.7}$$

where indices k, l label one-particle states and α_{kl} is a transition amplitude between two one-particle states labeled by k and l. So, to find a particle interpretation of the free scalar field theory we need to construct such creation and annihilation operators from our basic observable $\hat{\Phi}$. The construction which we will describe below is motivated by [9].

First we describe the way in which we will label one-particle states. Particles used for the description of a scalar field are scalar particles without any inner degrees of freedom. This means that on the classical level the position and momenta at one time are sufficient for the determination of the state of one particle. Therefore the quantum space $\mathcal{H}_1$ of one-particle states should be "∞^3" dimensional (one vector of a base for each space point) as a *complex* vector space (let's denote it $\mathbb{C}$-dimensionality). It means that as a real vector space it has "the same" $\mathbb{R}$-dimension as the phase space $\boldsymbol{\mathcal{S}}$ of the scalar field — "$2\infty^3$". These formal considerations suggest the use of the space $\boldsymbol{\mathcal{S}}$

for labeling of one-particle states. More precisely, we would like to find a one-to-one map between spaces $\mathcal{H}_1$ and $\boldsymbol{\mathcal{S}}$.

This presents us with a problem. Some vectors in $\mathcal{H}_1$ are related only by a phase and essentially represent the same physical state. But their images (labels) in $\boldsymbol{\mathcal{S}}$ are different. We would like to know how these different labels are related. This means that we need to introduce a structure of a Hilbert space to the phase space $\boldsymbol{\mathcal{S}}$ in such way that our mapping between $\boldsymbol{\mathcal{S}}$ and $\mathcal{H}_1$ will be an isomorphism of Hilbert spaces. But we already described such a structure at the end of the chapter (4) — we are looking for a complex structure J_p on the phase space $\boldsymbol{\mathcal{S}}$ which turns it into the Hilbert space $\boldsymbol{\mathcal{S}}_p$.

Now we can proceed and define creation and annihilation operators acting on $\mathcal{H}$ which are labeled by vectors from $\boldsymbol{\mathcal{S}}$:

$$\begin{aligned} \hat{\mathrm{a}}_p[\phi] &= \langle \phi, \hat{\Phi} \rangle_p \quad , \\ \hat{\mathrm{a}}_p[\phi]^\dagger &= \langle \hat{\Phi}, \phi \rangle_p \end{aligned} \tag{6.8}$$

for any $\phi \in \boldsymbol{\mathcal{S}}$. We can also express creation and annihilation operators using $\mathsf{P}_p^\pm$

$$\begin{aligned} \hat{\mathrm{a}}_p[\phi] &= -i\, \phi_p^- \circ \overleftrightarrow{\omega} \circ \hat{\Phi} = -i\, \phi \circ \overleftrightarrow{\omega} \circ \hat{\Phi}_p^+ \quad , \\ \hat{\mathrm{a}}_p[\phi]^\dagger &= i\, \phi_p^+ \circ \overleftrightarrow{\omega} \circ \hat{\Phi} = i\, \phi \circ \overleftrightarrow{\omega} \circ \hat{\Phi}_p^- \quad . \end{aligned} \tag{6.9}$$

This means that the positive (or negative) frequency part of the field operator $\hat{\Phi}$ is composed only from annihilation (or creation) operators and vice versa. Using these expressions we can compute the commutation relations of the introduced operators. For example,

$$\begin{aligned} \left[\hat{\mathrm{a}}_p[\phi_1], \hat{\mathrm{a}}_p[\phi_2]^\dagger\right] &= -i\, \phi_1 \circ \mathsf{P}_p^- \circ \overleftrightarrow{\omega} \circ \left[\hat{\Phi}, \hat{\Phi}\right] \circ \overleftrightarrow{\omega}^\top \circ \mathsf{P}_p^+ \circ \phi_2\, i = \\ &= \phi_1 \circ \mathsf{P}_p^- \circ \overleftrightarrow{\omega} \circ iG_c \circ \overleftrightarrow{\omega} \circ \mathsf{P}_p^+ \circ \phi_2\, \hat{\mathbb{1}} = -i\, \phi_1 \circ \mathsf{P}_p^- \circ \overleftrightarrow{\omega} \circ \mathsf{P}_p^+ \circ \phi_2\, \hat{\mathbb{1}} = \\ &= \langle \phi_1, \phi_2 \rangle_p\, \hat{\mathbb{1}} \quad . \end{aligned} \tag{6.10}$$

Similarly we get the complete set of commutation relations:

$$\begin{gathered} \left[\hat{\mathrm{a}}_p[\phi_1], \hat{\mathrm{a}}_p[\phi_2]\right] = 0 \quad , \quad \left[\hat{\mathrm{a}}_p[\phi_1]^\dagger, \hat{\mathrm{a}}_p[\phi_2]^\dagger\right] = 0 \quad , \\ \left[\hat{\mathrm{a}}_p[\phi_1], \hat{\mathrm{a}}_p[\phi_2]^\dagger\right] = \langle \phi_1, \phi_2 \rangle_p\, \hat{\mathbb{1}} \quad . \end{gathered} \tag{6.11}$$

We see that these are really the commutation relations of creation and annihilation operators.

We can define a vacuum state by the condition

$$\begin{gathered} \hat{\mathrm{a}}_p[\phi] |p : vac\rangle = 0 \quad \text{for each } \phi \in \boldsymbol{\mathcal{S}} \quad , \\ \langle p : vac | p : vac \rangle = 1 \end{gathered} \tag{6.12}$$

and multiple particle states by

$$\hat{\mathrm{a}}_p[\phi_1]^\dagger \hat{\mathrm{a}}_p[\phi_2]^\dagger \ldots |p : vac\rangle \quad . \tag{6.13}$$

The mapping between the phase space $\boldsymbol{\mathcal{S}}_p$ and the one-particle space $\mathcal{H}_1$ is given by

$$\phi \quad \leftrightarrow \quad \hat{\mathrm{a}}_p[\phi]^\dagger |p : vac\rangle \tag{6.14}$$

and is really an isomorphism of Hilbert spaces

$$\langle p : vac | \hat{\mathrm{a}}_p[\phi_1] \hat{\mathrm{a}}_p[\phi_2]^\dagger | p : vac\rangle = \langle p : vac | [\hat{\mathrm{a}}_p[\phi_1], \hat{\mathrm{a}}_p[\phi_2]^\dagger] | p : vac\rangle = \langle \phi_1, \phi_2 \rangle_p \quad , \tag{6.15}$$

$$i \star \phi \quad \leftrightarrow \quad \hat{\mathrm{a}}_p[i \star \phi]^\dagger\, |p : vac\rangle = i \hat{\mathrm{a}}_p[\phi]^\dagger\, |p : vac\rangle \quad . \tag{6.16}$$

We implicitly assumed that condition (6.12) selects a unique vacuum state (up to a phase) and creation operators acting on the vacuum state generate a complete set of vectors in $\mathcal{H}$. This assumption corresponds to the assumption that the set of observables $\hat{\Phi}$ (or $\hat{\mathsf{L}}_\phi$) is a sufficient set of observables for the description of our system, i.e. that we do not have any other degrees of freedom which are not reflected in the field observables $\hat{\Phi}$. In the opposite case we should use another kind of field.

Finally we can write the linear observables $\hat{\mathsf{L}}_\phi$ using annihilation and creation operators as

$$\hat{\mathsf{L}}_\phi = i(\hat{\mathrm{a}}_p[\phi] - \hat{\mathrm{a}}_p[\phi]^\dagger) = \hat{\mathrm{a}}_p[-\mathsf{J}_p \circ \phi] + \hat{\mathrm{a}}_p[-\mathsf{J}_p\phi]^\dagger) \quad . \tag{6.17}$$

We have successfully found a Fock structure in our quantum space $\mathcal{H}$ with one-particle states labeled by vectors from the classical phase space of the scalar field $\boldsymbol{\mathcal{S}}$. Or, in other words, we have constructed a particular representation of the quantum algebra of observables generated by $\hat{\mathsf{L}}_\phi$ on a Hilbert space given by the Fock space based on one-particle space isomorphic with $\boldsymbol{\mathcal{S}}_p$. We will call such construction a *particle interpretation* of the scalar field theory. For this construction we have used a new element — the complex structure J_p. We can expect that different complex structures can give us different Fock structures in $\mathcal{H}$, and we will investigate their relations in chapter 8.

To conclude, we show a connection to the usual mode decomposition. We choose a p-orthonormal $\mathbb{C}$-base $\mathbf{u} = \{u_\mathrm{k}; \mathrm{k} \in \mathcal{I}\}$ in $\boldsymbol{\mathcal{S}}_p$ with, for simplicity a discrete, index set $\mathcal{I}$, as was discussed before. It satisfies (4.27) and (4.28). These are standard properties [6] of modes which are used for the expansion of a field operator. We can decompose $\hat{\Phi}$ using the base $\{u_{\mathrm{k}}{}^+_p, u_{\mathrm{k}}{}^-_p; \mathrm{k} \in \mathcal{I}\}$

$$\hat{\Phi} = \sum_{\mathrm{k}\in\mathcal{I}} \big(\hat{\mathrm{a}}_\mathrm{k} u_{\mathrm{k}}{}^+_p + \hat{\mathrm{a}}_\mathrm{k}^\dagger u_{\mathrm{k}}{}^-_p\big) \quad , \tag{6.18}$$

where operator valued coefficients can be found using the relations (4.28)

$$\begin{aligned} \hat{\mathrm{a}}_\mathrm{k} &= -i\, u_{\mathrm{k}}{}^-_p \circ \overset{\leftrightsquigarrow}{\omega} \circ \hat{\Phi} = \hat{\mathrm{a}}_p[u_\mathrm{k}] \quad , \\ \hat{\mathrm{a}}_\mathrm{k}^\dagger &= -i\, \hat{\Phi} \circ \overset{\leftrightsquigarrow}{\omega} \circ u_{\mathrm{k}}{}^+_p = \hat{\mathrm{a}}_p[u_\mathrm{k}]^\dagger \quad . \end{aligned} \tag{6.19}$$

We see that the usual mode expansion gives nothing other than our creation and annihilation operators for a chosen base $\mathbf{u}$ in the phase space $\boldsymbol{\mathcal{S}}$. This connection also justifies using the words *positive* and *negative frequency part* respectively for vectors from spaces $\boldsymbol{\mathcal{S}}_p^\pm$.

Green functions

We can ask whether the construction of the Fock structure in $\mathcal{H}$ using the complex structure is not artificial. Does J_p have any physical meaning? Is it connected with any interesting physical quantity? The answer is yes. The complex structure has a rather simple interpretation. To show it we have to introduce Green functions associated with a particular choice of vacuum state. They are tensor objects from $\boldsymbol{\mathcal{S}}_0^2$ which we represents, similarly to the causal Green function, as objects from $\boldsymbol{\mathcal{P}}_0^2$ which satisfy free equation of motion in both indices.

The Wightman functions are defined by

$$\begin{aligned} G_p^{+\boldsymbol{xy}} &= \langle p : vac|\hat{\Phi}^{\boldsymbol{x}}\hat{\Phi}^{\boldsymbol{y}}|p : vac\rangle \quad , \\ G_p^{-\boldsymbol{xy}} &= \langle p : vac|\hat{\Phi}^{\boldsymbol{y}}\hat{\Phi}^{\boldsymbol{x}}|p : vac\rangle \quad . \end{aligned} \tag{6.20}$$

The Hadamard Green function is

$$G_p^{H\boldsymbol{xy}} = \langle p : vac|\hat{\Phi}^{\boldsymbol{x}}\hat{\Phi}^{\boldsymbol{y}} + \hat{\Phi}^{\boldsymbol{y}}\hat{\Phi}^{\boldsymbol{x}}|p : vac\rangle \quad . \tag{6.21}$$

The causal Green function can be written as

$$-iG_c^{\boldsymbol{xy}} = \langle p : vac|\hat{\Phi}^{\boldsymbol{x}}\hat{\Phi}^{\boldsymbol{y}} - \hat{\Phi}^{\boldsymbol{y}}\hat{\Phi}^{\boldsymbol{x}}|p : vac\rangle \quad . \tag{6.22}$$

Relations among these Green functions are

$$
\begin{aligned}
G_p^H &= G_p^+ + G_p^- \quad , \quad G_c = i(G_p^+ - G_p^-) \quad , && (6.23)\\
G_p^+ &= \frac{1}{2}(G_p^H - iG_c) \quad , \quad G_p^- = \frac{1}{2}(G_p^H + iG_c) \quad , && (6.24)\\
G_p^{+\top} &= G_p^- \quad , \quad G_p^{H\top} = G_p^H \quad , \quad G_c{}^\top = -G_c \quad , && (6.25)\\
G_p^{+*} &= G_p^- \quad , \quad G_p^{H*} = G_p^H \quad , \quad G_c{}^* = G_c \quad . && (6.26)
\end{aligned}
$$

Let's note that the causal Green function G_c is independent of the choice of the complex structure J_p, but the Green functions G_p^+, G_p^- and G_p^H depend of the choice of the vacuum state and therefore on the choice of the particle interpretation.

Using the definition of the vacuum state (6.12) and equations (6.9) we can write

$$
G_p^+ = \langle p:vac|(\hat\Phi_p^+ + \hat\Phi_p^-)(\hat\Phi_p^+ + \hat\Phi_p^-)|p:vac\rangle = \langle p:vac|\hat\Phi_p^+\hat\Phi_p^-|p:vac\rangle \quad . \tag{6.27}
$$

This means that

$$
G_p^+ = \mathsf{P}_p^+ \circ G_p^+ \circ \mathsf{P}_p^- \quad , \quad G_p^- = \mathsf{P}_p^- \circ G_p^- \circ \mathsf{P}_p^+ \quad . \tag{6.28}
$$

Using equations (6.23), (4.12) and (4.10) we find

$$
\begin{aligned}
G_p^\pm &= \mp i\, \mathsf{P}_p^\pm \circ G_c \circ \mathsf{P}_p^\mp = \mp i\, \mathsf{P}_p^\pm \circ G_c \quad , && (6.29)\\
G_p^H &= -i\,(\mathsf{P}_p^+ - \mathsf{P}_p^-) \circ G_c = -\mathsf{J}_p \circ G_c = \bar\omega_p^{-1} && (6.30)
\end{aligned}
$$

or

$$
\begin{aligned}
\mathsf{P}_p^\pm &= \mp i\, G_p^\pm \circ \overleftrightarrow{\omega} \quad , && (6.31)\\
\mathsf{J}_p &= G_p^H \circ \overleftrightarrow{\omega} \quad . && (6.32)
\end{aligned}
$$

This means that the complex structure J_p is essentially the Hadamard Green function. Or, more precisely, the action of J_p on a solution $\phi \in \boldsymbol{\mathcal{S}}$ is given by the Klein-Gordon product of the Hadamard Green function with the solution ϕ. Wightman functions are in similar relation to the projection operators $\mathsf{P}_p^\pm$.

We can use this relation to derive compositions laws for Green functions. The translation of equations (4.10), (4.2) to the language of Green functions gives us

$$
\begin{aligned}
G_p^\pm \circ \overleftrightarrow{\omega} \circ G_p^\pm &= \pm i\, G_p^\pm \quad , \quad G_p^\pm \circ \overleftrightarrow{\omega} \circ G_p^\mp = 0 \quad , && (6.33)\\
G_p^H \circ \overleftrightarrow{\omega} \circ G_p^H &= G_c \quad . && (6.34)
\end{aligned}
$$

We have seen that Green functions $G_p^\pm, G_p^H, G_p^F$ are associated with each particle interpretation. The Green functions of the same kind for different particle interpretations satisfy the same equations and symmetry conditions. They differ by boundary conditions. If we choose a Cauchy hypersurface Σ, we can define the value and the momentum forms $\underline{\varphi}[\Sigma]$ and $\underline{\pi}[\Sigma]$. In chapter 4 we have found that the complex structure can be written in the form (4.30), and the positive and negative frequency parts are given by conditions (4.37). So, thanks to (6.28), we can write the conditions on the Wightman Green functions using quantities on the hypersurface Σ,

$$
\begin{aligned}
(\theta_p^* \cdot \underline{\varphi} - i\underline{\pi}) \circ G_p^+ = 0 \quad &, \quad G_p^+ \circ (\underline{\varphi} \cdot \theta_p + i\underline{\pi}) = 0 \quad ,\\
(\theta_p \cdot \underline{\varphi} + i\underline{\pi}) \circ G_p^- = 0 \quad &, \quad G_p^- \circ (\underline{\varphi} \cdot \theta_p^* - i\underline{\pi}) = 0 \quad .
\end{aligned} \tag{6.35}
$$

If the complex structure J_p is chosen using some physical structure *on the hypersurface* Σ (as in the case of the complex structure obtained by diagonalization of the Hamiltonian as will be defined below), these equations gives the meaningful boundary conditions for Wightman Green functions.

Total particle-number observable

We can define a *quantum observable of the number of particles* in a state labeled by a solution ϕ:

$$\hat{\mathrm{n}}_p[\phi] = \frac{\hat{\mathrm{a}}_p[\phi]^\dagger \hat{\mathrm{a}}_p[\phi]}{\langle\phi,\phi\rangle_p} \quad . \tag{6.36}$$

It satisfies

$$\hat{\mathrm{n}}_p[\phi]\, \hat{\mathrm{a}}_p[\phi]^{\dagger\, m} |p : vac\rangle = m\, \hat{\mathrm{a}}_p[\phi]^{\dagger\, m} |p : vac\rangle \quad . \tag{6.37}$$

Let's choose again a p-orthonormal $\mathbb{C}$-base $\mathbf{u} = \{u_\mathrm{k}; \mathrm{k} \in \mathcal{I}\}$ in $\boldsymbol{\mathcal{S}}_p$. It generates an orthonormal base in the quantum space $\mathcal{H}$ composed of *particle states*

$$|p\,\mathbf{u} : \boldsymbol{m}\rangle = \frac{1}{\sqrt{\boldsymbol{m}!}} \hat{\mathrm{a}}_p[\mathbf{u}]^{\dagger\,\boldsymbol{m}} |p : vac\rangle \quad . \tag{6.38}$$

Here $\boldsymbol{m} = \{m_\mathrm{k}; \mathrm{k} \in \mathcal{I}\}$ is a *multi-index* and we are using the shorthand

$$\boldsymbol{m}! = \prod_{\mathrm{k}\in\mathcal{I}} m_\mathrm{k}! \quad , \quad \hat{\mathrm{a}}[\mathbf{u}]^{\dagger\,\boldsymbol{m}} = \prod_{\mathrm{k}\in\mathcal{I}} \hat{\mathrm{a}}_p[u_\mathrm{k}]^{\dagger\, m_\mathrm{k}} = \prod_{\mathrm{k}\in\mathcal{I}} \hat{\mathrm{a}}_\mathrm{k}^{\dagger\, m_\mathrm{k}} \quad , \tag{6.39}$$

where creation operators $\hat{\mathrm{a}}_\mathrm{k}$ are defined by equation (6.19). The combinatoric factor is chosen so that states are normalized:

$$\langle p\,\mathbf{u} : \boldsymbol{m} | p\,\mathbf{u} : \boldsymbol{m'}\rangle = \delta_{\boldsymbol{m}\boldsymbol{m'}} \quad . \tag{6.40}$$

$\boldsymbol{m}$ is also called the *occupation number*, and $\langle p\,\mathbf{u} : \boldsymbol{m}|state\rangle$ and $\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle$ are called the *occupation number representation* or the *particle representation* of a state $|state\rangle$ and an operator $\hat{\mathrm{A}}$.

The observable of the number of particles in a mode u_k is

$$\hat{\mathrm{n}}_{p\,\mathrm{k}} = \hat{\mathrm{n}}_p[u_\mathrm{k}] = \hat{\mathrm{a}}_\mathrm{k}^\dagger \hat{\mathrm{a}}_\mathrm{k} \quad , \tag{6.41}$$

and it satisfies

$$\hat{\mathrm{n}}_{p\,\mathrm{k}} |p\,\mathbf{u} : \boldsymbol{m}\rangle = m_\mathrm{k} |p\,\mathbf{u} : \boldsymbol{m}\rangle \quad . \tag{6.42}$$

Now we can define the *observable of the total number of p-particles*

$$\hat{\mathrm{N}}_p = \sum_{\mathrm{k}\in\mathcal{I}} \hat{\mathrm{n}}_{p\,\mathrm{k}} \quad . \tag{6.43}$$

Using definitions (6.19) of creation and annihilation operators and orthonormality of the base $\mathbf{u}$ we get

$$\hat{\mathrm{N}}_p = \sum_{\mathrm{k}\in\mathcal{I}} \hat{\mathrm{a}}_p[u_\mathrm{k}]^\dagger \hat{\mathrm{a}}_p[u_\mathrm{k}] = \sum_{\mathrm{k}\in\mathcal{I}} \langle\hat{\Phi}, u_\mathrm{k}\rangle_p \langle u_\mathrm{k}, \hat{\Phi}\rangle_p = \langle\hat{\Phi},\hat{\Phi}\rangle_p \quad . \tag{6.44}$$

We see that $\hat{\mathrm{N}}_p$ is independent of the choice of the base $\mathbf{u}$ but it depends on the complex structure J_p through the scalar product and therefore it depends on the particle interpretation. It will be useful to write down also another representation of $\hat{\mathrm{N}}_p$. First let's note that using the commutator relation (6.1), antisymmetry of the symplectic form and definition of causal Green function (2.21) we can get

$$\hat{\Phi} \circ \widetilde{\widetilde{\omega}} \circ \hat{\Phi} = -i\big(\frac{1}{2}\,\mathrm{tr}_{\boldsymbol{\mathcal{S}}}\,\delta_{\boldsymbol{\mathcal{S}}}\big)\, \hat{\mathbb{1}} = -i\big(\mathrm{tr}_{\boldsymbol{\mathcal{S}}_p}\,\delta_{\boldsymbol{\mathcal{S}}_p}\big)\, \hat{\mathbb{1}} \quad . \tag{6.45}$$

So

$$\begin{aligned} \hat{\mathrm{N}}_p = \langle\hat{\Phi},\hat{\Phi}\rangle_p &= \frac{1}{2}\hat{\Phi} \circ (\bar{\omega}_p - i\,\widetilde{\widetilde{\omega}}) \circ \hat{\Phi} = \\ &= \frac{1}{2}\hat{\Phi} \circ \bar{\omega}_p \circ \hat{\Phi} - \frac{1}{2}\big(\mathrm{tr}_{\boldsymbol{\mathcal{S}}_p}\,\delta_{\boldsymbol{\mathcal{S}}_p}\big)\, \hat{\mathbb{1}} \quad . \end{aligned} \tag{6.46}$$

Here the trace of the unit operator on $\boldsymbol{\mathcal{S}}$ is, of course, infinite; but it does not change the following reasoning.

We see that $\hat{\mathrm{N}}_p$ is a quantum version of a classical quadratic observable

$$N_p = \frac{1}{2}\Phi \circ \bar{\omega}_p \circ \Phi \tag{6.47}$$

with a special operator ordering. This operator ordering is called p-normal ordering and is defined by the condition that in any product of operators all p-creation operators are on the left of all p-annihilation operators. We denote a quantum version of a classical observable $F(\Phi)$ in p-normal ordering by

$$\hat{\mathrm{F}} = \boldsymbol{:}F(\hat{\Phi})\boldsymbol{:}_p \quad . \tag{6.48}$$

It can be written more explicitly for any quadratic observable defined using a symmetric bi-form $k \in \boldsymbol{\mathcal{S}}_2^0$

$$K(\Phi) = \frac{1}{2}\Phi \circ k \circ \Phi = \frac{1}{2}\Phi_p^+ \circ k \circ \Phi_p^+ + \frac{1}{2}\Phi_p^- \circ k \circ \Phi_p^- + \Phi_p^- \circ k \circ \Phi_p^+ \quad , \tag{6.49}$$

for which the p-normal ordered quantum version is

$$\hat{\mathrm{K}} = \boldsymbol{:}K(\hat{\Phi})\boldsymbol{:}_p = \frac{1}{2}\hat{\Phi}_p^+ \circ k \circ \hat{\Phi}_p^+ + \frac{1}{2}\hat{\Phi}_p^- \circ k \circ \hat{\Phi}_p^- + \hat{\Phi}_p^- \circ k \circ \hat{\Phi}_p^+ \quad . \tag{6.50}$$

For the observable $N_p(\Phi)$ using (4.13) we get

$$\hat{\mathrm{N}}_p = \hat{\Phi}_p^- \circ \bar{\omega}_p \circ \hat{\Phi}_p^+ = \boldsymbol{:}N_p(\hat{\Phi})\boldsymbol{:}_p \quad . \tag{6.51}$$

We will discuss p-normal ordering in more detail in connection with the holomorphic representation.

Diagonalization of Hamiltonian

Let's assume that a classical quadratic positive definite Hamiltonian is given,

$$H(\Phi) = \frac{1}{2}\Phi \circ \mathcal{H} \circ \Phi \quad , \tag{6.52}$$

where $\mathcal{H}$ is a positive definite symmetric bi-form from $\boldsymbol{\mathcal{S}}_2^0$ given, for example, by equation (2.60). We can ask whether there exists a particle interpretation such that particle states have definite energy and the energy is additive with respect to the number of particles. More precisely, we will look for such a complex structure J_h and h-orthonormal base $\mathbf{u} = \{u_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$ which satisfy

$$\hat{\mathrm{H}}\,|h\,\mathbf{u} : \boldsymbol{m}\rangle = \Big(\sum_{\mathrm{k}\in\mathcal{I}} \omega_{\mathrm{k}} m_{\mathrm{k}}\Big)\,|h\,\mathbf{u} : \boldsymbol{m}\rangle \quad , \tag{6.53}$$

where $\omega_{\mathrm{k}} \in \mathbb{R}^+$ is the energy of the one-particle state $\hat{\mathrm{a}}_{\mathrm{k}}^\dagger\,|h : vac\rangle$

$$\hat{\mathrm{H}}\,\hat{\mathrm{a}}_{\mathrm{k}}^\dagger\,|h : vac\rangle = \omega_{\mathrm{k}}\,\hat{\mathrm{a}}_{\mathrm{k}}^\dagger\,|h : vac\rangle \quad . \tag{6.54}$$

This requirement is equivalent to the requirement that the Hamiltonian have the form

$$\hat{\mathrm{H}} = \sum_{\mathrm{k}\in\mathcal{I}} \omega_{\mathrm{k}} \hat{\mathrm{n}}_{h\,\mathrm{k}} \quad . \tag{6.55}$$

Using the definition of $\hat{\mathrm{n}}_{h\,\mathrm{k}}$ (6.41) and the orthonormality of the base $\mathbf{u}$, we get

$$\hat{\mathrm{H}} = \sum_{\mathrm{k}\in\mathcal{I}} \langle\hat{\Phi}, u_{\mathrm{k}}\rangle_h \omega_{\mathrm{k}} \langle u_{\mathrm{k}}, \hat{\Phi}\rangle_h = \langle\hat{\Phi}, \Omega \circ \hat{\Phi}\rangle_h = \boldsymbol{:}\hat{\Phi} \circ \bar{\omega}_h \circ \Omega \circ \hat{\Phi}\boldsymbol{:}_h \quad , \tag{6.56}$$

where Ω is a h-linear hermitian positive definite operator on $\boldsymbol{\mathcal{S}}_h$ given by

$$\Omega \circ u_{\mathrm{k}} = \omega_{\mathrm{k}}\, u_{\mathrm{k}} \quad . \tag{6.57}$$

h-linearity gives us the condition

$$\big[\Omega, \mathsf{J}_h\big] = 0 \quad . \tag{6.58}$$

Hermicity $\Omega^{\langle\dagger\rangle} = \Omega$ (following from $\omega_{\mathrm{k}} \in \mathbb{R}^+$) gives

$$\overset{\leftrightsquigarrow}{\omega} \circ \Omega = \Omega \circ \overset{\leftrightsquigarrow}{\omega} \quad \Leftrightarrow \quad \bar{\omega}_h \circ \Omega = \Omega \circ \bar{\omega}_h \quad . \tag{6.59}$$

The quantum observable $\hat{\mathrm{H}}$ should be a quantum version of the classical observable $H(\Phi)$ in some operator ordering. As we have discussed, any two quantum versions of $H(\Phi)$ defined using two different operator orderings can differ only by multiple of the unit operator. Therefore we can write

$$\hat{\mathrm{H}} = \boldsymbol{:}H(\hat{\Phi})\boldsymbol{:}_h + \alpha\hat{\mathbb{1}} = \boldsymbol{:}\hat{\Phi} \circ \mathcal{H} \circ \hat{\Phi}\boldsymbol{:}_h + \alpha\hat{\mathbb{1}} \quad . \tag{6.60}$$

From a comparison with equation (6.56) we see that we need to satisfy

$$\mathcal{H} = \bar{\omega}_h \circ \Omega \quad , \tag{6.61}$$

which is equivalent to

$$G_c \circ \mathcal{H} = \mathsf{J}_h \circ \Omega \quad . \tag{6.62}$$

Let's summarize. We are looking for a complex structure J_h and a positive definite operator Ω which satisfy conditions (4.3), (4.4), (6.58), (6.59) and (6.62). We can get such a J_h and Ω using a polar decomposition[7] of the operator $(G_c \circ \mathcal{H})$. For a polar decomposition we need a transposition of operators. Let us use the transposition defined using a positive definite symmetric bi-form $\mathcal{H}$

$$A^{\mathbf{T}} = \mathcal{H}^{-1} \circ A \circ \mathcal{H} \qquad \text{for any operator } A \text{ on } \boldsymbol{\mathcal{S}} \quad . \tag{6.63}$$

Because

$$(G_c \circ \mathcal{H})^{\mathbf{T}} = -(G_c \circ \mathcal{H}) \quad , \tag{6.64}$$

left and right polar decompositions of $(G_c \circ \mathcal{H})$ coincide and we can define

$$\Omega = |G_c \circ \mathcal{H}| = \big((G_c \circ \mathcal{H})^{\mathbf{T}} \circ (G_c \circ \mathcal{H})\big)^{\frac{1}{2}} = \big((G_c \circ \mathcal{H}) \circ (G_c \circ \mathcal{H})^{\mathbf{T}}\big)^{\frac{1}{2}} \quad , \tag{6.65}$$

$$\mathsf{J}_h = \operatorname{sign}\big(G_c \circ \mathcal{H}\big) = (G_c \circ \mathcal{H}) \circ \Omega^{-1} = \Omega^{-1} \circ (G_c \circ \mathcal{H}) \quad , \tag{6.66}$$

$$G_c \circ \mathcal{H} = \mathsf{J}_h \circ \Omega = \Omega \circ \mathsf{J}_h \quad . \tag{6.67}$$

It is straightforward to check all conditions on J_h and Ω. Positive definiteness and symmetry ($\Omega^{\mathbf{T}} = \Omega$) of Ω follows from the definition of square root, the compatibility of J_h and $\overset{\leftrightsquigarrow}{\omega}$ follows from (6.66) and symmetry of Ω, positive definiteness of $\bar{\omega}_h$ follows from (6.66) and positive definiteness of Ω, (6.58) and (6.62) are the same as equation (6.67).

We have finally proved that the positive quadratic classical Hamiltonian $H(\Phi)$ picks up uniquely the particle interpretation in which it is possible to diagonalize the quantum Hamiltonian, i.e. to write

$$\hat{\mathrm{H}} = \boldsymbol{:}H(\hat{\Phi})\boldsymbol{:}_h = \sum_{\mathrm{k} \in \mathcal{I}} \omega_{\mathrm{k}} \hat{\mathrm{n}}_{h\,\mathrm{k}} \quad , \tag{6.68}$$

where $\hat{\mathrm{n}}_{h\,\mathrm{k}}$ are observables of number of particle in modes u_{k} which are eigenvectors of the operator Ω with eigenvalues ω_{k}. A similar result can be found in [9, 10].

Unfortunately we do not have a preferred $3+1$ splitting in a general spacetime, and for a general $3+1$ splitting the Hamiltonian is time dependent. This means that the diagonalization criterion picks up different particle interpretations at different times. This reflects the fact that in a general spacetime we do not have a preferred particle interpretation, and if we decide to choose particle interpretations, connected with the Hamiltonian of some $3+1$ decomposition, we have to expect particle creation as will be described in chapter 8.

Connection with value representation

Now we turn to investigate the connection of the introduced particle base with the value representation defined in the previous chapter. We will find the wave functional of the vacuum and one particle states.

As we already mentioned, we can define $\boldsymbol{\mathcal{V}}$ and $\tilde{\boldsymbol{\mathcal{V}}}$-valued forms $\underline{\varphi}$ and $\underline{\pi}$ on the phase space $\boldsymbol{\mathcal{S}}$ and using them we can express the quantum version of the value and momentum observables as

$$\hat{\varphi}[\Sigma] = \underline{\varphi}[\Sigma] \circ \hat{\Phi} \quad , \quad \hat{\pi}[\Sigma] = \underline{\pi}[\Sigma] \circ \hat{\Phi} \quad . \tag{6.69}$$

They satisfy the commutation relation (5.57), and we can construct the *value base* $|val : \varphi\rangle$ as defined in (5.58).

We express the creation and annihilation operators using $\hat{\varphi}$ and $\hat{\pi}$ as

$$\begin{aligned} \hat{\mathrm{a}}_p[\phi] &= \langle\phi, \hat{\Phi}\rangle_p = \underline{\psi}_p^-[\phi] \cdot (\theta_p \cdot \hat{\varphi} + i\, \hat{\pi}) \quad , \\ \hat{\mathrm{a}}_p[\phi]^\dagger &= \langle\hat{\Phi}, \phi\rangle_p = (\hat{\varphi} \cdot \theta_p^* - i\hat{\pi}) \cdot \underline{\psi}_p^+[\phi] \quad . \end{aligned} \tag{6.70}$$

The condition on the vacuum state (6.12) gives

$$0 = \langle val : \varphi|(\theta_p \cdot \hat{\varphi} + i\hat{\pi})|p : vac\rangle = (\theta_p \cdot \varphi + \mathrm{d})\langle val : \varphi|p : vac\rangle \quad . \tag{6.71}$$

The solution of this variation equation is

$$\Psi_{|p:vac\rangle}(\varphi) = \langle val : \varphi|p : vac\rangle = \mathrm{const}\ \exp\bigl(-\frac{1}{2}\varphi \cdot \theta_p \cdot \varphi\bigr) \quad . \tag{6.72}$$

Normalization gives us the prefactor:

$$\begin{aligned} 1 = \langle p : vac|p : vac\rangle &= \int_{\varphi\in\boldsymbol{\mathcal{V}}} \mathfrak{Q}\ \langle p : vac|val : \varphi\rangle\langle val : \varphi|p : vac\rangle = \\ &= \int_{\varphi\in\boldsymbol{\mathcal{V}}} \mathfrak{Q}\ |\mathrm{const}|^2 \exp\bigl(-\frac{1}{2}\varphi \cdot (\theta_p + \theta_p^*) \cdot \varphi\bigr) = \int_{\varphi\in\boldsymbol{\mathcal{V}}} \mathfrak{Q}\ |\mathrm{const}|^2 \exp\bigl(-\varphi \cdot \mathcal{B}_p^{-1} \cdot \varphi\bigr) = \\ &= \mathfrak{Q}\ |\mathrm{const}|^2 \bigl(\mathrm{Det}\,\pi\mathcal{B}_p\bigr)^{\frac{1}{2}} \quad . \end{aligned} \tag{6.73}$$

Finally, the wave functional of the vacuum state is, dropping an arbitrary phase factor,

$$\Psi_{|p:vac\rangle}(\varphi) = \mathfrak{Q}^{-\frac{1}{2}} \bigl(\mathrm{Det}\,\pi\mathcal{B}_p\bigr)^{-\frac{1}{4}} \exp\bigl(-\frac{1}{2}\varphi \cdot \theta_p \cdot \varphi\bigr) \quad . \tag{6.74}$$

The action of the creation operator gives the wave functional of one particle states

$$\begin{aligned} \Psi_{\hat{\mathrm{a}}_p[\phi]^\dagger|p:vac\rangle}(\varphi) &= \underline{\psi}_p^+[\phi] \cdot \langle val : \varphi|(\theta_p^* \cdot \hat{\varphi} - i\,\hat{\pi})|p : vac\rangle = \\ &= \underline{\psi}_p^+[\phi] \cdot (\theta_p^* \cdot \varphi - \mathrm{d})\langle val : \varphi|p : vac\rangle = \\ &= \bigl(2\underline{\psi}_p[\phi] \cdot \theta_p \cdot \varphi\bigr)\ \Psi_{|p:vac\rangle}(\varphi) \quad , \end{aligned} \tag{6.75}$$

and similarly for the wave functional of multiple particle states.

We have found that the wave functional of particle states is given by a Gaussian exponent $\Psi_{|p:vac\rangle}(\varphi)$ multiplied by a polynomial expression in φ. For such a wave functional the integral (5.60) makes sense, as we promised above.

7 Holomorphic representation

Coherent states

In the previous chapter we have defined the particle states depending on the choice of the particle representation. It is useful to introduce other states connected with the particle interpretation, the so-called *coherent states*. They allow us to skip making a particular choice of a base of modes to form particle states and skip unpleasant expressions with sums over occupation numbers. Instead we will be able to define a holomorphic representation of the quantum space $\mathcal{H}$. We will be very formal in our considerations, and basically we will ignore the infinite dimensional nature of our phase space $\boldsymbol{\mathcal{S}}$.

Coherent states associated with the particle representation are defined by

$$|p\,coh:\phi\rangle = \exp\big(\frac{1}{2}\langle\phi,\phi\rangle_p\big)\ \hat{\mathrm{W}}[\phi]\,|p:vac\rangle \tag{7.1}$$

for any $\phi\in\boldsymbol{\mathcal{S}}$. Here the *displacement operator* $\hat{\mathrm{W}}[\phi]$ is defined by

$$\hat{\mathrm{W}}[\phi] = \exp\big(i\,\phi\circ\overleftrightarrow{\omega}\circ\hat{\Phi}\big) = \exp\big(i\hat{\mathsf{L}}_\phi\big) \quad . \tag{7.2}$$

It is a unitary operator, and the name *displacement* operator is justified by the property

$$\hat{\mathrm{W}}[\phi]^\dagger\,\hat{\Phi}\,\hat{\mathrm{W}}[\phi] = \hat{\Phi} + \phi\,\hat{\mathbb{1}} \quad . \tag{7.3}$$

Using the known identity

$$\begin{gathered}\exp\big(\hat{\mathrm{A}}+\hat{\mathrm{B}}\big) = \exp\big(-\frac{1}{2}[\hat{\mathrm{A}},\hat{\mathrm{B}}]\big)\exp(\hat{\mathrm{A}})\exp(\hat{\mathrm{B}})\\ \text{for }\hat{\mathrm{A}},\hat{\mathrm{B}}\text{ satisfying}\quad \big[\hat{\mathrm{A}},[\hat{\mathrm{A}},\hat{\mathrm{B}}]\big]=0\quad\text{and}\quad\big[\hat{\mathrm{B}},[\hat{\mathrm{A}},\hat{\mathrm{B}}]\big]=0\quad ,\end{gathered} \tag{7.4}$$

we can write exponential versions of the commutation relations (6.1) and (6.11)

$$\hat{\mathrm{W}}[\phi_1]\hat{\mathrm{W}}[\phi_2] = \exp\big(i\,\phi_1\circ\overleftrightarrow{\omega}\circ\phi_2\big)\hat{\mathrm{W}}[\phi_2]\hat{\mathrm{W}}[\phi_1] \quad , \tag{7.5}$$

$$\exp\big(\hat{\mathrm{a}}_p[\phi_1]\big)\exp\big(\hat{\mathrm{a}}_p[\phi_2]^\dagger\big) = \exp\big(\langle\phi_1,\phi_2\rangle_p\big)\exp\big(\hat{\mathrm{a}}_p[\phi_2]^\dagger\big)\exp\big(\hat{\mathrm{a}}_p[\phi_1]\big) \quad , \tag{7.6}$$

p-normal ordering of the displacement operator and an additivity property

$$\hat{\mathrm{W}}[\phi] = \exp\big(\hat{\mathrm{a}}_p[\phi]^\dagger - \hat{\mathrm{a}}_p[\phi]\big) = \exp\big(-\frac{1}{2}\langle\phi,\phi\rangle_p\big)\exp\big(\hat{\mathrm{a}}_p[\phi]^\dagger\big)\exp\big(-\hat{\mathrm{a}}_p[\phi]\big) \quad , \tag{7.7}$$

$$\hat{\mathrm{W}}[\phi_1]\hat{\mathrm{W}}[\phi_2] = \exp\big(i\,\frac{1}{2}\phi_1\circ\overleftrightarrow{\omega}\circ\phi_2\big)\hat{\mathrm{W}}[\phi_1+\phi_2] \quad . \tag{7.8}$$

Using this relation we get

$$|p\,coh:\phi\rangle = \exp\big(\hat{\mathrm{a}}_p[\phi]^\dagger\big)\,|p:vac\rangle \quad . \tag{7.9}$$

Here we have used

$$\exp\big(\hat{\mathrm{a}}_p[\phi]\big)\,|p:vac\rangle = \Big(\sum_{n=0}^{\infty}\frac{1}{n!}\hat{\mathrm{a}}_p[\phi]^n\Big)\,|p:vac\rangle = |p:vac\rangle \quad . \tag{7.10}$$

We see that a coherent state $|p\,coh:\phi\rangle$ contains only particles in the ϕ mode. It is a superposition of particle states with any number of particles, and the mean value of particles in the mode ϕ_1 is given by

$$\langle p\,coh:\phi|\hat{\mathrm{n}}_p[\phi_1]|p\,coh:\phi\rangle = \frac{\langle\phi,\phi_1\rangle_p\langle\phi_1,\phi\rangle_p}{\langle\phi_1,\phi_1\rangle_p} \quad . \tag{7.11}$$

The scalar product of two coherent states is (using equations (7.9), (7.6), (7.10))

$$\langle p\,coh:\phi_1|p\,coh:\phi_2\rangle = \exp\bigl(\langle\phi_1,\phi_2\rangle_p\bigr) \tag{7.12}$$

This means that coherent states are not orthogonal. However, coherent states form a overcomplete set in the quantum space $\mathcal{H}$. This can be seen from the important completeness relation

$$\hat{\mathbb{1}} = \int\limits_{\phi\in\boldsymbol{S}} \mathfrak{H}_p(\phi)\,|p\,coh:\phi\rangle\langle p\,coh:\phi| \quad , \tag{7.13}$$

where the measure $\mathfrak{H}_p$ on the phase space $\boldsymbol{S}$ is given by

$$\mathfrak{H}_p(\phi) = \exp\bigl(-\langle\phi,\phi\rangle_p\bigr)\,d\Gamma \quad . \tag{7.14}$$

and $d\Gamma$ is the canonical measure (B.8) on phase space $\boldsymbol{S}$

$$d\Gamma = \bigl(\mathrm{Det}\,\frac{\overset{\leftrightarrow}{\omega}}{2\pi}\bigr)^{\frac{1}{2}} = \bigl(\mathrm{Det}\,\frac{\bar{\omega}_p}{2\pi}\bigr)^{\frac{1}{2}} \quad . \tag{7.15}$$

We will prove the identity (7.13) later (see equation (7.34)).

Finally, the coherent states are eigenvectors of the annihilation operators

$$\begin{aligned}
&\hat{\mathrm{a}}_p[\phi_1]\,|p\,coh:\phi\rangle = \\
&\quad = \mathrm{const}\,\langle\phi_1,\hat{\Phi}\rangle_p\,\hat{\mathrm{W}}[\phi]\,|p:vac\rangle = \mathrm{const}\,\hat{\mathrm{W}}[\phi]\bigl(\langle\phi_1,\hat{\Phi}\rangle_p + \langle\phi_1,\phi\rangle_p\hat{\mathbb{1}}\bigr)|p:vac\rangle = \\
&\quad = \langle\phi_1,\phi\rangle_p\,|p\,coh:\phi\rangle \quad ,
\end{aligned} \tag{7.16}$$

where we have used equation (7.3). The action of a creation operator on a coherent state is given by

$$\begin{aligned}
&\hat{\mathrm{a}}_p[\phi_1]^\dagger\,|p\,coh:\phi\rangle = \\
&\quad = \Bigl(\hat{\mathrm{a}}_p[\phi_1]^\dagger\exp\bigl(\hat{\mathrm{a}}_p[\phi]^\dagger\bigr)\Bigr)|p:vac\rangle = \Bigl(\phi_1\circ\mathrm{d}\,\exp\bigl(\hat{\mathrm{a}}_p[\phi]^\dagger\bigr)\Bigr)|p:vac\rangle = \\
&\quad = \phi_1\circ\mathrm{d}\,|p\,coh:\phi\rangle \quad .
\end{aligned} \tag{7.17}$$

Holomorphic representation

First we recall the definition of a holomorphic function on complex vector spaces. A function $F: V \mapsto \mathbb{C}$ on a complex vector space V is *holomorphic* or *antiholomorphic* respectively, if for any vector $\phi\in V$ a function $F(z\phi)$ is holomorphic or antiholomorphic in the complex variable z.

We will call a function $F:\boldsymbol{S}\mapsto\mathbb{C}$ on the phase space $\boldsymbol{S}$ *p-holomorphic* or *p-antiholomorphic* respectivelly if it is holomorphic or antiholomorphic on the complex space $\boldsymbol{S}_p$ with the multiplication $\star$, i.e. if for any $\phi\in\boldsymbol{S}$ a function $F(z\star\phi)$ is holomorphic or antiholomorphic in complex variable z.

A function $F:\boldsymbol{S}\mapsto\mathbb{C}$ is called *analytical* on $\boldsymbol{S}$ if it is possible to extend it to a holomorphic function on $\boldsymbol{S}^{\mathbb{C}}$ (holomorphic in the sense of $\boldsymbol{S}^{\mathbb{C}}$). This extension is called the analytical extension of F, and we will use the same letter F for it.

Using relations valid for any $\phi\in\boldsymbol{S}$ (see eq. (4.10)),

$$\mathsf{P}^+_p\circ(z\star\phi) = z\phi^+_p \quad , \quad \mathsf{P}^-_p\circ(z\star\phi) = z^*\phi^-_p \quad , \tag{7.18}$$

we can find that an analytical function F on $\boldsymbol{\mathcal{S}}$ is p-holomorphic or p-antiholomorphic respectively, if and only if its analytical extension on $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$ depends only on the p-positive or p-negative frequency part of its argument

$$\begin{aligned} &F \quad \text{is } p\text{-holomorphic} &&\Leftrightarrow \quad F(\phi) = F(\phi_p^+) \quad , \\ &F \quad \text{is } p\text{-antiholomorphic} &&\Leftrightarrow \quad F(\phi) = F(\phi_p^-) \quad . \end{aligned} \tag{7.19}$$

Now we will introduce the *holomorphic representation* of quantum space $\mathcal{H}$. Any state $|state\rangle$ can be represented by p-antiholomorphic function $\mathfrak{f}_p\left[|state\rangle\right] : \boldsymbol{\mathcal{S}} \mapsto \mathbb{C}$ on the phase space

$$\mathfrak{f}_p\left[|state\rangle\right](\phi) = \langle p\,coh : \phi|state\rangle = \langle p : vac|\exp\bigl(\hat{\mathrm{a}}_p[\phi]\bigr)|state\rangle \quad . \tag{7.20}$$

Similarly we introduce p-holomorphic function $\mathfrak{f}_p\left[\langle state|\right] : \boldsymbol{\mathcal{S}} \mapsto \mathbb{C}$ for a covector $\langle state|$ and the function $\mathfrak{f}_p\left[\hat{\mathrm{A}}\right] : \boldsymbol{\mathcal{S}}\times\boldsymbol{\mathcal{S}} \mapsto \mathbb{C}$ p-antiholomorphic in the first and p-holomorphic in the second argument for an operator $\hat{\mathrm{A}}$

$$\mathfrak{f}_p\left[\langle state|\right](\phi) = \langle state|p\,coh : \phi\rangle = \mathfrak{f}_p\left[|state\rangle\right](\phi)^* \quad , \tag{7.21}$$

$$\mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi_1, \phi_2) = \langle p\,coh : \phi_1|\hat{\mathrm{A}}|p\,coh : \phi_2\rangle \quad . \tag{7.22}$$

Using the completeness relation (7.13) it is trivial to prove the compositions laws

$$\begin{aligned} \langle state1|state2\rangle &= \int\limits_{\phi\in\boldsymbol{\mathcal{S}}} \mathfrak{H}_p(\phi)\; \mathfrak{f}_p\left[\langle state1|\right](\phi)\; \mathfrak{f}_p\left[|state2\rangle\right](\phi) \quad , \\ \mathfrak{f}_p\left[\hat{\mathrm{A}}|state\rangle\right](\phi) &= \int\limits_{\phi'\in\boldsymbol{\mathcal{S}}} \mathfrak{H}_p(\phi')\; \mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi,\phi')\; \mathfrak{f}_p\left[|state\rangle\right](\phi') \quad , \\ \mathfrak{f}_p\left[\hat{\mathrm{A}}\hat{\mathrm{B}}\right](\phi_1,\phi_2) &= \int\limits_{\phi\in\boldsymbol{\mathcal{S}}} \mathfrak{H}_p(\phi)\; \mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi_1,\phi)\; \mathfrak{f}_p\left[\hat{\mathrm{B}}\right](\phi,\phi_2) \quad , \\ \operatorname{Tr}\hat{\mathrm{A}} &= \int\limits_{\phi\in\boldsymbol{\mathcal{S}}} \mathfrak{H}_p(\phi)\; \mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi,\phi) \quad . \end{aligned} \tag{7.23}$$

Next we will find the action of annihilation and creation operators. Using equations (7.16), (7.17) we obtain

$$\begin{aligned} \mathfrak{f}_p\left[\hat{\mathrm{a}}_p[\phi]^\dagger|state\rangle\right](\phi_1) &= \langle\phi_1,\phi\rangle_p\, \mathfrak{f}_p\left[|state\rangle\right](\phi_1) \quad , \\ \mathfrak{f}_p\left[\hat{\mathrm{a}}_p[\phi]^\dagger\hat{\mathrm{A}}\right](\phi_1,\phi_2) &= \langle\phi_1,\phi\rangle_p\, \mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi_1,\phi_2) \quad , \\ \mathfrak{f}_p\left[\hat{\mathrm{a}}_p[\phi]|state\rangle\right](\phi_1) &= \phi\circ\bigl(\mathrm{d}\,\mathfrak{f}_p\left[|state\rangle\right]\bigr)(\phi_1) \quad , \\ \mathfrak{f}_p\left[\hat{\mathrm{a}}_p[\phi]\hat{\mathrm{A}}\right](\phi_1,\phi_2) &= \phi\circ\bigl(\mathrm{d}_1\,\mathfrak{f}_p\left[\hat{\mathrm{A}}\right]\bigr)(\phi_1,\phi_2) \quad . \end{aligned} \tag{7.24}$$

Here d_1 is the variation with respect to the left argument. Similar relations hold for $\mathfrak{f}_p\left[\langle state|\hat{\mathrm{a}}_p[\phi]\right]$, $\mathfrak{f}_p\left[\hat{\mathrm{A}}\hat{\mathrm{a}}_p[\phi]\right]$ and so on.

Let us list the holomorphic representations of some states and operators:

$$\mathfrak{f}_p\left[|p : vac\rangle\right](\phi) = 1 \quad , \tag{7.25}$$

$$\mathfrak{f}_p\left[\hat{\mathrm{a}}_p[\phi]^{\dagger\,n}|p : vac\rangle\right](\phi_1) = \langle\phi_1,\phi\rangle_p^{\;n} \quad , \tag{7.26}$$

$$\mathfrak{f}_p\left[|p\,coh : \phi\rangle\right](\phi_1) = \exp\bigl(\langle\phi_1,\phi\rangle_p\bigr) \quad , \tag{7.27}$$

$$\mathfrak{f}_p\left[|p : vac\rangle\langle p : vac|\right](\phi_1,\phi_2) = 1 \quad , \tag{7.28}$$

$$\mathfrak{f}_p\left[\hat{1\!\!1}\right](\phi_1,\phi_2) = \exp\bigl(\langle\phi_1,\phi_2\rangle_p\bigr) \quad , \tag{7.29}$$

$$\mathfrak{f}_p\left[\hat{\mathrm{n}}_p[\phi]\right](\phi_1,\phi_2) = \frac{\langle\phi_1,\phi\rangle_p\langle\phi,\phi_2\rangle_p}{\langle\phi,\phi\rangle_p}\exp\bigl(\langle\phi_1,\phi_2\rangle_p\bigr) \quad , \tag{7.30}$$

$$\mathfrak{f}_p\left[\hat{\mathrm{N}}_p\right](\phi_1,\phi_2) = \langle\phi_1,\phi_2\rangle_p \exp\bigl(\langle\phi_1,\phi_2\rangle_p\bigr) \quad , \tag{7.31}$$

$$\mathfrak{f}_p\left[|p\,coh:\phi\rangle\langle p\,coh:\phi|\right](\phi_1,\phi_2) = \exp\bigl(\langle\phi_1,\phi\rangle_p + \langle\phi,\phi_2\rangle_p\bigr) \quad , \tag{7.32}$$

$$\mathfrak{f}_p\left[\hat{\mathrm{W}}[\phi]\right](\phi_1,\phi_2) = \exp\bigl(-\frac{1}{2}\langle\phi,\phi\rangle_p + \langle\phi_1,\phi\rangle_p - \langle\phi,\phi_2\rangle_p + \langle\phi_1,\phi_2\rangle_p\bigr) \quad . \tag{7.33}$$

To conclude, we will prove the completeness relation (7.13):

$$\begin{aligned}
&\mathfrak{f}_p\Biggl[\int\limits_{\phi\in\boldsymbol{\mathcal{S}}} \mathfrak{H}(\phi)\,|p\,coh:\phi\rangle\langle p\,coh:\phi|\Biggr](\phi_1,\phi_2) = \\
&\quad= \int\limits_{\phi\in\boldsymbol{\mathcal{S}}} d\Gamma\;\; \exp\bigl(-\langle\phi,\phi\rangle_p + \langle\phi_1,\phi\rangle_p + \langle\phi,\phi_2\rangle_p\bigr) = \\
&\quad= \int\limits_{\phi\in\boldsymbol{\mathcal{S}}} d\Gamma\;\; \exp\bigl(-\frac{1}{2}\phi\circ\bar{\omega}_p\circ\phi + \phi\circ\bar{\omega}_p\circ({\phi_1}_p^- + {\phi_2}_p^+)\bigr) = \\
&\quad= \exp\bigl(\frac{1}{2}({\phi_1}_p^- + {\phi_2}_p^+)\circ\bar{\omega}_p\circ({\phi_1}_p^- + {\phi_2}_p^+)\bigr) = \\
&\quad= \exp\bigl(\langle\phi_1,\phi_2\rangle_p\bigr) \quad ,
\end{aligned} \tag{7.34}$$

where we used equations (7.32), (7.15) and Gaussian integration. Comparing with equation (7.29) we get exactly the completeness relation (7.13).

p-normal ordering

Holomorphic representation of operators on $\mathcal{H}$ is closely related with p-normal ordering of the operators. We will investigate this connection now. Let's choose again a p-orthonormal $\mathbb{C}$-base $\mathbf{u} = \{u_{\mathrm{k}};\mathrm{k}\in\mathcal{I}\}$ in $\boldsymbol{\mathcal{S}}_p$. It generates the particle base (6.38) in $\mathcal{H}$

$$|p\,\mathbf{u}:\boldsymbol{m}\rangle = \frac{1}{\sqrt{\boldsymbol{m}!}}\hat{\mathrm{a}}_p[\mathbf{u}]^{\dagger\,\boldsymbol{m}}|p:vac\rangle \quad . \tag{7.35}$$

We are using the shorthands (6.39). Any operator $\hat{\mathrm{A}}$ generated analytically by $\hat{\Phi}$ (i.e. defined by a sum of products, maybe infinite, of $\hat{\Phi}$) can be expressed in p-normal ordered form

$$\hat{\mathrm{A}} = \sum_{\boldsymbol{m},\boldsymbol{n}} a_{\boldsymbol{m},\boldsymbol{n}}\,\hat{\mathrm{a}}_p[\mathbf{u}]^{\dagger\,\boldsymbol{m}}\hat{\mathrm{a}}_p[\mathbf{u}]^{\boldsymbol{n}} \quad , \tag{7.36}$$

where $a_{\boldsymbol{m},\boldsymbol{n}}$ are some complex valued coefficients. If we introduce the *generating function* $\tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\phi_1,\phi_2)$ by[8]

$$\tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\phi_1,\phi_2) = \sum_{\boldsymbol{m},\boldsymbol{n}} a_{\boldsymbol{m},\boldsymbol{n}}\,\langle\phi_1,\mathbf{u}\rangle_p^{\boldsymbol{m}}\langle\mathbf{u},\phi_2\rangle_p^{\boldsymbol{n}} \tag{7.37}$$

we can write

$$\hat{\mathrm{A}} = \boldsymbol{:}\tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\hat{\Phi},\hat{\Phi})\boldsymbol{:}_p = \boldsymbol{:}\tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\hat{\Phi}_p^-,\hat{\Phi}_p^+)\boldsymbol{:}_p \quad . \tag{7.38}$$

The generating function is given by the previous equation uniquely. More precisely, if an operator $\hat{\mathrm{A}}$ can be written as

$$\hat{\mathrm{A}} = \boldsymbol{:}F(\hat{\Phi}_p^-,\hat{\Phi}_p^+)\boldsymbol{:}_p \quad , \tag{7.39}$$

where $F(\phi_1, \phi_2)$ is a holomorphic function on $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$ in both arguments, than the function F restricted on $\boldsymbol{\mathcal{S}}$ is the generating function of the operator $\hat{\mathrm{A}}$

$$F(\phi_1, \phi_2) = \tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\phi_1, \phi_2) \quad . \tag{7.40}$$

The generating function is independent of the choice of base $\mathbf{u}$ as can be seen from the following.

We will find a relation between the generating function $\tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right]$ and the holomorphic representation $\mathfrak{f}_p\left[\hat{\mathrm{A}}\right]$ of an operator $\hat{\mathrm{A}}$. Using equations (7.36), (7.16), (7.37) we get

$$\begin{aligned}
\mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi_1, \phi_2) &= \langle p\, coh : \phi_1|\hat{\mathrm{A}}|p\, coh : \phi_2\rangle = \\
&= \sum_{\boldsymbol{m},\boldsymbol{n}} \langle p\, coh : \phi_1|a_{\boldsymbol{m},\boldsymbol{n}}\, \hat{\mathrm{a}}_p[\mathbf{u}]^{\dagger\,\boldsymbol{m}}\hat{\mathrm{a}}_p[\mathbf{u}]^{\boldsymbol{n}}|p\, coh : \phi_2\rangle = \\
&= \sum_{\boldsymbol{m},\boldsymbol{n}} a_{\boldsymbol{m},\boldsymbol{n}}\, \langle\phi_1, \mathbf{u}\rangle_p^{\boldsymbol{m}}\langle\mathbf{u}, \phi_2\rangle_p^{\boldsymbol{n}}\langle p\, coh : \phi_1|p\, coh : \phi_2\rangle = \\
&= \exp\bigl(\langle\phi_1, \phi_2\rangle_p\bigr)\, \tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\phi_1, \phi_2) \quad .
\end{aligned} \tag{7.41}$$

This means

$$\hat{\mathrm{A}} = \boldsymbol{:}\exp\bigl(-\langle\hat{\Phi}, \hat{\Phi}\rangle_p\bigr)\, \mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\hat{\Phi}, \hat{\Phi})\boldsymbol{:}_p \quad . \tag{7.42}$$

As useful examples we can find (using equations (7.28), (7.32)) p-normal ordered expressions for projectors on the vacuum state and on a coherent state

$$|p : vac\rangle\langle p : vac| = \boldsymbol{:}\exp\bigl(-\langle\hat{\Phi}, \hat{\Phi}\rangle_p\bigr)\boldsymbol{:}_p \quad , \tag{7.43}$$

$$|p\, coh : \phi\rangle\langle p\, coh : \phi| = \boldsymbol{:}\exp\bigl(-\langle\hat{\Phi} - \phi\hat{\mathbb{1}}, \hat{\Phi} - \phi\hat{\mathbb{1}}\rangle_p + \langle\phi, \phi\rangle_p\hat{\mathbb{1}}\bigr)\boldsymbol{:}_p \quad . \tag{7.44}$$

Relation between holomorphic and particle representations

Finally we derive a relation between the holomorphic representation and the occupation number representation of an operator. Using the base $|p\,\mathbf{u} : \boldsymbol{m}\rangle$ we can write

$$\begin{aligned}
\hat{\mathrm{A}} &= \sum_{\boldsymbol{m},\boldsymbol{n}} |p\,\mathbf{u} : \boldsymbol{m}\rangle\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle\langle p\,\mathbf{u} : \boldsymbol{n}| = \\
&= \sum_{\boldsymbol{m},\boldsymbol{n}} \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}}\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle\; \hat{\mathrm{a}}_p[\mathbf{u}]^{\dagger\,\boldsymbol{m}}|p : vac\rangle\langle p : vac|\hat{\mathrm{a}}_p[\mathbf{u}]^{\boldsymbol{n}} = \\
&= \sum_{\boldsymbol{m},\boldsymbol{n}} \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}}\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle\; \boldsymbol{:}\langle\hat{\Phi}, \mathbf{u}\rangle_p^{\boldsymbol{m}}\exp\bigl(-\langle\hat{\Phi}, \hat{\Phi}\rangle_p\bigr)\langle\mathbf{u}, \hat{\Phi}\rangle_p^{\boldsymbol{n}}\boldsymbol{:}_p \quad .
\end{aligned} \tag{7.45}$$

We have expressed the operator $\hat{\mathrm{A}}$ in the form (7.39); therefore, we can use equation (7.40)

$$\tilde{\mathfrak{f}}_p\left[\hat{\mathrm{A}}\right](\phi_1, \phi_2) = \Bigl(\sum_{\boldsymbol{m},\boldsymbol{n}} \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}}\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle\langle\phi_1, \mathbf{u}\rangle_p^{\boldsymbol{m}}\langle\mathbf{u}, \phi_2\rangle_p^{\boldsymbol{n}}\Bigr)\exp\bigl(-\langle\phi_1, \phi_2\rangle_p\bigr) \tag{7.46}$$

and finally we get expression for the holomorphic representation $\mathfrak{f}_p\left[\hat{\mathrm{A}}\right]$ in terms of the occupation number representation $\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle$

$$\mathfrak{f}_p\left[\hat{\mathrm{A}}\right](\phi_1, \phi_2) = \sum_{\boldsymbol{m},\boldsymbol{n}} \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}}\langle p\,\mathbf{u} : \boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u} : \boldsymbol{n}\rangle\langle\phi_1, \mathbf{u}\rangle_p^{\boldsymbol{m}}\langle\mathbf{u}, \phi_2\rangle_p^{\boldsymbol{n}} \quad . \tag{7.47}$$

Inverse relations can be obtained by repeated variation and setting arguments to zero at the end[8]

$$\langle p\,\mathbf{u}:\boldsymbol{m}|\hat{\mathrm{A}}|p\,\mathbf{u}:\boldsymbol{n}\rangle = \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}}\Big(\big[\mathbf{u}\circ \mathrm{d}_{\mathrm{l}}\big]^{\boldsymbol{m}}\,\big[\mathbf{u}\circ \mathrm{d}_{\mathrm{r}}\big]^{\boldsymbol{n}}\,\mathfrak{f}_p\,\Big[\hat{\mathrm{A}}\Big]\Big)(0,0) \quad . \tag{7.48}$$

We could have found relation (7.47) faster — using (6.8), (7.9) and an expansion to the base we get

$$|p\,coh:\phi\rangle = \sum_{\boldsymbol{m}} \frac{1}{\sqrt{\boldsymbol{m}!}}\langle \mathbf{u},\phi\rangle_p^{\boldsymbol{m}}|p\,\mathbf{u}:\boldsymbol{m}\rangle \quad . \tag{7.49}$$

Substituting to the definition of the holomorphic representation (7.22) we immediately get (7.47) and similary also

$$\mathfrak{f}_p\,[|st\rangle](\phi) = \sum_{\boldsymbol{m}} \frac{1}{\sqrt{\boldsymbol{m}!}}\langle \phi,\mathbf{u}\rangle_p^{\boldsymbol{m}}\langle p\,\mathbf{u}:\boldsymbol{m}|st\rangle \quad . \tag{7.50}$$

The inverse relation is

$$\langle p\,\mathbf{u}:\boldsymbol{m}|st\rangle = \frac{1}{\sqrt{\boldsymbol{m}!}}\Big(\big[\mathbf{u}\circ \mathrm{d}\big]^{\boldsymbol{m}}\,\mathfrak{f}_p\,[|st\rangle]\Big)(0) \quad . \tag{7.51}$$

8 Transition amplitudes

Two particle interpretations

Until now we have not addressed dynamical questions in the quantum theory. We have found several methods for identifying some special observables or states in our quantum system, but we have not studied their development. Because covariant phase space quantization is essentially in the Heisenberg picture, the dynamics should be formulated as finding the time evolution of the quantum observables. If we restrict to the situation in which we perform experiments only at the beginning and at the end, we want to find relations between "the same kind" of observables defined at the initial and final times.

In the previous chapter we have investigated a single particle interpretation of the scalar field theory. But there exist a lot of different particle interpretations, each corresponding to a different complex structure on the phase space, and in a general situation none of them has a preferred status. However in most physical situations, we are dealing with a spacetime which has special properties at least in the remote past and future. For example, the spacetime may be static in these regions. This gives us usually the possibility to choose a preferred notion of particles in the past and in the future. These particle interpretations are not generally the same. And their relation is exactly the sort of dynamical question which we want to investigate. The dynamical information is hidden in the comparison of objects built using these two particle interpretations — as particle or coherent states, observables of number of particles, etc..

Therefore we need to investigate the relation between two different particle interpretations. This problem is usually described in terms of Bogoljubov coefficients. We will reformulate the theory using quantities independent of the choice of modes, and we will also find connections among different in-out Green functions and find their geometrical interpretation, similar to the interpretation of Green functions associated with the one particle interpretation. We will also find that given a Green function with certain properties, we are able to reconstruct two different particle interpretations for which the Green function is an in-out Green function.

Green functions

Let us choose two particle interpretations given by two complex structures J_i and J_f. We will change the letter p to the letters i and f in all quantities defined in the previous chapter. This means that we have two, generally different, vacuum states $|i : vac\rangle$, $|f : vac\rangle$, two sets of creation and annihilation operators etc..

We can define new Green functions, beside G_i^H, $G_i^{\pm}$, G_f^H, $G_f^{\pm}$. Let's define the in-out Hadamard Green function

$$G_{fi}^{H\,\boldsymbol{xy}} = \frac{\langle f : vac|\hat{\Phi}^{\boldsymbol{x}}\hat{\Phi}^{\boldsymbol{y}} + \hat{\Phi}^{\boldsymbol{y}}\hat{\Phi}^{\boldsymbol{x}}|i : vac\rangle}{\langle f : vac|i : vac\rangle} \quad , \tag{8.1}$$

and Wightman functions

$$G^{+\,\boldsymbol{xy}}_{fi} = \frac{\langle f : vac|\hat{\Phi}^{\boldsymbol{x}}\hat{\Phi}^{\boldsymbol{y}}|i : vac\rangle}{\langle f : vac|i : vac\rangle} \quad ,$$
$$G^{-\,\boldsymbol{xy}}_{fi} = \frac{\langle f : vac|\hat{\Phi}^{\boldsymbol{y}}\hat{\Phi}^{\boldsymbol{x}}|i : vac\rangle}{\langle f : vac|i : vac\rangle} \quad . \tag{8.2}$$

For simplicity of the notation in the rest of this chapter we will skip the index fi which these functions and related objects defined below should carry.

Relations similar to equations (6.23), (6.24) and (6.25) hold:

$$G^H = G^+ + G^- \quad , \quad G_c = i(G^+ - G^-) \quad , \tag{8.3}$$
$$G^+ = \frac{1}{2}(G^H - iG_c) \quad , \quad G^- = \frac{1}{2}(G^H + iG_c) \quad , \tag{8.4}$$
$$G^{+\top} = G^- \quad , \quad G^{H\top} = G^H \quad , \quad G_c{}^\top = -G_c \quad . \tag{8.5}$$

These Green functions are again elements from $\boldsymbol{\mathcal{S}}_0^2 \subset \boldsymbol{\mathcal{P}}_0^2$, i.e as bi-scalars they satisfy homogeneous equations of motion in both arguments.

Let us define operators J and $\mathsf{P}^\pm$ on $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$ using equations similar to equations (6.31), (6.32):

$$\mathsf{P}^\pm = \mp i\, G^\pm \circ \overset{\leftrightarrow}{\omega} \quad , \tag{8.6}$$
$$\mathsf{J} = G^H \circ \overset{\leftrightarrow}{\omega} = i\,(\mathsf{P}^+ - \mathsf{P}^-) \quad . \tag{8.7}$$

Using the properties of the f and i vacuum states we get

$$G^+ = \mathsf{P}_f^+ \circ G^+ = G^+ \circ \mathsf{P}_i^- \quad ,$$
$$G^- = \mathsf{P}_i^- \circ G^- = G^- \circ \mathsf{P}_f^+ \quad . \tag{8.8}$$

From this follows

$$\mathsf{P}^+ = \mathsf{P}_f^+ \circ \mathsf{P}^+ = \mathsf{P}^+ \circ \mathsf{P}_i^+ \quad , \quad 0 = \mathsf{P}_f^- \circ \mathsf{P}^+ = \mathsf{P}^+ \circ \mathsf{P}_i^- \quad ,$$
$$\mathsf{P}^- = \mathsf{P}_i^- \circ \mathsf{P}^- = \mathsf{P}^- \circ \mathsf{P}_f^- \quad , \quad 0 = \mathsf{P}_i^+ \circ \mathsf{P}^- = \mathsf{P}^- \circ \mathsf{P}_f^+ \quad , \tag{8.9}$$
$$\mathsf{P}^\pm \circ \mathsf{P}^\mp = 0 \quad , \quad G^\pm \circ \overset{\leftrightarrow}{\omega} \circ G^\mp = 0 \quad . \tag{8.10}$$

From equation (8.3) we get

$$\mathsf{P}^+ + \mathsf{P}^- = \delta_{\boldsymbol{\mathcal{S}}} \quad , \tag{8.11}$$

and it, together with the previous equations, give

$$\mathsf{P}^\pm \circ \mathsf{P}^\pm = \mathsf{P}^\pm \quad , \quad G^\pm \circ \overset{\leftrightarrow}{\omega} \circ G^\pm = \pm i\, G^\pm \quad , \tag{8.12}$$
$$\mathsf{J} \circ \mathsf{J} = -\delta_{\boldsymbol{\mathcal{S}}} \quad , \quad G^H \circ \overset{\leftrightarrow}{\omega} \circ G^H = G_c \quad . \tag{8.13}$$

We can further show

$$\mathsf{P}^\pm \circ \overset{\leftrightarrow}{\omega} \circ \mathsf{P}^\pm = 0 \quad ,$$
$$\overset{\leftrightarrow}{\omega} = \mathsf{P}^+ \circ \overset{\leftrightarrow}{\omega} \circ \mathsf{P}^- + \mathsf{P}^- \circ \overset{\leftrightarrow}{\omega} \circ \mathsf{P}^+ \quad , \tag{8.14}$$
$$\mathsf{J} \circ \overset{\leftrightarrow}{\omega} = -\overset{\leftrightarrow}{\omega} \circ \mathsf{J} \quad . \tag{8.15}$$

We see that J is a complex structure compatible with $\overset{\leftrightarrow}{\omega}$, and $\mathsf{P}^\pm$ are its eigenspace projectors. However, there is a difference from the complex structures J_i or J_f — the complex structure J does not act on the space $\boldsymbol{\mathcal{S}}$ but on the complexified space $\boldsymbol{\mathcal{S}}^{\mathbb{C}}$. More precisely, in general $\mathsf{J}^* \neq \mathsf{J}$, $G^{H*} \neq G^H$, $\mathsf{P}^{\pm *} \neq \mathsf{P}^\mp$, $G^{\pm *} \neq G^\mp$. Therefore the complex structure J does not define a particle interpretation (except, of course, in the degenerate case $\mathsf{J}_f = \mathsf{J}_i = \mathsf{J}$).

We can define real and imaginary parts of the complex structure J by

$$\begin{gathered}\mathsf{J} = M + iN \quad , \\ M = \operatorname{Re}\mathsf{J} = \frac{1}{2}(\mathsf{J}+\mathsf{J}^*) \quad , \quad N = \operatorname{Im}\mathsf{J} = -i\frac{1}{2}(\mathsf{J}-\mathsf{J}^*) \quad .\end{gathered} \tag{8.16}$$

Using equations (8.11), (8.9) and their complex conjugates and previous definitions we get

$$\begin{aligned} M &= i\,(\mathsf{P}^+ - \mathsf{P}^{-*}) = i\,(\mathsf{P}^{-*} - \mathsf{P}^-) \quad , \\ N &= \mathsf{P}^+ + \mathsf{P}^{+*} - \delta_{\mathcal{S}} = \delta_{\mathcal{S}} - \mathsf{P}^- - \mathsf{P}^{-*} \quad , \end{aligned} \tag{8.17}$$

and

$$-\mathsf{J}_f \circ M = -M \circ \mathsf{J}_i = \delta_{\mathcal{S}} + N \quad , \quad -M \circ \mathsf{J}_f = -\mathsf{J}_i \circ M = \delta_{\mathcal{S}} - N \quad . \tag{8.18}$$

This gives us the important relation

$$\big[-\frac{1}{2}(\mathsf{J}_i + \mathsf{J}_f)\big] \circ M = M \circ \big[-\frac{1}{2}(\mathsf{J}_i + \mathsf{J}_f)\big] = \delta_{\mathcal{S}} \tag{8.19}$$

or

$$\frac{1}{2}(G^H + G^{H*}) = \big[\frac{1}{2}(\bar{\omega}_i + \bar{\omega}_f)\big]^{-1} = -\,G_c \circ \big[\frac{1}{2}(G^H_i + G^H_f)\big]^{-1} \circ G_c \quad . \tag{8.20}$$

We will define a real symmetric bi-form $\bar{\omega}$

$$\bar{\omega} = \big[\operatorname{Re} G^H\big]^{-1} = \big[\frac{1}{2}(G^H + G^{H*})\big]^{-1} = \overleftrightarrow{\omega} \circ M^{-1} \quad . \tag{8.21}$$

Using the previous identity we get

$$\bar{\omega} = \frac{1}{2}(\bar{\omega}_i + \bar{\omega}_f) \quad . \tag{8.22}$$

This means that $\bar{\omega}$, and therefore also $\operatorname{Re} G^H$, are positive definite.

The relations among the projectors $\mathsf{P}^\pm, \mathsf{P}^\pm_i, \mathsf{P}^\pm_f$ and the operator J can be translated into composition laws among Green function. Beside equations (8.12), (8.13) we have, for example (using equation (8.8)),

$$G^+_f \circ \overleftrightarrow{\omega} \circ G^+ = i\,G^+ \quad , \quad G^+ \circ \overleftrightarrow{\omega} \circ G^+_i = iG^+ \quad . \tag{8.23}$$

Reconstruction of initial and final particle interpretations

We have found that the Hadamard Green function G^H defined by equation (8.1) satisfies

$$\overleftrightarrow{\mathcal{F}} \bullet G^H = 0 \quad , \quad G^{H\top} = G^H \quad , \tag{8.24}$$

$$G^H \circ \overleftrightarrow{\omega} \circ G^H = G_c \quad , \tag{8.25}$$

$$\bar{\omega} = \big[\operatorname{Re} G^H\big]^{-1} \quad \text{is positive definite} \quad . \tag{8.26}$$

Now we will show the opposite — that any Green function which satisfies these conditions can be written in the form (8.1). This means that for given a Green function G^H which satisfies the conditions above, it is possible to find particle interpretations given by complex structures $\mathsf{J}_i, \mathsf{J}_f$ such that

$$G^{H\boldsymbol{xy}} = \frac{\langle f : vac|\hat{\Phi}^{\boldsymbol{x}}\hat{\Phi}^{\boldsymbol{y}} + \hat{\Phi}^{\boldsymbol{y}}\hat{\Phi}^{\boldsymbol{x}}|i : vac\rangle}{\langle f : vac|i : vac\rangle} \quad . \tag{8.27}$$

Starting from G^H we will define operators $\mathsf{J}, M, N, \bar{\omega}$ in the same way as in the previous section and operators $\mathsf{P}^\pm$ as projectors on eigenspaces of J. From conditions (8.24), (8.25) follow equations (8.13), (8.15), (8.17) and

$$M \circ \overleftrightarrow{\omega} = -\overleftrightarrow{\omega} \circ M \quad , \quad N \circ \overleftrightarrow{\omega} = -\overleftrightarrow{\omega} \circ N \quad . \tag{8.28}$$

Using equation (8.13) we get

$$-\delta_{\boldsymbol{\mathcal{S}}} = M \circ M - N \circ N + i(M \circ N + N \circ M) \tag{8.29}$$

or

$$N \circ N = \delta_{\boldsymbol{\mathcal{S}}} + M \circ M \quad , \tag{8.30}$$

$$M \circ N = -N \circ M \quad . \tag{8.31}$$

It will be helpful in the following derivation to define a real scalar product on the phase space $\boldsymbol{\mathcal{S}}$ and a corresponding transposition using the bi-form $\bar{\omega}$

$$\begin{aligned} (\phi_1, \phi_2) = \phi_1^{\mathrm{T}} \circ \phi_2 = \phi_1 \circ \bar{\omega} \circ \phi_2 \qquad &\text{for} \quad \phi_1, \phi_2 \in \boldsymbol{\mathcal{S}} \quad , \\ A^{\mathrm{T}} = \bar{\omega}^{-1} \circ A \circ \bar{\omega} \qquad &\text{for} \quad A \in \boldsymbol{\mathcal{S}}^1_1 \quad . \end{aligned} \tag{8.32}$$

It is straightforward to show

$$N^{\mathrm{T}} = N \quad , \quad M^{\mathrm{T}} = -M \quad . \tag{8.33}$$

If we define the absolute value $|M|$ and signum σ of the operator M as[7]

$$|M| = (M^{\mathrm{T}} \circ M)^{\frac{1}{2}} = (-M \circ M)^{\frac{1}{2}} \quad , \tag{8.34}$$

$$\sigma = \operatorname{sign} M = M \circ |M|^{-1} = |M|^{-1} \circ M \quad , \tag{8.35}$$

$$M = \sigma \circ |M| = |M| \circ \sigma \tag{8.36}$$

we find

$$\sigma^{\mathrm{T}} = \sigma^{-1} \quad , \quad \sigma^* = \sigma \quad , \tag{8.37}$$

$$\sigma \circ \overset{\leftrightsquigarrow}{\omega} = -\overset{\leftrightsquigarrow}{\omega} \circ \sigma \quad , \tag{8.38}$$

$$\sigma \circ \sigma = -\delta_{\boldsymbol{\mathcal{S}}} \quad , \tag{8.39}$$

$$\sigma \circ \overset{\leftrightsquigarrow}{\omega} \quad \text{is positive definite} \quad , \tag{8.40}$$

$$\sigma \circ N = -N \circ \sigma \tag{8.41}$$

and

$$|M|^{\mathrm{T}} = |M| \quad , \quad |M|^* = |M| \quad , \tag{8.42}$$

$$|M| \circ \overset{\leftrightsquigarrow}{\omega} = \overset{\leftrightsquigarrow}{\omega} \circ |M| \quad , \tag{8.43}$$

$$\big[|M|, N\big] = 0 \quad . \tag{8.44}$$

Therefore $|M|$ and N have common eigenvectors and can be written as functions of a single operator. We can find these operators by solving equation (8.30):

$$N = \operatorname{th}\mathcal{X} \quad , \quad |M| = \big[\operatorname{ch}\mathcal{X}\big]^{-1} \quad . \tag{8.45}$$

The operator $\mathcal{X}$ satisfies

$$\big[N, \mathcal{X}\big] = 0 \quad , \quad \big[|M|, \mathcal{X}\big] = 0 \quad , \tag{8.46}$$

$$\mathcal{X}^{\mathrm{T}} = \mathcal{X} \quad , \quad \mathcal{X}^* = \mathcal{X} \quad , \tag{8.47}$$

$$\mathcal{X} \circ \overset{\leftrightsquigarrow}{\omega} = -\overset{\leftrightsquigarrow}{\omega} \circ \mathcal{X} \quad , \tag{8.48}$$

$$\mathcal{X} \circ \sigma = -\sigma \circ \mathcal{X} \quad . \tag{8.49}$$

The Green function G^H can be written using the operators $\mathcal{X}$ and σ as

$$G^H \circ \overleftrightarrow{\omega} = \sigma \circ \left[\mathrm{ch}\mathcal{X}\right]^{-1} + i\,\mathrm{th}\mathcal{X} \quad . \tag{8.50}$$

We will see below that the operator $\mathcal{X}$ is closely connected with the Bogoljubov transformation and we will call it the *Bogoljubov operator*.

Finally we can define initial and final complex structures

$$\begin{aligned} \mathsf{J}_i &= \exp(-\mathcal{X}) \circ \sigma = \sigma \circ \exp(\mathcal{X}) \quad , \\ \mathsf{J}_f &= \exp(\mathcal{X}) \circ \sigma = \sigma \circ \exp(-\mathcal{X}) \quad . \end{aligned} \tag{8.51}$$

Clearly, they are real complex structures. Compatibility with the symplectic structure follows from equations (8.38), (8.48) and positive definiteness from equation (8.40) and positivity of the exponential function. Therefore J_i and J_f define particle interpretations. Next we have to check equation (8.27). But it is straightforward to show that the real and imaginary parts M, N of the given Green function G^H are the same as the real and imaginary parts of $\frac{\langle f:vac|(\hat{\Phi}\hat{\Phi})+(\hat{\Phi}\hat{\Phi})^{\top}|i:vac\rangle}{\langle f:vac|i:vac\rangle}$ constructed using equations (8.19) and (8.18). For example for the operator M,

$$-\frac{1}{2}(\mathsf{J}_i + \mathsf{J}_f) = -\frac{1}{2}\big(\exp(\mathcal{X}) + \exp(-\mathcal{X})\big) \circ \sigma = \sigma^{-1} \circ \mathrm{ch}\mathcal{X} = M^{-1} \quad , \tag{8.52}$$

which is we wanted to prove.

We have proved that if a Green function G^H satisfying conditions (8.24), (8.25) and (8.24) is given, it is possible to find initial and final particle interpretations defined by equations (8.51) for which the Green function G^H is given by equation (8.27). Similar result can be found in [11].

Additionally, we can prove new properties of the operator $\mathcal{X}$. Using the relations (8.51) and properties of $\mathcal{X}$ (8.48), and (8.49), we find that $\mathcal{X}$ is i-antilinear, f-antilinear and symmetric:

$$\mathcal{X} \circ \mathsf{J}_i = -\mathsf{J}_i \circ \mathcal{X} \quad , \quad \mathcal{X} \circ \mathsf{J}_f = -\mathsf{J}_f \circ \mathcal{X} \quad , \quad \mathcal{X}^{\langle\top\rangle} = \mathcal{X} \quad . \tag{8.53}$$

Bogoljubov operators

We have studied the relation of two particle interpretations from the point of view of Green functions. Now we will compare initial and final creation and annihilation operators.

Because the particle states defined using initial and final particle interpretations are generated by creation and annihilation operators which satisfy the same commutation relations, we can expect that they are related by a unitary transformation. In other words, for any experiment formulated using the initial notion of particles, we can construct an experiment formulated in the same way using the final notion of particles. These experiments will be generally different, but their description should be related by a unitary transformation.

However this "translation" of the initial experiment to the final one is not unique. We have to specify which initial and final states correspond to each other, which states have "the same physical meaning" at the beginning and at the end. We have to specify, for example, how we change modes which we use for labeling of one-particle states.

More precisely, we write a relation of initial and final particle states in following way

$$|f:vac\rangle = \hat{\mathrm{S}}^{\dagger}\,|i:vac\rangle \quad , \tag{8.54}$$

$$\hat{\mathrm{a}}_f[s\circ\phi]^{\dagger}|f:vac\rangle = \hat{\mathrm{S}}^{\dagger}\,\hat{\mathrm{a}}_i[\phi]^{\dagger}|i:vac\rangle \quad , \tag{8.55}$$

where $\hat{\mathrm{S}}$ is a unitary operator on the quantum space $\mathcal{H}$ called the *S-matrix*,

$$\hat{\mathrm{S}}^{\dagger} = \hat{\mathrm{S}}^{-1} \tag{8.56}$$

and s is a *transition operator* on the phase space $\boldsymbol{\mathcal{S}}$ which "translates" initial modes to final modes as we discussed above. This means that an initial one-particle state labeled by a mode ϕ is related by a unitary transformation given by the S-matrix with a final one-particle state labeled by the mode $s\circ\phi$. Of course, the S-matrix depends on a choice of the operator s.

The relation (8.54), (8.55) are equivalent to

$$\begin{aligned}\hat{\mathrm{a}}_f[s\circ\phi] &= \hat{\mathrm{S}}^\dagger\hat{\mathrm{a}}_i[\phi]\hat{\mathrm{S}} \quad ,\\ \hat{\mathrm{a}}_f[s\circ\phi]^\dagger &= \hat{\mathrm{S}}^\dagger\hat{\mathrm{a}}_i[\phi]^\dagger\hat{\mathrm{S}} \quad .\end{aligned} \tag{8.57}$$

Using the commutation relation (6.11) and unitarity of the S-matrix we get a condition on the operator s,

$$\langle s\circ\phi_1, s\circ\phi_2\rangle_f = \langle\phi_1,\phi_2\rangle_i \quad . \tag{8.58}$$

The operator s changes the initial scalar product on the phase space $\boldsymbol{\mathcal{S}}$ to the final one. This is a natural condition which expresses a meaning of the transition operator s — this operator translates the initial labeling of one-particle states to the final one, and therefore it has to map all initial structures on the phase space to the final ones. Consequences of the last equation are

$$s\circ\bar{\omega}_f\circ s = \bar{\omega}_i \quad , \tag{8.59}$$

$$s\circ\overset{\leftrightarrow}{\omega}\circ s = \overset{\leftrightarrow}{\omega} \quad , \tag{8.60}$$

$$\mathsf{J}_f\circ s = s\circ\mathsf{J}_i \quad . \tag{8.61}$$

Using these relations and equation (8.57) we can get another relation between the S-matrix and the operator s,

$$s\circ\hat{\Phi} = \hat{\mathrm{S}}\,\hat{\Phi}\,\hat{\mathrm{S}}^\dagger \quad . \tag{8.62}$$

The transition operator s is closely related to Bogoljubov coefficients between initial and final bases of modes. It can be seen from a decomposition of s to i-linear and i-antilinear parts (see equations (4.17), (4.19))

$$s = \alpha+\beta \quad , \tag{8.63}$$

$$\alpha\circ\mathsf{J}_i = \mathsf{J}_i\circ\alpha \quad , \quad \beta\circ\mathsf{J}_i = -\mathsf{J}_i\circ\beta \quad . \tag{8.64}$$

Explicitly,

$$\begin{aligned}\alpha &= \frac{1}{2}(s-\mathsf{J}_i\circ s\circ\mathsf{J}_i) = \mathsf{P}_i^+\circ s\circ\mathsf{P}_i^+ + \mathsf{P}_i^-\circ s\circ\mathsf{P}_i^- \quad ,\\ \beta &= \frac{1}{2}(s+\mathsf{J}_i\circ s\circ\mathsf{J}_i) = \mathsf{P}_i^+\circ s\circ\mathsf{P}_i^- + \mathsf{P}_i^-\circ s\circ\mathsf{P}_i^+ \quad .\end{aligned} \tag{8.65}$$

This allows us to write relations of initial and final positive and negative frequency projectors,

$$\begin{aligned}\mathsf{P}_f^+\circ s &= \mathsf{P}_i^+\circ\alpha + \mathsf{P}_i^-\circ\beta \quad ,\\ \mathsf{P}_f^-\circ s &= \mathsf{P}_i^-\circ\alpha + \mathsf{P}_i^+\circ\beta\end{aligned} \tag{8.66}$$

and relations of initial and final creation and annihilation operators,

$$\begin{aligned}\hat{\mathrm{a}}_f[s\circ\phi] &= \hat{\mathrm{a}}_i[\alpha\circ\phi] - \hat{\mathrm{a}}_i[\beta\circ\phi]^\dagger \quad ,\\ \hat{\mathrm{a}}_f[s\circ\phi]^\dagger &= \hat{\mathrm{a}}_i[\alpha\circ\phi]^\dagger - \hat{\mathrm{a}}_i[\beta\circ\phi] \quad .\end{aligned} \tag{8.67}$$

This expresses the final creation and annihilation operators as a mixture of both initial creation and annihilation operators. It shows explicitly that the initial and final notion of particles are really different for $\beta\neq 0$. The relations (8.67) are a base-independent definition of the Bogoljubov transformation, and we will call the operators α,β also *Bogoljubov operators*.

Now we will investigate properties of Bogoljubov operators. It is straightforward to show (see equations (4.22), (4.24) and (4.25) for definitions of the operations used) that

$$s^{-1} = -\mathsf{J}_i \circ s^{\mathrm{T}_i} \circ \mathsf{J}_i = \alpha^{\langle\dagger\rangle} - \beta^{\langle\top\rangle} \quad , \tag{8.68}$$

$$s \circ s^{\mathrm{T}_i} = -\mathsf{J}_f \circ \mathsf{J}_i \quad . \tag{8.69}$$

Substituting this and equation (8.63) into $\delta_{\boldsymbol{\mathcal{S}}} = s \circ s^{-1} = s^{-1} \circ s$ and taking i-linear and i-antilinear parts, we get identities

$$\alpha \circ \alpha^{\langle\dagger\rangle} - \beta \circ \beta^{\langle\top\rangle} = \delta_{\boldsymbol{\mathcal{S}}} \quad , \quad \alpha^{\langle\dagger\rangle} \circ \alpha - \beta^{\langle\top\rangle} \circ \beta = \delta_{\boldsymbol{\mathcal{S}}} \quad , \tag{8.70}$$

$$\beta \circ \alpha^{\langle\dagger\rangle} = \alpha \circ \beta^{\langle\top\rangle} \quad , \quad \alpha^{\langle\dagger\rangle} \circ \beta = \beta^{\langle\top\rangle} \circ \alpha \quad , \tag{8.71}$$

and their consequences

$$\alpha^{-1\,\langle\dagger\rangle} = \alpha - \beta \circ \alpha^{-1} \circ \beta \quad , \tag{8.72}$$

$$\beta \circ \alpha^{-1} = \left[\beta \circ \alpha^{-1}\right]^{\langle\top\rangle} \quad , \quad \alpha^{-1} \circ \beta = \left[\alpha^{-1} \circ \beta\right]^{\langle\top\rangle} \quad . \tag{8.73}$$

The transition operator s is not fixed by equation (8.58) uniquely; we have some freedom in the selection of this operator. It corresponds to the freedom in the labeling of our one-particle states. We can change the labeling of initial one-particle states by an i-unitary transformation of the phase space without changing the initial notion of particles and similarly with the final particles. If we have two different transition operators s_a and s_b for translation of initial modes to final modes, they both have to satisfy equation (8.58), and we easily see that they have to be related by

$$s_a = s_b \circ u_i = u_f \circ s_b \quad , \tag{8.74}$$

where u_i (u_f respectively) is an i-linear and i-unitary (f-linear and f-unitary respectively) operator on the phase space $\boldsymbol{\mathcal{S}}$ (see equations (4.17), (4.22))

$$\begin{aligned} u_i \circ \mathsf{J}_i = \mathsf{J}_i \circ u_i \quad &, \quad u_i^{\langle\dagger\rangle} = u_i^{-1} \quad , \\ u_f \circ \mathsf{J}_f = \mathsf{J}_f \circ u_f \quad &, \quad u_f^{\langle\dagger\rangle} = u_f^{-1} \quad . \end{aligned} \tag{8.75}$$

All these equations can be simplified if we choose a special transition operator s. The operator

$$s_o = \exp \mathcal{X} = -\sigma \circ \mathsf{J}_i = -\mathsf{J}_f \circ \sigma = \left[-\mathsf{J}_f \circ \mathsf{J}_i\right]^{\frac{1}{2}} \tag{8.76}$$

satisfies conditions (8.60) and (8.61) and therefore also the condition (8.58), and so we can use it as a special transition operator for the translation of initial to final modes. We will call this choice *canonical*. We can define canonical Bogoljubov operators α_o, β_o by equation (8.65), and than by using equation (8.59), we get

$$\begin{gathered} s_o = \exp(\mathcal{X}) = \alpha_o + \beta_o \quad , \quad s_o^{-1} = \exp(-\mathcal{X}) = \alpha_o - \beta_o \quad , \\ \alpha_o = \mathrm{ch}\mathcal{X} \quad , \quad \beta_o = \mathrm{sh}\mathcal{X} \quad , \\ \alpha_o \circ \mathsf{J}_{i,f} = \mathsf{J}_{i,f} \circ \alpha_o \quad , \quad \beta_o \circ \mathsf{J}_{i,f} = -\mathsf{J}_{i,f} \circ \beta_o \quad , \end{gathered} \tag{8.77}$$

$$\begin{gathered} s_o^{\mathrm{T}_i} = s_o \quad , \quad s_o^{\mathrm{T}_f} = s_o \quad , \\ \alpha_o^{\langle\dagger\rangle} = \alpha_o \quad , \quad \beta_o^{\langle\top\rangle} = \beta_o \quad . \end{gathered} \tag{8.78}$$

We also see that the operators α_o and $-\beta_o$ play the role of inverse canonical Bogoljubov operators for the transformation from final to initial particle states.

A weaker version of these relations can be derived for general Bogoljubov operators α, β. Using eqs. (8.68), (8.74) and (8.77) we find

$$\begin{aligned} s &= \exp(\mathcal{X}) \circ u_i = \alpha + \beta \quad , \\ s^{\text{-}1\,\mathrm{T}_i} &= \exp(-\mathcal{X}) \circ u_i = \alpha - \beta \quad . \end{aligned} \tag{8.79}$$

This immediately gives

$$\begin{gathered} \alpha = \mathrm{ch}\mathcal{X} \circ u_i \quad , \quad \beta = \mathrm{sh}\mathcal{X} \circ u_i \quad , \\ \beta \circ \alpha^{\text{-}1} = \mathrm{th}\mathcal{X} \quad . \end{gathered} \tag{8.80}$$

Now we will show a connection with standard Bogoljubov coefficients. Let's assume that i-orthonormal and f-orthonormal bases $\mathbf{u} = \{u_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$ and $\mathbf{v} = \{v_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$, respectively, for the description of initial and final modes, are chosen. These define the transition operator s by the conditions

$$v_{\mathrm{k}} = s \circ u_{\mathrm{k}} \quad , \quad \mathsf{J}_f \circ v_{\mathrm{k}} = s \circ \mathsf{J}_i \circ u_{\mathrm{k}} \tag{8.81}$$

for all $\mathrm{k} \in \mathcal{I}$. The Bogoljubov coefficients $\alpha_{\mathrm{kl}}, \beta_{\mathrm{kl}}$ are defined by equations [7]

$$v_{\mathrm{k}}{}^{+}_{f} = \sum_{\mathrm{k}\in\mathcal{I}} \big(u_{\mathrm{l}}{}^{+}_{i}\, \alpha_{\mathrm{lk}} + u_{\mathrm{l}}{}^{-}_{i}\, \beta_{\mathrm{lk}} \big) \quad . \tag{8.82}$$

Using equation (8.66) we see

$$\alpha_{\mathrm{kl}} = \langle u_{\mathrm{k}}, \alpha \circ u_{\mathrm{l}} \rangle_i \quad , \quad \beta_{\mathrm{kl}} = \langle u_{\mathrm{k}}, \beta \circ u_{\mathrm{l}} \rangle_i \quad , \tag{8.83}$$

i.e., the Bogoljubov coefficients are matrix elements of the Bogoljubov operators in a chosen base.

We can use eigenvectors of the operator $\mathcal{X}$ to define special bases of initial and final modes — so called *canonical bases* [12]. Because the operator $\mathcal{X}$ is i-symmetric it has a complete set of eigenvectors. From i-antilinearity follows that for each eigenvector u the vector $\mathsf{J}_i \circ u$ is also an eigenvector with the opposite sign of the eigenvalue. Therefore we can choose an $\mathbb{R}$-base $\{u_{\mathrm{k}}, \mathsf{J}_i \circ u_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$ such that

$$\begin{aligned} \mathcal{X} \circ u_{\mathrm{k}} &= \chi_{\mathrm{k}}\, u_{\mathrm{k}} \quad , \qquad \chi_{\mathrm{k}} \geqslant 0 \quad , \\ \mathcal{X} \circ \mathsf{J}_i \circ u_{\mathrm{k}} &= -\chi_{\mathrm{k}}\, \mathsf{J}_i \circ u_{\mathrm{k}} \quad . \end{aligned} \tag{8.84}$$

The base can be chosen orthonormal with respect to the real scalar product defined by the bi-form $\bar{\omega}_i$,

$$u_{\mathrm{k}} \circ \bar{\omega}_i \circ u_{\mathrm{l}} = \delta_{\mathrm{kl}} \quad , \quad u_{\mathrm{k}} \circ \bar{\omega}_i \circ \mathsf{J}_i \circ u_{\mathrm{l}} = 0 \quad . \tag{8.85}$$

If the operator $\mathcal{X}$ is non-degenerate with different eigenvalues, the base is fixed uniquely. The subset $\{u_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$ of this $\mathbb{R}$-base forms the i-orthonormal $\mathbb{C}$-base. It will be used for labeling of initial particles. The final f-orthonormal $\mathbb{C}$-base $\{v_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}\}$ will be generated by the canonical transition operator s_o,

$$v_{\mathrm{k}} = s_o \circ u_{\mathrm{k}} = \exp(\chi_{\mathrm{k}})\, u_{\mathrm{k}} \quad . \tag{8.86}$$

The Bogoljubov transformation between these two bases is

$$v_{\mathrm{k}}{}^{+}_{f} = u_{\mathrm{k}}{}^{+}_{i}\, \mathrm{ch}(\chi_{\mathrm{k}}) + u_{\mathrm{k}}{}^{-}_{i}\, \mathrm{sh}(\chi_{\mathrm{k}}) \quad , \tag{8.87}$$

and the final and initial creation and annihilation operators are related by

$$\begin{aligned} \hat{\mathrm{a}}_f[v_{\mathrm{k}}] &= \hat{\mathrm{a}}_i[u_{\mathrm{k}}]\mathrm{ch}(\chi_{\mathrm{k}}) - \hat{\mathrm{a}}_i[u_{\mathrm{k}}]^\dagger \mathrm{sh}(\chi_{\mathrm{k}}) \quad , \\ \hat{\mathrm{a}}_f[v_{\mathrm{k}}]^\dagger &= \hat{\mathrm{a}}_i[u_{\mathrm{k}}]^\dagger \mathrm{ch}(\chi_{\mathrm{k}}) - \hat{\mathrm{a}}_i[u_{\mathrm{k}}]\mathrm{sh}(\chi_{\mathrm{k}}) \quad . \end{aligned} \tag{8.88}$$

Elementary transition amplitudes

Now we are prepared to calculate in-out transition amplitudes, i.e., amplitudes between initial and final particle states. In the next section we show (see also [7]) that amplitudes between many-particle states can be reduced to one-particle transition amplitudes. Therefore we will calculate only these simple amplitudes. First, using equation (8.67) and its inverse, we get the identities

$$\begin{aligned} \hat{\mathrm{a}}_i[\phi]^\dagger &= \hat{\mathrm{a}}_f[s\circ\alpha^{-1}\circ\phi]^\dagger + \hat{\mathrm{a}}_i[\beta\circ\alpha^{-1}\circ\phi] \quad , \\ \hat{\mathrm{a}}_f[\phi] &= \hat{\mathrm{a}}_i[s^{-1}\circ\alpha^{-1\,\langle\dagger\rangle}\circ\phi] - \hat{\mathrm{a}}_f[\beta^{\langle\top\rangle}\circ\alpha^{-1\,\langle\dagger\rangle}\circ\phi]^\dagger \quad . \end{aligned} \tag{8.89}$$

Now it is easy to check that vacuum – one-particle transition amplitudes vanish

$$\begin{aligned} &\langle f:vac|\hat{\mathrm{a}}_i[\phi]^\dagger|i:vac\rangle = \langle f:vac|\big(\hat{\mathrm{a}}_f[s\circ\alpha^{-1}\circ\phi]^\dagger + \hat{\mathrm{a}}_i[\beta\circ\alpha^{-1}]\big)|i:vac\rangle = 0 \quad , \\ &\langle f:vac|\hat{\mathrm{a}}_f[\phi]|i:vac\rangle = 0 \quad . \end{aligned} \tag{8.90}$$

The one-particle to one-particle transition amplitude is

$$\begin{aligned} &\frac{\langle f:vac|\hat{\mathrm{a}}_f[s\circ\phi_1]\hat{\mathrm{a}}_i[\phi_2]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &\quad = \frac{\langle f:vac|\hat{\mathrm{a}}_f[s\circ\phi_1]\big(\hat{\mathrm{a}}_f[s\circ\alpha^{-1}\circ\phi_2]^\dagger + \hat{\mathrm{a}}_i[\beta\circ\alpha^{-1}\circ\phi_2]\big)|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &\quad = \langle s\circ\phi_1, s\circ\alpha^{-1}\circ\phi_2\rangle_f = \langle\phi_1,\alpha^{-1}\circ\phi_2\rangle_i \quad , \end{aligned} \tag{8.91}$$

where we have used the commutation relation (6.11). Vacuum to two-particle transition amplitudes are

$$\begin{aligned} &\frac{\langle f:vac|\hat{\mathrm{a}}_i[\phi_1]^\dagger\hat{\mathrm{a}}_i[\phi_2]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &\quad = \frac{\langle f:vac|\big(\hat{\mathrm{a}}_f[s\circ\alpha^{-1}\circ\phi_1]^\dagger + \hat{\mathrm{a}}_i[\beta\circ\alpha^{-1}\circ\phi_1]\big)\hat{\mathrm{a}}_i[\phi_2]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &\quad = \langle\beta\circ\alpha^{-1}\circ\phi_1,\phi_2\rangle_i \quad , \end{aligned} \tag{8.92}$$

$$\frac{\langle f:vac|\hat{\mathrm{a}}_f[s\circ\phi_1]\hat{\mathrm{a}}_f[s\circ\phi_2]|i:vac\rangle}{\langle f:vac|i:vac\rangle} = -\langle\phi_1,\alpha^{-1}\circ\beta\circ\phi_2\rangle_i \quad . \tag{8.93}$$

These expressions are connected more closely with initial modes — we have used a transition operator s to generate final modes. It is also possible to obtain translation amplitudes without this asymmetry. Simply choosing the canonical operator s_o and doing some algebra, we can get

$$\begin{aligned} \phi_1\circ\mathrm{I}\circ\phi_2 &\overset{\text{def}}{=} \frac{\langle f:vac|\hat{\mathrm{a}}_f[\phi_1]\hat{\mathrm{a}}_i[\phi_2]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &= \langle(\delta_{\boldsymbol{\mathcal{S}}}-\mathrm{th}\mathcal{X})\circ\phi_1,\phi_2\rangle_i = \langle\phi_1,(\delta_{\boldsymbol{\mathcal{S}}}+\mathrm{th}\mathcal{X})\circ\phi_2\rangle_f = \\ &= -\phi_1\circ\overset{\leftrightsquigarrow}{\omega}\circ G^+\circ\overset{\leftrightsquigarrow}{\omega}\circ\phi_2 \quad , \end{aligned} \tag{8.94}$$

$$\begin{aligned} \phi_1\circ\Lambda\circ\phi_2 &\overset{\text{def}}{=} \frac{\langle f:vac|\hat{\mathrm{a}}_i[\phi_1]^\dagger\hat{\mathrm{a}}_i[\phi_2]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &= \langle\mathrm{th}(\mathcal{X})\circ\phi_1,\phi_2\rangle_i = \frac{1}{2}\,\phi_1\circ\mathsf{P}_i^+\circ\overset{\leftrightsquigarrow}{\omega}\circ G^H\circ\overset{\leftrightsquigarrow}{\omega}\circ\mathsf{P}_i^+\circ\phi_2 \quad , \end{aligned} \tag{8.95}$$

$$\begin{aligned} \phi_1\circ\mathrm{V}\circ\phi_2 &\overset{\text{def}}{=} \frac{\langle f:vac|\hat{\mathrm{a}}_f[\phi_1]\hat{\mathrm{a}}_f[\phi_2]|i:vac\rangle}{\langle f:vac|i:vac\rangle} = \\ &= -\langle\phi_1,\mathrm{th}(\mathcal{X})\circ\phi_2\rangle_f = \frac{1}{2}\phi_1\circ\mathsf{P}_f^-\circ\overset{\leftrightsquigarrow}{\omega}\circ G^H\circ\overset{\leftrightsquigarrow}{\omega}\circ\mathsf{P}_f^-\circ\phi_2 \quad . \end{aligned} \tag{8.96}$$

We have thus calculated the in-out one-particle transition amplitudes, except for calculating the normalization factor $\langle f : vac | i : vac\rangle$. We will derive it in the next section — see equation (8.110).

Other interesting physical quantities are the mean number of final particles in the initial vacuum. Using the identities (8.67) we get

$$\begin{aligned}
&\langle i : vac|\hat{\mathrm{n}}_f[s_o \circ \phi]|i : vac\rangle = \\
&= \frac{\langle i : vac|\hat{\mathrm{a}}_f[s_o \circ \phi]^\dagger \hat{\mathrm{a}}_i[s_o \circ \phi]|i : vac\rangle}{\langle \phi, \phi\rangle_i} = \\
&= \frac{\langle i : vac|\big(\hat{\mathrm{a}}_i[\alpha_o \circ \phi]^\dagger - \hat{\mathrm{a}}_i[\beta_o \circ \phi]\big)\big(\hat{\mathrm{a}}_i[\alpha_o \circ \phi] - \hat{\mathrm{a}}_i[\beta_o \circ \phi]^\dagger\big)|i : vac\rangle}{\langle \phi, \phi\rangle_i} = \\
&= \frac{\langle \beta_o \circ \phi, \beta_o \circ \phi\rangle_i}{\langle \phi, \phi\rangle_i} = \frac{\langle \mathrm{sh}(\mathcal{X}) \circ \phi, \mathrm{sh}(\mathcal{X}) \circ \phi\rangle_i}{\langle \phi, \phi\rangle_i} \quad .
\end{aligned} \tag{8.97}$$

This means

$$\langle i : vac|\hat{\mathrm{n}}_f[\phi]|i : vac\rangle = \frac{\langle \mathrm{sh}(\mathcal{X}) \circ \phi, \mathrm{sh}(\mathcal{X}) \circ \phi\rangle_f}{\langle \phi, \phi\rangle_f} \quad , \tag{8.98}$$

and similarly

$$\langle f : vac|\hat{\mathrm{n}}_i[\phi]|f : vac\rangle = \frac{\langle \mathrm{sh}(\mathcal{X}) \circ \phi, \mathrm{sh}(\mathcal{X}) \circ \phi\rangle_i}{\langle \phi, \phi\rangle_i} \quad . \tag{8.99}$$

The mean total number of particles is

$$\langle i : vac|\hat{\mathrm{N}}_f|i : vac\rangle = \sum_{\mathrm{k}\in\mathcal{I}} \langle i : vac|\hat{\mathrm{n}}_f[v_\mathrm{k}]|i : vac\rangle = \sum_{\mathrm{k}\in\mathcal{I}} \langle v_\mathrm{k}, (\mathrm{sh}\mathcal{X})^2 \circ v_\mathrm{k}\rangle_f \tag{8.100}$$

for some f-orthonormal $\mathbb{C}$-base, i.e.

$$\langle i : vac|\hat{\mathrm{N}}_f|i : vac\rangle = \mathrm{tr}_{\boldsymbol{\mathcal{S}}_f}(\mathrm{sh}\mathcal{X})^2 = \sum_{\mathrm{k}\in\mathcal{I}} (\mathrm{sh}\chi_\mathrm{k})^2 \tag{8.101}$$

and similarly

$$\langle f : vac|\hat{\mathrm{N}}_i|f : vac\rangle = \mathrm{tr}_{\boldsymbol{\mathcal{S}}_i}(\mathrm{sh}\mathcal{X})^2 = \sum_{\mathrm{k}\in\mathcal{I}} (\mathrm{sh}\chi_\mathrm{k})^2 \quad . \tag{8.102}$$

When this quantity is finite, one has a unitary equivalence of the initial and final particle representations of the quantum algebra and regularity of the vacuum – vacuum amplitude (8.110) (see [3,4]).

S-matrix

After computing the elementary transition amplitudes we turn to investigate the S-matrix in more detail, and we derive the structure of multiple-particle transition amplitudes. We will compute the S-matrix using the holomorphic representation to show the advantages of this method. We can write, combining equations (8.57) and (8.67),

$$\begin{aligned}
\hat{\mathrm{S}}\,(\hat{\mathrm{a}}_i[\alpha \circ \phi] - \hat{\mathrm{a}}_i[\beta \circ \phi]^\dagger) &= \hat{\mathrm{a}}_i[\phi]\,\hat{\mathrm{S}} \quad , \\
\hat{\mathrm{S}}\,(\hat{\mathrm{a}}_i[\alpha \circ \phi]^\dagger - \hat{\mathrm{a}}_i[\beta \circ \phi]) &= \hat{\mathrm{a}}_i[\phi]^\dagger\,\hat{\mathrm{S}} \quad .
\end{aligned} \tag{8.103}$$

The holomorphic representation of these equations using the action of the annihilation and creation operators (7.24) is

$$\begin{aligned}
\Big(\big[\langle \alpha \circ \phi, \phi_2\rangle_i - \phi \circ \beta \circ \mathrm{d}_\mathbf{r}\big]\mathfrak{f}_i\,\big[\hat{\mathrm{S}}\big]\Big)(\phi_1, \phi_2) &= \phi \circ \big(\mathrm{d}_\mathbf{l}\mathfrak{f}_i\,\big[\hat{\mathrm{S}}\big]\big)(\phi_1, \phi_2) \quad , \\
\Big(\big[\phi \circ \alpha \circ \mathrm{d}_\mathbf{r} - \langle \beta \circ \phi, \phi_2\rangle_i\big]\mathfrak{f}_i\,\big[\hat{\mathrm{S}}\big]\Big)(\phi_1, \phi_2) &= \langle \phi_1, \phi\rangle_i\,\mathfrak{f}_i\,\big[\hat{\mathrm{S}}\big](\phi_1, \phi_2) \quad .
\end{aligned} \tag{8.104}$$

Solving the latter equation with respect to the variation term, substituting it into the former and using identity (8.72), we get

$$\begin{aligned} \phi \circ \mathrm{d}_{\mathrm{l}}\, \mathfrak{f}_i \left[\hat{\mathrm{S}}\right] &= \left(\langle \phi, \alpha^{-1} \circ \phi_2 \rangle_i - \langle \phi_1, \alpha^{-1} \circ \beta \circ \phi \rangle_i\right) \mathfrak{f}_i \left[\hat{\mathrm{S}}\right] \quad , \\ \phi \circ \mathrm{d}_{\mathrm{r}}\, \mathfrak{f}_i \left[\hat{\mathrm{S}}\right] &= \left(\langle \phi_1, \alpha^{-1} \circ \phi \rangle_i + \langle \beta \circ \alpha^{-1} \circ \phi, \phi_2 \rangle_i\right) \mathfrak{f}_i \left[\hat{\mathrm{S}}\right] \quad . \end{aligned} \tag{8.105}$$

The solution to these variation equations is

$$\begin{aligned} &\mathfrak{f}_i \left[\hat{\mathrm{S}}\right](\phi_1, \phi_2) = \\ &\quad = \mathrm{o}\ \exp\left(-\frac{1}{2}\langle \phi_1, \alpha^{-1} \circ \beta \circ \phi_1 \rangle_i + \frac{1}{2}\langle \beta \circ \alpha^{-1} \circ \phi_2, \phi_2 \rangle_i + \langle \phi_1, \alpha^{-1} \circ \phi_2 \rangle_i\right) \quad , \end{aligned} \tag{8.106}$$

where we have used definitions (8.94-8.96) and the symmetry of V and Λ. The prefactor o can be obtained from the unitarity of the S-matrix,

$$\hat{\mathrm{S}}^\dagger \hat{\mathrm{S}} = \hat{1\!\!1} \quad . \tag{8.107}$$

The holomorphic representation of this condition leads to a Gaussian integral which can be done explicitly, giving the prefactor (with the simplest choice of the phase)

$$\mathrm{o} = \left(\det_{\boldsymbol{\mathcal{S}}}\ \mathrm{ch}\mathcal{X}\right)^{-\frac{1}{4}} = \left(\det_{\boldsymbol{\mathcal{S}}_i}\ \mathrm{ch}\mathcal{X}\right)^{-\frac{1}{2}} = \Big(\prod_{\mathrm{k}\in\mathcal{I}} \mathrm{ch}\chi_{\mathrm{k}}\Big)^{-\frac{1}{2}} \quad . \tag{8.108}$$

Note that this is nonzero if and only if the mean number of particles, given by (8.102) is finite, i.e., if and only if there is a unitary equivalence between the initial and final particle representations. If $\mathrm{o} = 0$, the equations of this section are merely formal.

From the holomorphic representation of the S-matrix, we can get a normal-ordered form of the S-matrix using equation (7.42):

$$\hat{\mathrm{S}} = \mathrm{o} \,\boldsymbol{:}\exp\Big(\frac{1}{2}\langle \beta \circ \alpha^{-1} \circ \hat{\Phi}, \hat{\Phi} \rangle_i - \frac{1}{2}\langle \hat{\Phi}, \alpha^{-1} \circ \beta \circ \hat{\Phi} \rangle_i + \langle \hat{\Phi}, \alpha^{-1} \circ \hat{\Phi} \rangle_i - \langle \hat{\Phi}, \hat{\Phi} \rangle_i\Big)\boldsymbol{:}_i \tag{8.109}$$

Now we can find a meaning of the prefactor o:

$$\langle f : vac | i : vac \rangle = \langle i : vac | \hat{\mathrm{S}} | i : vac \rangle = \mathrm{o} = \left(\det_{\boldsymbol{\mathcal{S}}_i}\ \mathrm{ch}\mathcal{X}\right)^{-\frac{1}{2}} \quad . \tag{8.110}$$

We can also express the final vacuum using initial particle states

$$| f : vac \rangle = \langle i : vac | f : vac \rangle \ \exp\left(\frac{1}{2}\hat{\Phi} \circ \Lambda^* \circ \hat{\Phi}\right) | i : vac \rangle \quad . \tag{8.111}$$

It is possible to find an explicit expression for the S-matrix without normal ordering. A derivation in appendix E gives the S-matrix associated with a transition operator s as

$$\hat{\mathrm{S}} = \exp\Big(-i\langle \hat{\Phi}, \psi \circ \hat{\Phi} \rangle_i\Big) \ \exp\left(\frac{1}{2}\langle \mathcal{X} \circ \hat{\Phi}, \hat{\Phi} \rangle_i - \frac{1}{2}\langle \hat{\Phi}, \mathcal{X} \circ \hat{\Phi} \rangle_i\right) \quad , \tag{8.112}$$

where ψ is an i-linear i-hermitian operator on the phase space $\boldsymbol{\mathcal{S}}$ defined by

$$\begin{aligned} s = s_o \circ u_i &= s_o \circ \exp\left(\mathsf{J}_i \circ \psi\right) \quad , \\ \psi \circ \mathsf{J}_i = \mathsf{J}_i \circ \psi \quad &, \quad \psi^{\langle\dagger\rangle} = \psi \quad . \end{aligned} \tag{8.113}$$

In-out holomorphic representation

The S-matrix formalism has a disadvantage of introducing an additional structure — the transition operator s. If we are interested in transition amplitudes of the type (8.94-8.96), we do not need to choose the transition operator. Therefore we introduce an *in-out holomorphic representation* which will be a better tool for the computation of general transition amplitudes between independently described initial and final states.

The in-out holomorphic representation can be introduced if we have two particle interpretations given by complex structures J_f, J_i. It is a mixture of the final and initial holomorphic representations — vectors from the quantum space are represented using the f-representation and covectors are represented using the i-holomorphic representation:

$$\begin{aligned} \mathfrak{f}\left[|st\rangle\right](\phi) &= \langle f\ coh : \phi|st\rangle \quad , \\ \mathfrak{f}\left[\langle st|\right](\phi) &= \langle st|i\ coh : \phi\rangle \quad , \\ \mathfrak{f}\left[\hat{\mathrm{A}}\right](\phi_{\mathrm{f}}, \phi_{\mathrm{i}}) &= \langle f\ coh : \phi_{\mathrm{f}}|\hat{\mathrm{A}}|i\ coh : \phi_{\mathrm{i}}\rangle \quad . \end{aligned} \tag{8.114}$$

It has properties similar to (7.24):

$$\begin{aligned} \mathfrak{f}\left[\hat{\mathrm{a}}_f[\phi]^\dagger|st\rangle\right](\phi_{\mathrm{f}}) &= \langle\phi_{\mathrm{f}}, \phi\rangle_f\, \mathfrak{f}\left[|st\rangle\right](\phi_{\mathrm{f}}) \quad , \\ \mathfrak{f}\left[\hat{\mathrm{a}}_f[\phi]|st\rangle\right](\phi_{\mathrm{f}}) &= \phi \circ \big(\mathrm{d}\, \mathfrak{f}\left[|st\rangle\right]\big)(\phi_{\mathrm{f}}) \quad , \\ \mathfrak{f}\left[\langle st|\hat{\mathrm{a}}_i[\phi]\right](\phi_{\mathrm{i}}) &= \langle\phi, \phi_{\mathrm{i}}\rangle_i\, \mathfrak{f}\left[\langle st|\right](\phi_{\mathrm{i}}) \quad , \\ \mathfrak{f}\left[\langle st|\hat{\mathrm{a}}_i[\phi]^\dagger\right](\phi_{\mathrm{i}}) &= \phi \circ \big(\mathrm{d}\, \mathfrak{f}\left[\langle st|\right]\big)(\phi_{\mathrm{i}}) \quad . \end{aligned} \tag{8.115}$$

We can also find equivalents to expressions (7.25-7.28):

$$\mathfrak{f}\left[|f : vac\rangle\right](\phi) = 1 \quad , \quad \mathfrak{f}\left[\langle i : vac|\right](\phi) = 1 \quad , \tag{8.116}$$

$$\mathfrak{f}\left[\hat{\mathrm{a}}_f[\phi]^{\dagger\, n}|f : vac\rangle\right](\phi_{\mathrm{f}}) = \langle\phi_{\mathrm{f}}, \phi\rangle_f{}^n \quad , \quad \mathfrak{f}\left[\langle i : vac|\hat{\mathrm{a}}_i[\phi]^n\right](\phi_{\mathrm{i}}) = \langle\phi, \phi_{\mathrm{i}}\rangle_i{}^n \quad , \tag{8.117}$$

$$\mathfrak{f}\left[|f\ coh : \phi\rangle\right](\phi_{\mathrm{f}}) = \exp\big(\langle\phi_{\mathrm{f}}, \phi\rangle_f\big) \quad , \quad \mathfrak{f}\left[\langle i\ coh : \phi|\right](\phi_{\mathrm{i}}) = \exp\big(\langle\phi, \phi_{\mathrm{i}}\rangle_i\big) \quad , \tag{8.118}$$

$$\mathfrak{f}\left[|f : vac\rangle\langle i : vac|\right](\phi_{\mathrm{f}}, \phi_{\mathrm{i}}) = 1 \quad . \tag{8.119}$$

We can formulate the following "trace-composition law":

$$\mathrm{Tr}\big(\hat{\mathrm{A}}_1^\dagger \hat{\mathrm{A}}_2\big) = \int\limits_{\phi_f ix, \phi_{\mathrm{i}} \in \boldsymbol{S}} \mathfrak{H}_f(\phi_{\mathrm{f}})\mathfrak{H}_i(\phi_{\mathrm{i}})\, \mathfrak{f}\left[\hat{\mathrm{A}}_1\right](\phi_{\mathrm{f}}, \phi_{\mathrm{i}})^*\, \mathfrak{f}\left[\hat{\mathrm{A}}_2\right](\phi_{\mathrm{f}}, \phi_{\mathrm{i}})^* \quad , \tag{8.120}$$

which is a consequence of (7.23). But it is not straightforward to find composition laws more similar to (7.23).

Now we compute the in-out holomorphic representation of the unit operator. From eq. (8.55) follows

$$\langle f\ coh : \phi| = \langle i\ coh : s^{-1} \circ \phi|\, \hat{\mathrm{S}} \quad , \tag{8.121}$$

and therefore, using (8.109) and definitions (8.94-8.96) of I, V, Λ, we get

$$\begin{aligned} \langle f\ coh : \phi_{\mathrm{f}}|i\ coh : \phi_{\mathrm{i}}\rangle &= \mathfrak{f}\left[\hat{\mathbb{1}}\right](\phi_{\mathrm{f}}, \phi_{\mathrm{i}}) = \mathfrak{f}_i\left[\hat{\mathrm{S}}\right](s^{-1} \circ \phi_{\mathrm{f}}, \phi_{\mathrm{i}}) = \\ &= \mathrm{o}\ \exp\Big(\frac{1}{2}\phi_{\mathrm{f}} \circ \mathrm{V} \circ \phi_{\mathrm{f}} + \frac{1}{2}\phi_{\mathrm{i}} \circ \Lambda \circ \phi_{\mathrm{i}} + \phi_{\mathrm{f}} \circ \mathrm{I} \circ \phi_{\mathrm{i}}\Big) \quad . \end{aligned} \tag{8.122}$$

As we will see in the next section, this is a generating function for the multiple-particle amplitudes.

Next we can find the in-out holomorphic representation of the displacement operator. Using again the definition of coherent states, the additivity property of the displacement operator (7.8) and properties of the amplitudes I, V and Λ, we obtain

$$
\begin{aligned}
&\langle f\, coh : \phi_{\mathrm{f}} | \hat{\mathrm{W}}[\phi] | i\, coh : \phi_{\mathrm{i}} \rangle = \langle f : vac | \hat{\mathrm{W}}[\phi] | i : vac \rangle \times \\
&\quad \times \exp\big(\tfrac{1}{2}\phi_{\mathrm{f}} \circ \mathrm{V} \circ \phi_{\mathrm{f}} + \tfrac{1}{2}\phi_{\mathrm{i}} \circ \Lambda \circ \phi_{\mathrm{i}} + \phi_{\mathrm{f}} \circ \mathrm{I} \circ \phi_{\mathrm{i}} + \phi_{\mathrm{f}} \circ \mathrm{I} \circ \phi - \phi \circ \mathrm{I} \circ \phi_{\mathrm{i}}\big) \quad .
\end{aligned}
\tag{8.123}
$$

A similar calculation shows

$$
\langle f : vac | \hat{\mathrm{W}}[\phi] | i : vac \rangle = \mathrm{o}\, \exp\big(-\phi \circ \mathrm{I} \circ \phi\big) \quad . \tag{8.124}
$$

A slightly different calculation leads to the mean value of the field

$$
\begin{aligned}
&\frac{\langle f\, coh : \phi_{\mathrm{f}} | \hat{\Phi} | i\, coh : \phi_{\mathrm{i}} \rangle}{\langle f\, coh : \phi_{\mathrm{f}} | i\, coh : \phi_{\mathrm{i}} \rangle} = \frac{\langle f\, coh : \phi_{\mathrm{f}} | \big(\hat{\Phi}_i^{+} + \hat{\Phi}_i^{-}\big) | i\, coh : \phi_{\mathrm{i}} \rangle}{\langle f\, coh : \phi_{\mathrm{f}} | i\, coh : \phi_{\mathrm{i}} \rangle} = \\
&\quad = {\phi_{\mathrm{i}}}_i^{+} + G_i^{-} \circ \big(\mathrm{d}_{\mathrm{r}} \ln \mathfrak{f}\,[\hat{\mathbb{1}}]\big)(\phi_{\mathrm{f}}, \phi_{\mathrm{i}}) = {\phi_{\mathrm{i}}}_i^{+} + G_i^{-} \circ \Lambda \circ \phi_{\mathrm{i}} + \phi_{\mathrm{f}} \circ \mathrm{I} \circ G_i^{+} = \\
&\quad = -i\big(-G^{-} \circ \overset{\leftrightsquigarrow}{\omega} \circ \phi_{\mathrm{f}} + G^{+} \circ \overset{\leftrightsquigarrow}{\omega} \circ \phi_{\mathrm{i}}\big) \quad .
\end{aligned}
\tag{8.125}
$$

Here we have used properties of coherent states under the action of annihilation and creation operators (positive and negative frequancy parts of the field operator), the amplitude (8.122) and properties of Green functions and amplitudes Λ and I. See the end of this chapter (eq. (8.142)) for further possible simplification of this expression.

Finally we write down the relation of the in-out holomorphic representation to the particle representation. Let $\mathbf{v} = \{v_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}_{\mathrm{f}}\}$ and $\mathbf{u} = \{u_{\mathrm{k}}; \mathrm{k} \in \mathcal{I}_{\mathrm{i}}\}$ be f and i-orthonormal bases in $\boldsymbol{\mathcal{S}}$. Using (7.49) we obtain

$$
\begin{aligned}
&\mathfrak{f}\big[\hat{\mathrm{A}}\big](\phi_{\mathrm{f}}, \phi_{\mathrm{i}}) = \sum_{\boldsymbol{m},\boldsymbol{n}} \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}} \langle f\, \mathbf{u} : \boldsymbol{m} | \hat{\mathrm{A}} | i\, \mathbf{u} : \boldsymbol{n} \rangle \langle \phi_{\mathrm{f}}, \mathbf{u} \rangle_f^{\boldsymbol{m}} \langle \mathbf{u}, \phi_{\mathrm{i}} \rangle_i^{\boldsymbol{n}} \quad , \\
&\langle f\, \mathbf{u} : \boldsymbol{m} | \hat{\mathrm{A}} | i\, \mathbf{u} : \boldsymbol{n} \rangle = \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}} \Big(\big[\mathbf{u} \circ \mathrm{d}_{\mathrm{l}}\big]^{\boldsymbol{m}} \big[\mathbf{u} \circ \mathrm{d}_{\mathrm{r}}\big]^{\boldsymbol{n}}\, \mathfrak{f}\big[\hat{\mathrm{A}}\big]\Big)(0,0) \quad .
\end{aligned}
\tag{8.126}
$$

Transition amplitudes

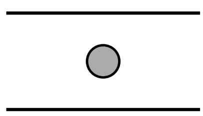
If we apply the last equation on the unit operator we get the *multiple-particle transition amplitudes* we are looking for:

$$
\langle f\, \mathbf{v} : \boldsymbol{m} | i\, \mathbf{u} : \boldsymbol{n} \rangle = \frac{1}{\sqrt{\boldsymbol{m}!\boldsymbol{n}!}} \Big(\big[\mathbf{v} \circ \mathrm{d}_{\mathrm{l}}\big]^{\boldsymbol{m}} \big[\mathbf{u} \circ \mathrm{d}_{\mathrm{r}}\big]^{\boldsymbol{n}}\, \mathfrak{f}\,[\hat{\mathbb{1}}]\Big)(0,0) \quad , \tag{8.127}
$$

where $\mathfrak{f}\,[\hat{\mathbb{1}}]$ is given by (8.122). It is a variation of the exponential function with a quadratic exponent. It is easy to check that the result is given by all possible pairings of the bi-form in the exponent. It can be suggestively represented in a diagrammatical form.

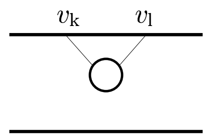
We will use the following dictionary between algebraic and diagrammatical forms[9]

$$
\langle f : vac | i : vac \rangle = \mathrm{o} \quad \leftrightarrow
$$



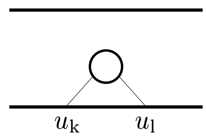
, (8.128)

$$\frac{\langle f:vac|\hat{\mathrm{a}}_f[v_\mathrm{k}]\hat{\mathrm{a}}_f[v_\mathrm{l}]|i:vac\rangle}{\langle f:vac|i:vac\rangle} = v_\mathrm{k}\circ \mathrm{V}\circ v_\mathrm{l} \quad \leftrightarrow$$



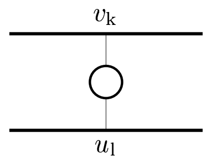
, (8.129)

$$\frac{\langle f:vac|\hat{\mathrm{a}}_i[u_\mathrm{k}]^\dagger\hat{\mathrm{a}}_i[u_\mathrm{l}]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = u_\mathrm{k}\circ \Lambda\circ u_\mathrm{l} \quad \leftrightarrow$$



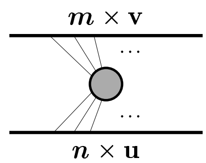
, (8.130)

$$\frac{\langle f:vac|\hat{\mathrm{a}}_f[v_\mathrm{k}]\hat{\mathrm{a}}_i[u_\mathrm{l}]^\dagger|i:vac\rangle}{\langle f:vac|i:vac\rangle} = v_\mathrm{k}\circ \mathrm{I}\circ u_\mathrm{l} \quad \leftrightarrow$$



, (8.131)

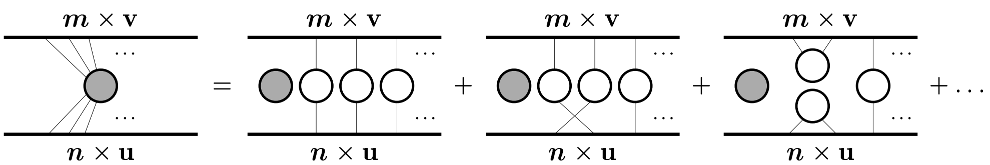
$$\langle f:vac|\hat{\mathrm{a}}_f[\mathbf{v}]^{\boldsymbol{m}}\hat{\mathrm{a}}_i[\mathbf{u}]^{\dagger\,\boldsymbol{n}}|i:vac\rangle = \sqrt{\boldsymbol{m}!\boldsymbol{n}!}\,\langle f\,\mathbf{v}:\boldsymbol{m}|i\,\mathbf{u}:\boldsymbol{n}\rangle \quad \leftrightarrow$$



. (8.132)

Here $\boldsymbol{n}\times\mathbf{u}$ symbolically represents a sequence of $\mathbf{u}$ modes in which a mode u_k is repeated n_k times. Multiplication will be represented simply by composition of diagrams.

The result for a general transition amplitude in the diagrammatical form is



, (8.133)

where the sum is over all possible connections of $\boldsymbol{n}\times\mathbf{u}$ initial particle states and $\boldsymbol{m}\times\mathbf{v}$ final particle states with three basic propagators (8.129), (8.130) and (8.131).

Feynman Green function

Until now in this part, we have worked mainly on the covariant phase space. It will be useful to introduce some related objects living in different spaces.

First we return to the note mentioned at the end of chapter 4. Using two complex structures J_f and J_i on the covariant phase space we can construct a complex structure J_q on the boundary phase space. We have natural isomorphisms $\underline{\partial\Phi}_\mathrm{f}$ and $\underline{\partial\Phi}_\mathrm{i}$ of the covariant phase space with the final and initial canonical phase spaces $\boldsymbol{\mathcal{B}}_\mathrm{f}$ and $\boldsymbol{\mathcal{B}}_\mathrm{i}$, and the boundary phase space $\boldsymbol{\mathcal{B}}$ is direct sum of these two. So, we can construct the complex structure on $\boldsymbol{\mathcal{B}}$ as

$$\mathsf{J}_q = -\mathsf{J}_f + \mathsf{J}_i \quad , \tag{8.134}$$

where J_f is acting on $\boldsymbol{\mathcal{B}}_{\mathrm{f}}$ and J_i is acting on $\boldsymbol{\mathcal{B}}_{\mathrm{i}}$. As we discussed, the notion of q-positive frequencies is equivalent to f-negative frequencies on Σ_{f} and i-positive frequencies on Σ_{i}.

The complex structure J_q allows us to introduce a notion of q-complex boundary conditions and associated objects as the wave operator $\mathcal{F}_q$, projector D_q or the Feynman Green function G_q^F. Now we prove that

$$G_q^F = i\frac{1}{2}G_q^H + G_{\mathrm{sym}} = iG_q^+ + G_{\mathrm{adv}} = iG_q^- + G_{\mathrm{ret}} \quad . \tag{8.135}$$

Here $G_q^H = G_{fi}^H$ is the in-out Hadamard Green function (8.1) associated with the complex structures J_f, and J_i and similarly for Wightman functions. The last two equalities follow from the first one using the relations (8.4) and (2.33), (2.30). So we shall prove the first one.

Feynman Green functions, similar to retarded and advanced Green functions, are defined by their actions on the smooth sources. Therefore we will prove the smoothed version of the statement. Clearly, for a smooth source J we have

$$\overset{\leadsto}{\mathcal{F}} \bullet (i\frac{1}{2}G_q^H + G_{\mathrm{sym}}) \bullet J = \overset{\leadsto}{\mathcal{F}} \bullet G_{\mathrm{sym}} \bullet J = J \quad . \tag{8.136}$$

Next we want to prove the boundary conditions

$$\begin{aligned} &\underline{\psi}_q^+[\partial\Omega] \bullet (i\frac{1}{2}G_q^H + G_{\mathrm{sym}}) \bullet J = \\ &\quad = \underline{\psi}_f^-[\Sigma_{\mathrm{f}}] \bullet (i\frac{1}{2}G_q^H + G_{\mathrm{sym}} - G_{\mathrm{adv}}) \bullet J + \underline{\psi}_i^+[\Sigma_{\mathrm{i}}] \bullet (i\frac{1}{2}G_q^H + G_{\mathrm{sym}} - G_{\mathrm{ret}}) \bullet J = \\ &\quad = i\underline{\psi}_f^-[\Sigma_{\mathrm{f}}] \bullet G_q^+ \bullet J + i\underline{\psi}_i^+[\Sigma_{\mathrm{i}}] \bullet G_q^- \bullet J = \\ &\quad = i\underline{\psi}_f^- \circ G_q^+ \bullet J + i\underline{\psi}_i^+ \circ G_q^- \bullet J = 0 \quad , \end{aligned} \tag{8.137}$$

where we used a decomposition of the form $\underline{\psi}_q^+[\partial\Omega]$ into parts on the final and initial hypersurfaces, added retarded and advanced Green functions (which do not contribute thanks to their boundary conditions), and used (8.8). Therefore we have proved

$$(i\frac{1}{2}G_q^H + G_{\mathrm{sym}}) \bullet J \in \boldsymbol{\mathcal{P}}_q = \boldsymbol{\mathcal{P}}_q^- \quad , \tag{8.138}$$

which, together with (3.43), proves equations (8.135).

From these relations we get

$$-iG_q^{F\,xy} = \begin{cases} G_q^{+\,xy} & \text{for } x \text{ after } y \quad , \\ G_q^{-\,xy} & \text{for } x \text{ befor } y \quad , \\ G_q^{+\,xy} = G_q^{-\,xy} = \frac{1}{2}G_q^{H\,xy} & \text{for } x,y \text{ space-like separated} \quad . \end{cases} \tag{8.139}$$

This means that the Feynman Green function is in-out vacuum mean value of the two time-ordered field observables,

$$G_q^F = \frac{\langle f : vac|\mathcal{T}\big(\hat{\Phi}\hat{\Phi}\big)|i : vac\rangle}{\langle f : vac|i : vac\rangle} \quad . \tag{8.140}$$

Using the relation between the Feynman and Hadamard Green functions we can rewrite the amplitudes (8.94-8.96) in the following symmetric way:

$$\begin{aligned} \Lambda_q &= \overset{\leadsto}{d\mathcal{F}}_q[\Sigma_{\mathrm{i}}] \bullet iG_q^F \bullet \overset{\leftsquigarrow}{d\mathcal{F}}_q[\Sigma_{\mathrm{i}}] \quad , \\ \mathrm{V}_q &= \overset{\leadsto}{d\mathcal{F}}_q[-\Sigma_{\mathrm{f}}] \bullet iG_q^F \bullet \overset{\leftsquigarrow}{d\mathcal{F}}_q[-\Sigma_{\mathrm{f}}] \quad , \\ \mathrm{I}_q &= \overset{\leadsto}{d\mathcal{F}}_q[-\Sigma_{\mathrm{f}}] \bullet iG_q^F \bullet \overset{\leftsquigarrow}{d\mathcal{F}}_q[\Sigma_{\mathrm{i}}] \quad . \end{aligned} \tag{8.141}$$

At the end we prove that

$$-i\big(-G_q^- \bullet \partial\mathcal{F}[\Sigma_\mathrm{f}] + G_q^+ \bullet \partial\mathcal{F}[\Sigma_\mathrm{i}]\big) = D_q[\partial\Omega] \quad . \tag{8.142}$$

A quick proof would be

$$\begin{aligned} & -i\big(-G_q^- \bullet \partial\mathcal{F}[\Sigma_\mathrm{f}] + G_q^+ \bullet \partial\mathcal{F}[\Sigma_\mathrm{i}]\big) = \\ & \quad = -\big((iG_q^- + G_\mathrm{ret}) \bullet \partial\mathcal{F}[-\Sigma_\mathrm{f}] + (iG_q^+ + G_\mathrm{adv}) \bullet \partial\mathcal{F}[\Sigma_\mathrm{i}]\big) = \\ & \quad = -G_q^F \bullet \partial\mathcal{F}[\partial\Omega] = D_q[\partial\Omega] \quad , \end{aligned} \tag{8.143}$$

with the help of (3.75). But here we implicitly assumed a smoothing with a smooth source, and we could have problems, for example, with the source $(\underline{\varphi}_q \cdot j)$ which is localized on the boundary, because of inconsistency discussed in (3.73).

Therefore we will prove the statement above in a more general situation. We show that D_q defined by the expression (8.142) satisfies all necessary properties of the desired projection operator. First $D_q \bullet \phi$ is clearly in $\boldsymbol{\mathcal{S}}$ because both $G_q^\pm$ act on $\boldsymbol{\mathcal{S}}$. Next, for $\phi \in \boldsymbol{\mathcal{S}}$ we have

$$-i\big(-G_q^- \bullet \partial\mathcal{F}[\Sigma_\mathrm{f}] + G_q^+ \bullet \partial\mathcal{F}[\Sigma_\mathrm{i}]\big) \bullet \phi = -i(G_q^+ - G_q^-) \circ \overleftrightarrow{\omega} \circ \phi = -G_c \circ \overleftrightarrow{\omega} \circ \phi = \phi \quad . \tag{8.144}$$

And finally, for $\phi \in \boldsymbol{\mathcal{P}}_q$ (i.e. $\underline{\psi}_f^-[\Sigma_\mathrm{f}] \bullet \phi = 0$ and $\underline{\psi}_i^+[\Sigma_\mathrm{i}] \bullet \phi = 0$), using again (8.8) and (3.79), we get

$$-i\big(-G_q^- \bullet \partial\mathcal{F}[\Sigma_\mathrm{f}] + G_q^+ \bullet \partial\mathcal{F}[\Sigma_\mathrm{i}]\big) \bullet \phi = -i\big(-G_q^- \bullet \overrightarrow{d\mathcal{F}}_f[\Sigma_\mathrm{f}] + G_q^+ \bullet \overleftarrow{d\mathcal{F}}_i[\Sigma_\mathrm{i}]\big) \bullet \phi = 0 \quad . \tag{8.145}$$

This concludes the proof that D_q is the projector on $\boldsymbol{\mathcal{S}}$ parallel to $\boldsymbol{\mathcal{P}}_q$.

9 Interaction with an external source

Quantization of a non-linear phase space

Until now we have worked with the free theory, i.e. we have set $J = 0$. In this chapter we generalize the formalism to the case of a non-zero source. We will work again on the fixed sandwich domain $\Omega = \langle \Sigma_{\rm f}, \Sigma_{\rm i} \rangle$, and we drop the domain dependence in the notation. But let us emphasize that some equations below make sense only on the domain Ω. For example $\overset{\rightsquigarrow}{\mathcal{F}} \bullet \phi = J$ means $\overset{\rightsquigarrow}{\mathcal{F}}[\Omega] \bullet \phi = J[\Omega]$ and so on.

In the case $J = 0$ we had an advantage that the covariant phase space, which we have used for quantization, was a linear space. It allowed us to define the basic quantum observable $\hat{\Phi}$ as an element of the tensor product $\boldsymbol{\mathcal{S}} \otimes \mathcal{H}$. For non-zero external source the covariant phase space $\boldsymbol{\mathcal{S}}_J$ is not a vector space. Therefore we have to move to the larger space and define the basic quantum observable as an element from $\boldsymbol{\mathcal{P}} \otimes \mathcal{H}$. (More precisely it is again an operator-valued distribution.) We require that it satisfy the equation of motion

$$\overset{\rightsquigarrow}{\mathcal{F}} \bullet \hat{\Phi} = J\,\hat{\mathbb{1}} \quad . \tag{9.1}$$

Luckily, the Poisson brackets of the basic field observable Φ (which can be defined thanks to the linearity of the space of histories $\boldsymbol{\mathcal{P}}$) are still

$$\{\Phi, \Phi\} = G_c \quad . \tag{9.2}$$

It is important that the right-hand side is a constant on $\boldsymbol{\mathcal{S}}_J$, so we will not have any problems with operator ordering of the basic commutator relations

$$[\hat{\Phi}, \hat{\Phi}] = -i G_c\,\hat{\mathbb{1}} \quad . \tag{9.3}$$

But the situation is not too bad — the space $\boldsymbol{\mathcal{S}}_J$ is parallel to the free phase space $\boldsymbol{\mathcal{S}}$. I.e. if we choose an origin $\bar{\phi}$ in $\boldsymbol{\mathcal{S}}_J$, any element ϕ from this space can be decomposed as

$$\phi = \phi_{\rm free} + \bar{\phi} \quad , \tag{9.4}$$

with $\phi_{\rm free}$ from the free space $\boldsymbol{\mathcal{S}}$. We will decomposite the quantum observable $\hat{\Phi}$ in a similar way:

$$\hat{\Phi} = \hat{\Phi}_{\rm free} + \bar{\phi}\,\hat{\mathbb{1}} \quad , \tag{9.5}$$

and we obtain a quantum observable $\hat{\Phi}_{\rm free}$ which satisfies the free field equation and the commutator relation (6.1) of the free field theory. Therefore we can apply the formalism of the previous chapters and build a quantum space using this observable.

But first we have to choose an origin $\bar{\phi}$ in $\boldsymbol{\mathcal{S}}_J$. Of course, the different choices gives unitarily equivalent theories; however, we have to identify the physical states. We have to specify, for example, which state is the vacuum at the beginning. But the vacuum state is dependent on the choice of the origin $\bar{\phi}$.

We have a natural choice for identification of the final and initial states — we choose the free fields $\hat{\Phi}_{\mathrm{f}}$ and $\hat{\Phi}_{\mathrm{i}}$ which are identical with a real quantum field $\hat{\Phi}$ on the final or intial hypersurface. It is equivalent to the choice

$$\hat{\Phi} = \hat{\Phi}_{\mathrm{f}} + \bar{\phi}_{\mathrm{adv}}(J)\,\hat{\mathbb{1}} = \hat{\Phi}_{\mathrm{i}} + \bar{\phi}_{\mathrm{ret}}(J)\,\hat{\mathbb{1}} \quad . \tag{9.6}$$

Now we can construct final states using $\hat{\Phi}_{\mathrm{f}}$, and similarly for initial states. To denote this dependence we add a new label to all objects defined using these free fields. For example, if we choose particle interpretations given by the complex structures $\mathsf{J}_{p_{\mathrm{f}}}$ and $\mathsf{J}_{p_{\mathrm{i}}}$ for final and initial states, we will write $|\mathrm{f}, p_{\mathrm{f}} : vac\rangle$, $|\mathrm{f}, p_{\mathrm{f}}\, coh : \phi\rangle$, $\hat{\mathrm{a}}_{\mathrm{f},p_{\mathrm{f}}}[\phi]$ or $\hat{\mathrm{W}}_{\mathrm{f}}[\phi]$ for objects constructed using $\hat{\Phi}_{\mathrm{f}}$ and similarly for $\hat{\Phi}_{\mathrm{i}}$.

Now we can compute transition amplitudes between such states. But it will be more symmetric if we choose some auxiliary free field which we use for the computation. We choose it in the following form (see eq. (3.39))

$$\hat{\Phi} = \hat{\Phi}_b + \bar{\phi}_b(J) \tag{9.7}$$

with some real b-boundary conditions. The physical results will be, of course, independent of this choice. Again, the objects constructed using this observable will carry an additional label b.

The relations between free quantum observables are (using (7.3))

$$\begin{aligned} \hat{\Phi}_{\mathrm{f}} &= \hat{\Phi}_b + \Delta\phi_{b\mathrm{f}}\,\hat{\mathbb{1}} = \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{f}}]^\dagger\, \hat{\Phi}_b\, \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{f}}] \quad , \\ \hat{\Phi}_{\mathrm{i}} &= \hat{\Phi}_b + \Delta\phi_{b\mathrm{i}}\,\hat{\mathbb{1}} = \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{i}}]^\dagger\, \hat{\Phi}_b\, \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{i}}] \quad , \end{aligned} \tag{9.8}$$

where

$$\Delta\phi_{b\mathrm{f}} = \bar{\phi}_b(J) - \bar{\phi}_{\mathrm{adv}}(J) \quad , \quad \Delta\phi_{b\mathrm{i}} = \bar{\phi}_b(J) - \bar{\phi}_{\mathrm{ret}}(J) \quad . \tag{9.9}$$

These elements of $\boldsymbol{\mathcal{S}}$ satisfy

$$\Delta\phi_{b\mathrm{f}} - \Delta\phi_{b\mathrm{i}} = \phi_c(J) \quad , \tag{9.10}$$

$$\Delta\phi_{b\mathrm{f}} \circ \overleftrightarrow{\omega} \circ \Delta\phi_{b\mathrm{i}} = J \bullet (G_b^F - G_{\mathrm{sym}}) \bullet J = i\frac{1}{2} J \bullet G_b^H \bullet J \quad , \tag{9.11}$$

with $\phi_c(J)$ defied in (2.31). Let's prove the last equation

$$\begin{aligned} \Delta\phi_{b\mathrm{f}} \circ \overleftrightarrow{\omega} \circ \Delta\phi_{b\mathrm{i}} &= (\bar{\phi}_b - \bar{\phi}_{\mathrm{adv}}) \bullet \partial\mathcal{F}[\Sigma] \bullet (\bar{\phi}_b - \bar{\phi}_{\mathrm{ret}}) = \\ &= \frac{1}{2}\bar{\phi}_b \bullet \big(\partial\mathcal{F}[-\Sigma_{\mathrm{f}}] \bullet \bar{\phi}_{\mathrm{ret}} + \partial\mathcal{F}[\Sigma_{\mathrm{i}}] \bullet \bar{\phi}_{\mathrm{adv}}\big) = \bar{\phi}_b \bullet \partial\mathcal{F}[\partial\Omega] \bullet \bar{\phi}_{\mathrm{sym}} = \\ &= \bar{\phi}_b \bullet (\overrightarrow{\mathcal{F}} - \overleftarrow{\mathcal{F}}) \bullet \bar{\phi}_{\mathrm{sym}} = \bar{\phi}_b \bullet J - J \bullet \bar{\phi}_{\mathrm{sym}} = J \bullet \big(G_b^F - G_{\mathrm{sym}}\big) \bullet J \quad . \end{aligned} \tag{9.12}$$

Vacuum-vacuum amplitude and the phase fixing

The equations (9.8) represent the unitary transformation between free quantum fields. We can transform states constructed using these fields, except that the transformation for quantum observables do not fix a phase for the transformation between states.

Let us choose the initial and final particle representations generated by the complex structures $\mathsf{J}_{p_{\mathrm{f}}}$ and $\mathsf{J}_{p_{\mathrm{i}}}$ which induce the complex structure J_p on the boundary phase space as discussed at the end of the previous chapter. We can write a relation between vacuum states of these particle interpretations defined using different free field observables

$$\begin{aligned} |\mathrm{f}, p_{\mathrm{f}} : vac\rangle &= c_{\mathrm{f}} \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{f}}]^\dagger |b, p_{\mathrm{f}} : vac\rangle \quad , \\ |\mathrm{i}, p_{\mathrm{i}} : vac\rangle &= c_{\mathrm{i}} \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{i}}]^\dagger |b, p_{\mathrm{i}} : vac\rangle \quad , \end{aligned} \tag{9.13}$$

with some phase factors c_{f}, c_{i}. The vacuum-vacuum amplitude is

$$
\begin{aligned}
\langle \mathrm{f}, p_{\mathrm{f}} : vac | \mathrm{i}, p_{\mathrm{i}} : vac\rangle &= c_{\mathrm{f}}^* c_{\mathrm{i}}\, \langle b, p_{\mathrm{f}} : vac | \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{f}}] \hat{\mathrm{W}}_b[-\Delta\phi_{b\mathrm{i}}] | b, p_{\mathrm{i}} : vac\rangle = \\
&= c_{\mathrm{f}}^* c_{\mathrm{i}}\, \exp\big(-i\frac{1}{2}\Delta\phi_{b\mathrm{f}} \circ \overset{\leftrightsquigarrow}{\omega} \circ \Delta\phi_{b\mathrm{i}}\big) \langle b, p_{\mathrm{f}} : vac | \hat{\mathrm{W}}_b[\phi_c] | b, p_{\mathrm{i}} : vac\rangle = \\
&= c_{\mathrm{f}}^* c_{\mathrm{i}}\, \exp\Big(-\frac{1}{2}\phi_c \bullet \mathrm{I}_p \bullet \phi_c + \frac{1}{2} J \bullet \frac{1}{2} G_b^H \bullet J\Big) \langle b, p_{\mathrm{f}} : vac | b, p_{\mathrm{i}} : vac\rangle = \\
&= c_{\mathrm{f}}^* c_{\mathrm{i}}\, \mathrm{o}_p\, \exp\Big(-\frac{1}{4} J \bullet (G_p^H - G_b^H) \bullet J\Big) = \\
&= c_{\mathrm{f}}^* c_{\mathrm{i}}\, \mathrm{o}_p\, \exp\big(-i\frac{1}{2} J \bullet G_b^F \bullet J\big) \exp\big(i\frac{1}{2} J \bullet G_p^F \bullet J\big) \quad .
\end{aligned}
\tag{9.14}
$$

Here we have used the additive property of the displacement operator (7.8), the transition amplitude (8.124), (8.108), (8.94), and properties of the Green functions.

In will be extremely useful to choose the phase factor $c_{\mathrm{f}}^* c_{\mathrm{i}}$ in such way that the the vacuum-vacuum amplitude does not depend on the choice of the auxiliary field $\hat{\Phi}_b$. Therefore we set

$$
c_{\mathrm{f}}^* c_{\mathrm{i}} = \exp\big(i\frac{1}{2} J \bullet G_b^F \bullet J\big) \quad . \tag{9.15}
$$

This gives us a simple form of the vacuum-vacuum amplitude,

$$
\mathrm{o}_p(J) \overset{\mathrm{def}}{=} \langle \mathrm{f}, p_{\mathrm{f}} : vac | \mathrm{i}, p_{\mathrm{i}} : vac\rangle = \mathrm{o}_p\, \exp\big(i\frac{1}{2} J \bullet G_p^F \bullet J\big) \quad . \tag{9.16}
$$

Transition amplitudes

Similar to the free field case we can obtain multi-particle transition amplitudes by the variation of the coherent states transition amplitude (see (8.126)). Therefore we will write down this amplitude. The relation between coherent states constructed using different free field observables is the same as for vacuum states thanks to the unitarity of the transformation. Therefore we can apply the same calculation as for vacuum-vacuum amplitude and obtain

$$
\begin{aligned}
&\langle \mathrm{f}, p_{\mathrm{f}}\, coh : \phi_{\mathrm{f}} | \mathrm{i}, p_{\mathrm{i}}\, coh : \phi_{\mathrm{i}}\rangle = \\
&\quad = \mathrm{o}_p(J)\, \exp\Big(\frac{1}{2}\phi_{\mathrm{f}} \circ \mathrm{V}_p \circ \phi_{\mathrm{f}} + \frac{1}{2}\phi_{\mathrm{i}} \circ \Lambda_p \circ \phi_{\mathrm{i}} + \phi_{\mathrm{f}} \circ \mathrm{I}_p \circ \phi_{\mathrm{i}} + \phi_{\mathrm{f}} \circ \mathrm{T}_p + \perp_p \circ \phi_{\mathrm{i}}\Big) \quad ,
\end{aligned}
\tag{9.17}
$$

where the amplitudes V_p, Λ_p, I_p are defined in (8.94-8.96) or in (8.141) and the new amplitudes T_p and $\perp_p$ are given by

$$
\begin{aligned}
\mathrm{T}_p &= \mathrm{I}_p \circ \phi_c(J) = \overset{\leftrightsquigarrow}{\omega} \circ G_p^+ \bullet J = -i\overset{\leftrightsquigarrow}{d\mathcal{F}}_p[-\Sigma_{\mathrm{f}}] \bullet G_p^F \bullet J \quad , \\
\perp_p &= \phi_c(J) \bullet \mathrm{I}_p = J \bullet G_p^+ \circ \overset{\leftrightsquigarrow}{\omega} = -J \bullet G_p^F \bullet i\overset{\leftrightsquigarrow}{d\mathcal{F}}_p[\Sigma_{\mathrm{i}}] \quad .
\end{aligned}
\tag{9.18}
$$

Using the relation (8.142) we get

$$
\phi_{\mathrm{f}} \circ \mathrm{T}_p + \perp_p \circ \phi_{\mathrm{i}} = -iJ \bullet G_p^F \bullet \partial\mathcal{F}[\partial\Omega]\phi = iJ \bullet D_p \bullet \partial\phi \quad , \tag{9.19}
$$

where $\partial\phi$ is the projection of ϕ_{i} on Σ_{i} and of ϕ_{f} on Σ_{f} to the boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ (information on the boundary phase space is sufficient for the action of D_p),

$$
\partial\phi = \underline{\partial\Phi}[\Sigma_{\mathrm{f}}] \bullet \phi_{\mathrm{f}} + \underline{\partial\Phi}[\Sigma_{\mathrm{i}}] \bullet \phi_{\mathrm{i}} \quad . \tag{9.20}
$$

Using the relations between Green functions and field operators, we can transform the transition amplitude to another form:

$$\begin{aligned}
&\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} | \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} \rangle = \\
&\quad = \mathrm{o}_p \,\exp\Big(\frac{1}{2}\mathcal{J}_p(J,\partial\phi) \bullet iG^F_p \bullet \mathcal{J}_p(J,\partial\phi)\Big) = \\
&\quad = \mathrm{o}_p \,\exp\Big(\frac{1}{2}\bar{\phi}_p(J,\partial\phi) \bullet i\mathcal{F}_{\sim p} \bullet \bar{\phi}_p(J,\partial\phi)\Big) = \\
&\quad = \mathrm{o}_p \,\exp\big(i\bar{S}_p(J,\partial\phi)\big) \quad ,
\end{aligned} \tag{9.21}$$

where the generalized source, the classical solution and the classical action associated with the p-boundary conditions are

$$\mathcal{J}_p(J,\partial\phi) = J - \partial\phi \bullet \overleftrightarrow{d}\mathcal{F}_p = \mathcal{F}_{\sim p} \bullet \bar{\phi}_p(J,\partial\phi) \quad , \tag{9.22}$$

$$\bar{\phi}_p(J,\partial\phi) = G^F_p \bullet J + D_p \bullet \partial\phi = G_{\sim p} \bullet \mathcal{J}_p(J,\partial\phi) \quad , \tag{9.23}$$

$$\bar{S}_p(J,\partial\phi) = -\frac{1}{2}\bar{\phi}_p(J,\partial\phi) \bullet \mathcal{F}_p \bullet \bar{\phi}_p(J,\partial\phi) + J \bullet \bar{\phi}_p(J,\partial\phi) \quad . \tag{9.24}$$

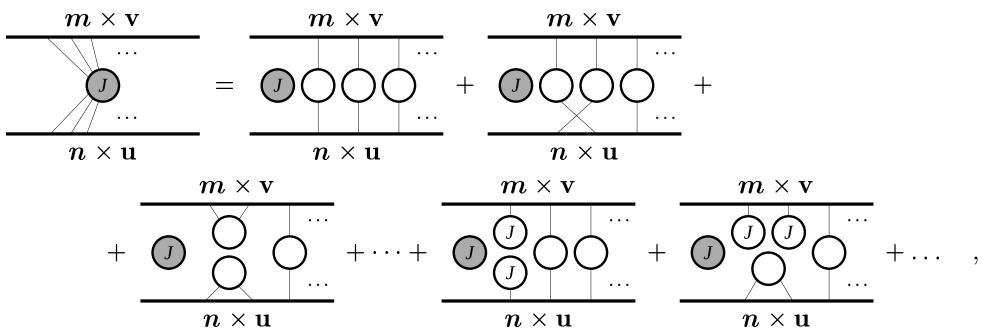
For the demonstration we compute also an in-out mean value of the quantum field

$$\begin{aligned}
&\frac{\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} | \hat{\Phi} | \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} \rangle}{\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} | \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} \rangle} = \\
&\quad = \frac{\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} | \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{f}}] \hat{\Phi}_b \hat{\mathrm{W}}_b[-\Delta\phi_{b\mathrm{i}}] | \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} \rangle}{\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} | \hat{\mathrm{W}}_b[\Delta\phi_{b\mathrm{f}}] \hat{\mathrm{W}}_b[-\Delta\phi_{b\mathrm{i}}] | \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} \rangle} + \bar{\phi}_b(J) = \\
&\quad = \frac{\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} - \Delta\phi_{b\mathrm{f}} | \hat{\Phi}_b | \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} - \Delta\phi_{b\mathrm{i}} \rangle}{\langle \mathrm{f}, p_{\mathrm{f}}\; coh : \phi_{\mathrm{f}} - \Delta\phi_{b\mathrm{f}} || \mathrm{i}, p_{\mathrm{i}}\; coh : \phi_{\mathrm{i}} - \Delta\phi_{b\mathrm{i}} \rangle} + \bar{\phi}_b(J) = \\
&\quad = D_p \bullet \big(\partial\phi - \underline{\partial\Phi} \bullet \bar{\phi}_b(J)\big) + \bar{\phi}_b(J) = \\
&\quad = \bar{\phi}_p(J,\partial\phi) \quad ,
\end{aligned} \tag{9.25}$$

where again $\partial\phi$ is given by eq. (9.20). Here we have used $\underline{\partial\Phi}[\Sigma_{\mathrm{f}}] \bullet \Delta\phi_{b\mathrm{f}} = \underline{\partial\Phi}[\Sigma_{\mathrm{f}}] \bullet \bar{\phi}_b(J)$ and similarly on Σ_{i}.

The multi-particle amplitude (8.133) in the presence of the external source has the form

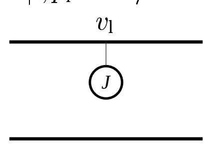
$$\langle \mathrm{f}, p_{\mathrm{f}} : vac | \hat{\mathrm{a}}_{\mathrm{f},p_{\mathrm{f}}}[\mathbf{v}]^{\boldsymbol{m}} \hat{\mathrm{a}}_{\mathrm{i},p_{\mathrm{i}}}[\mathbf{u}]^{\dagger\,\boldsymbol{n}} | \mathrm{i}, p_{\mathrm{i}} : vac \rangle = \sqrt{\boldsymbol{m}!\boldsymbol{n}!}\, \langle \mathrm{f}, p_{\mathrm{f}}\; \mathbf{v} : \boldsymbol{m} | \mathrm{i}, p_{\mathrm{i}}\; \mathbf{u} : \boldsymbol{n} \rangle \quad \leftrightarrow$$



(9.26)

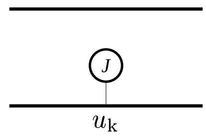
where we have introduced the following diagrammatical representations of T_p, L_p, and $\mathrm{o}_p(J)$ amplitudes

$$\frac{\langle \mathrm{f}, p_\mathrm{f} : vac | \hat{\mathrm{a}}_{\mathrm{f},p_\mathrm{f}}[v_\mathrm{l}] | \mathrm{i}, p_\mathrm{i} : vac\rangle}{\langle \mathrm{f}, p_\mathrm{f} : vac | \mathrm{i}, p_\mathrm{i} : vac\rangle} = v_\mathrm{k} \circ \mathrm{T} \quad \leftrightarrow$$



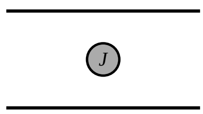
$$, \tag{9.27}$$

$$\frac{\langle \mathrm{f}, p_\mathrm{f} : vac | \hat{\mathrm{a}}_{\mathrm{i},p_\mathrm{i}}[u_\mathrm{k}]^\dagger | \mathrm{i}, p_\mathrm{i} : vac\rangle}{\langle \mathrm{f}, p_\mathrm{f} : vac | \mathrm{i}, p_\mathrm{i} : vac\rangle} = \mathrm{L} \circ u_\mathrm{k} \quad \leftrightarrow$$



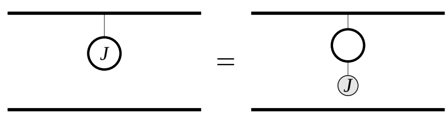
$$, \tag{9.28}$$

$$\langle \mathrm{f}, p_\mathrm{f} : vac | \mathrm{i}, p_\mathrm{i} : vac\rangle = \mathrm{o}(J) \quad \leftrightarrow$$

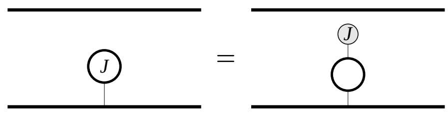


$$. \tag{9.29}$$

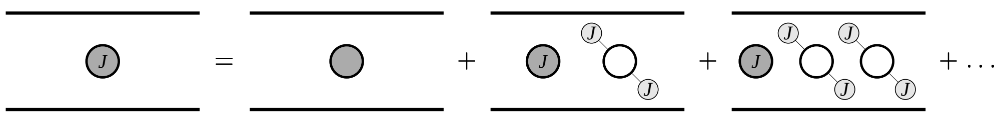
We can be even more explicit and decompose diagrams for elementary transition amplitudes T_p, L_p, and $\mathrm{o}_p(J)$ using (9.18) and (9.16) as



$$, \tag{9.30}$$



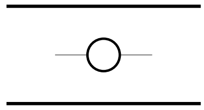
$$, \tag{9.31}$$



$$, \tag{9.32}$$

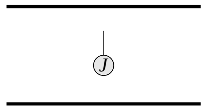
where we understand

$$-i\,G^F_p \quad \leftrightarrow$$



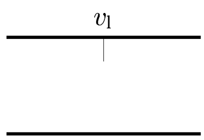
, (9.33)

$$i\,J \quad \leftrightarrow$$



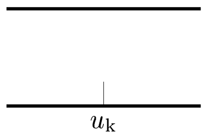
, (9.34)

$$-i\,v_{\mathrm{l}} \bullet \overset{\rightsquigarrow}{d}\mathcal{F}_p[-\Sigma_{\mathrm{f}}] \quad \leftrightarrow$$



, (9.35)

$$-i\,u_{\mathrm{k}} \bullet \overset{\rightsquigarrow}{d}\mathcal{F}_p[\Sigma_{\mathrm{i}}] \quad \leftrightarrow$$



. (9.36)

Thanks to (8.141) the diagrams for the amplitudes V_p, Λ_p, and I_p can be also viewed as composed from the elements above.

Part III

QFT — Boundary Quantum Mechanics

10 General formulation

Introduction

In this part we will develop *boundary quantum mechanics* — a variation of quantum mechanics based on the quantization of the boundary phase space. First we present a general overview of the method, and next we apply it to scalar field theory.

Let start with the quantum theory described in chapter 5. There we have quantized observables F_f and G_a on a phase space with the cotangent bundle structure. We have found their quantum forms $\hat{\mathsf{F}}_f$ and $\hat{\mathsf{G}}_a$, and we have constructed the special position base $|pos : \mathrm{x}\rangle$. We have not formulated the dynamical part of the theory, so we touch this question 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 only in observables with support on the initial and final hypersurfaces of the sandwich domain $\Omega = \langle\Sigma_\mathrm{f}, \Sigma_\mathrm{i}\rangle$ in a globally hyperbolic spacetime. In this case we can quantize the initial and final canonical phase spaces $\boldsymbol{\mathcal{B}}_\mathrm{i} = \boldsymbol{\mathcal{B}}[\Sigma_\mathrm{i}]$ and $\boldsymbol{\mathcal{B}}_\mathrm{f} = \boldsymbol{\mathcal{B}}[\Sigma_\mathrm{f}]$ — i.e. we construct the quantum observables $\hat{\mathsf{F}}_{\mathrm{f}\,f}$, $\hat{\mathsf{G}}_{\mathrm{f}\,a}$ and $\hat{\mathsf{F}}_{\mathrm{i}\,f}$, $\hat{\mathsf{G}}_{\mathrm{i}\,a}$ on the quantum space $\mathcal{H}$ satisfying the conditions (5.2-5.11) with the ordering parameters $\gamma_\mathrm{f} = -\gamma_\mathrm{i}$, and the corresponding bases[10] $|\mathrm{f}\,pos : \mathrm{x}_\mathrm{f}\rangle$ and $|\mathrm{i}\,pos : \mathrm{x}_\mathrm{i}\rangle$ in the space $\mathcal{H}$. The dynamics reduces to the investigation of the relations between these two sets of observables or the relations between objects generated by them — for example the position bases. We can say we have solved the dynamical problem if we find in-out transition amplitudes $\langle\mathrm{f}\,pos : \mathrm{x}_\mathrm{f}|\mathrm{i}\,pos : \mathrm{x}_\mathrm{i}\rangle$ for all $\mathrm{x}_\mathrm{f} \in \boldsymbol{\mathcal{V}}[\Sigma_\mathrm{f}]$ and $\mathrm{x}_\mathrm{i} \in \boldsymbol{\mathcal{V}}[\Sigma_\mathrm{i}]$.

We do not attempt to find the transition amplitudes in a general situation (but we have proceeded in a similar way for the scalar field already). However we reformulate this setting in a slightly different language.

Construction of the boundary quantum space

We have represented the quantization of both $\boldsymbol{\mathcal{B}}_\mathrm{f}$ and $\boldsymbol{\mathcal{B}}_\mathrm{i}$ on a common quantum Hilbert space $\mathcal{H}$. Let us construct another representation on the *boundary quantum space*

$$\mathcal{H}_{\boldsymbol{\mathcal{B}}} = \mathcal{H}^\dagger \otimes \mathcal{H} \tag{10.1}$$

(the space of tensor products of covector and vector elements of the form $\langle\mathrm{f}| \otimes |\mathrm{i}\rangle$, i.e. essentially operators on $\mathcal{H}$). We use the notation $|state)$ for vectors from $\mathcal{H}_{\boldsymbol{\mathcal{B}}}$, and we use the accent $\hat{}$ to denote observables on this space.

We interpret the boundary quantum space in the following way: We assign to any pair of f-dependent and i-dependent vectors $|\mathrm{f}\rangle$ and $|\mathrm{i}\rangle$ the vector $|\mathrm{fi})$ from $\mathcal{H}_{\boldsymbol{\mathcal{B}}}$ by mapping

$$|\mathrm{fi}) = \langle\mathrm{f}| \otimes |\mathrm{i}\rangle \quad . \tag{10.2}$$

Here f-*dependent vector* suggests that the vector is identified using quantum observables on Σ_f, but of course, it can be any vector from $\mathcal{H}$. Particularly we define for $\mathrm{x} = [\mathrm{x}_\mathrm{f}, \mathrm{x}_\mathrm{i}] \in \boldsymbol{\mathcal{V}}[\partial\Omega] = \boldsymbol{\mathcal{V}}[\Sigma_\mathrm{f}] \times \boldsymbol{\mathcal{V}}[\sigma_\mathrm{i}]$ the vector in $\mathcal{H}_{\boldsymbol{\mathcal{B}}}$

$$|pos : \mathrm{x}) = \langle\mathrm{f}\,pos : x_\mathrm{f}| \otimes |\mathrm{i}\,pos : \mathrm{x}_\mathrm{i}\rangle \quad . \tag{10.3}$$

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 $\mathcal{H}_{\mathcal{B}}$

$$\begin{aligned} \hat{A}_f &= \hat{A}_f^\dagger \otimes \mathbb{1}_i & \hat{A}_f|fi) &= \langle f|\hat{A}_f^\dagger \otimes |i\rangle \quad , \\ \hat{A}_i &= \mathbb{1}_f \otimes \hat{A}_f & \hat{A}_i|fi) &= \langle f| \otimes \hat{A}_i|i\rangle \quad . \end{aligned} \tag{10.4}$$

Using these definitions we find

$$[\hat{A}_f, \hat{A}_i] = 0 \quad . \tag{10.5}$$

We apply this method to construct observables $\hat{\mathsf{F}}_{f\,f_f}$, $\hat{\mathsf{G}}_{f\,a_f}$ and $\hat{\mathsf{F}}_{i\,f_i}$, $\hat{\mathsf{G}}_{i\,a_i}$ for any functions and vector fields f_f, a_f or f_i, a_i on the value spaces $\boldsymbol{\mathcal{V}}[\Sigma_f]$ or $\boldsymbol{\mathcal{V}}[\Sigma_i]$. Next we want to construct a generalization of these observables $\hat{\mathsf{F}}_f$ and $\hat{\mathsf{G}}_a$ for any function f and vector field a on the value space $\boldsymbol{\mathcal{V}}[\partial\Omega] = \boldsymbol{\mathcal{V}}[\Sigma_f] \times \boldsymbol{\mathcal{V}}[\Sigma_i]$. Thanks to (5.4) for both $\hat{\mathsf{F}}_{f\,f}$ and $\hat{\mathsf{F}}_{i\,f}$ and to equation (10.5), we do not have ordering problems with $\hat{\mathsf{F}}_f$ for $f(x) = f(x_f, x_i)$

$$\begin{aligned} \hat{\mathsf{F}}_f &= \int\limits_{\substack{x_f \in \boldsymbol{\mathcal{V}}[\Sigma_f] \\ x_i \in \boldsymbol{\mathcal{V}}[\Sigma_i]}} |f\,pos : x_f\rangle\langle f\,pos : x_f| \otimes |i\,pos : x_i\rangle\langle i\,pos : x_i|\, f(x_f, x_i) = \\ &= \int\limits_{x \in \boldsymbol{\mathcal{V}}[\partial\Omega]} |pos : x)(pos : x|\, f(x) \quad . \end{aligned} \tag{10.6}$$

Similarily, for any vector field $a(x) = a_f(x_f) \oplus a_i(x_i)$ on $\boldsymbol{\mathcal{V}}[\partial\Omega]$ where $a_f \in \mathfrak{T}\,\boldsymbol{\mathcal{V}}[\Sigma_f]$ and $a_i \in \mathfrak{T}\,\boldsymbol{\mathcal{V}}[\Sigma_i]$, motivated by (1.22), we can write

$$\hat{\mathsf{G}}_a = -\hat{\mathsf{G}}_{f\,a_f} + \hat{\mathsf{G}}_{i\,a_i} \quad . \tag{10.7}$$

It is straightforward to check that $\hat{\mathsf{F}}_f$, $\hat{\mathsf{G}}_a$ are quantizations of the observables F_f, G_a on the boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$; i.e. they satisfy (5.2-5.11) with the ordering parameter $\gamma = \gamma_i = \gamma_f$. Note that different orientation of the bounary $\partial\Omega$ and the final hypersurface Σ_f, which translates to the different sign of the symplectic structures (1.21) and to the definition of the momenta (1.22), is compensated by the covector representation of f-dependent vectors.

Let us summarize: quantization of the basic observables on the final and initial hypersurfaces Σ_f and Σ_i gives arise to the quantization of the basic observables F_f, G_a on the whole boundary $\partial\Omega$. I.e. we are able to formulate the "kinematics" of the theory using quantization of the boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ — which we call the *boundary quantum mechanics*. The boundary quantum space $\mathcal{H}_{\mathcal{B}}$ represents all possible quantum states at the beginning and at the end chosen independently on a real evolution of the system. Essentially we are treating the initial and final experiments as experiments on independent systems. States in $\mathcal{H}_{\mathcal{B}}$ represents outputs of such understood measurements.

Before we turn to the dynamics let us list some properties of the space $\mathcal{H}_{\mathcal{B}} = \mathcal{H}^\dagger \otimes \mathcal{H}$. For vectors and operators in the "product" form

$$\begin{aligned} |fi) &= \langle f| \otimes |i\rangle \quad , \\ \hat{O}_{fi} &= \hat{O}_f^\dagger \otimes \hat{O}_i \quad , \end{aligned} \tag{10.8}$$

we can write

$$\begin{gathered} (fi\,st1|fi\,st2) = \langle f\,st2|f\,st1\rangle\,\langle i\,st1|i\,st2\rangle = \mathrm{Tr}_{\mathcal{H}}\big((|f\,st2\rangle\langle f\,st1|)^\dagger\,(|i\,st2\rangle\langle i\,st1|)\big) \quad , \\ (fi| = |fi)^\dagger = |f\rangle \otimes \langle i| \quad , \quad \hat{A}_{fi}\hat{B}_{fi} = (\hat{B}_f^\dagger\hat{A}_f^\dagger) \otimes (\hat{B}_i\hat{A}_i) \quad , \\ \hat{O}_{fi}|fi) = \langle f|\hat{O}_f^\dagger \otimes \hat{O}_i|i\rangle \quad , \quad \mathrm{Tr}_{\mathcal{H}_{\mathcal{B}}}\hat{O}_{fi} = \mathrm{Tr}_{\mathcal{H}}\,\hat{O}_f^\dagger\ \mathrm{Tr}_{\mathcal{H}}\,\hat{O}_i \quad . \end{gathered} \tag{10.9}$$

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 sketched, the dynamical information is hidden in the in-out transition amplitudes $\langle \mathrm{f}|\mathrm{i}\rangle$. Such an amplitude can be written as

$$\langle \mathrm{f}|\mathrm{i}\rangle = \mathrm{Tr}_{\mathcal{H}}\big(\hat{\mathbb{1}}^{\dagger}\,|\mathrm{i}\rangle\langle \mathrm{f}|\big) = (phys|\mathrm{fi}) \quad , \tag{10.10}$$

where $|\mathrm{fi})$ is as in (10.8) and the *physical state* $|phys)$ is given by

$$|phys) = \sum_{\mathrm{k}} \langle \mathrm{k}| \otimes |\mathrm{k}\rangle = \hat{\mathbb{1}} \tag{10.11}$$

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

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

$$A(state) = (phys|state) \quad . \tag{10.12}$$

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

$$A_{pos}(\mathrm{x}) = A_{pos}(\mathrm{x_f}|\mathrm{x_i}) = (phys|pos:\mathrm{x}) = \langle \mathrm{f}\, pos:\mathrm{x_f}|\mathrm{i}\, pos:\mathrm{x_i}\rangle \quad . \tag{10.13}$$

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

Boundary quantum mechanics

In the previous sections we have 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 $\boldsymbol{\mathcal{B}}[\partial\Omega]$. It is a phase space with a cotangent bundle structure, so we can apply the general formalism and obtain the quantum observables $\hat{\mathsf{F}}_f$ and $\hat{\mathsf{G}}_a$. We can also construct the position base $|pos:\mathrm{x})$. And we do not need any causal information for this; we do not need any global time flow on the underlying manifold or a causal decomposition of the boundary.

This 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 for Euclidian theories. Therefore we will call the boundary quantum mechanics also *time-symmetric quantum mechanics*.

But in this setting we have to find the physical state $|phys)$ without reference to the initial and final decomposition[11]. Again we cannot expect an answer on a general level — this is a question equivalent to a solution of the quantum evolution. But we suggest a method for determination of the physical state and in the next chapter we apply this method in the case of the non-interacting scalar field theory.

The classical evolution in the boundary phase space $\boldsymbol{\mathcal{B}}[\partial\Omega]$ is determined by specification of the physical phase space $\boldsymbol{\mathcal{S}}$ as a subspace of $\boldsymbol{\mathcal{B}}[\partial\Omega]$. It can be done, for example, by condition (1.15), or, expressed using observables F_f, G_a by the condition

$$\mathsf{G}_a + \mathsf{F}_{a\bullet \mathrm{d}\bar{S}} = 0 \qquad \text{for all} \quad a \in \mathfrak{T}\boldsymbol{\mathcal{V}}[\partial\Omega] \quad . \tag{10.14}$$

I.e., on the classical level we have specified physical states by the constraints in the phase space. In the usual canonical quantization one tries to quantize the constrained subspace $\boldsymbol{\mathcal{S}}$. In the boundary quantum mechanics we quantize the full boundary phase space and impose conditions on the physical state inspired by the classical constraints

$$\big(\hat{\mathsf{G}}_a + \hat{\mathsf{F}}_{a\cdot \mathrm{d}\bar{S}}\big)|phys) = 0 \tag{10.15}$$

for at least some vector field on the value space $\boldsymbol{\mathcal{V}}[\partial\Omega]$.

We cannot expect the condition above to be satisfied for all vector fields a due to the noncommutativity of the position and momentum observables ($\hat{\mathsf{G}}_a$ is some ordering of "$a(\mathbf{x})\cdot\mathbf{p}$" observable). We will see that such strong requirement would be inconsistent. It will turn out that the choice of the class of vector fields for which the condition (10.15) is required to hold (i.e. the choice of the 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.

Let us look at the position representation of the constraint conditions. Using (5.14) and (5.43) we find

$$(phys|\big(\hat{\mathsf{G}}_a + \hat{\mathsf{F}}_{a\cdot \mathrm{d}\bar{S}}\big)|pos:.) = \big(i\mathcal{L}_a + a\cdot \mathrm{d}\bar{S}\big)(phys|pos:.) = 0 \quad . \tag{10.16}$$

If we represent the position transition amplitude as

$$A_{pos}(\mathrm{x}) = \mathfrak{a}(\mathrm{x})\ \exp\big(i\bar{S}(\mathrm{x})\big) \tag{10.17}$$

with $\mathfrak{a}(\mathrm{x})$ a density of the weight $(\frac{1}{2} - i\gamma)$, the condition above translates to

$$\mathcal{L}_a \mathfrak{a} = 0 \quad . \tag{10.18}$$

This confirms that the constraint conditions cannot be satisfied for all vector fields a. And if we find a linearly complete set of vector fields for which the constraint conditions should be satisfied, it determines the density $\mathfrak{a}$ up to a constant multiplicative factor completely. The freedom is, of course, equivalent to the right normalization and the choice of a relative phase factor which is unphysical.

The density $\mathfrak{a}$ contains all quantum corrections to the transition amplitude A_{pos}. So we can expect that for a non-interacting theory there should exists a natural choice of a "constant" density $\mathfrak{a}_o$ — constant with respect of a set of some natural vector fields a. This is true for the scalar field, as we will see in the next chapter.

Path integral

There exists another approach to the quantization of the system. This is 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,

$$\langle \mathrm{f}\,pos:\mathrm{x_f}|\mathrm{i}\,pos:\mathrm{x_i}\rangle = A_{pos}(\mathrm{x_f}|\mathrm{x_i}) = \int\limits_{\substack{\mathrm{h}\in\boldsymbol{\mathcal{H}}\\ \mathbf{x}(\mathrm{h})=[\mathrm{x_f},\mathrm{x_i}]}} \mathfrak{M}^F(\mathrm{h})\ \exp\big(iS(\mathrm{h})\big) \quad . \tag{10.19}$$

We will discuss this method more in the last part.

The integral over the space of histories faces serious problems due to the infinite dimension of this space and the oscillatory character of the integrand. A technical solution usually leads to the computation of some Euclidian equivalent of this integral, which is usually better defined, and performance of some transformation from the Euclidian to the Lorentzian theory. We can view this as only a technical detour without a physical interpretation. Only after the computation of the integral are we able to identify the results with the transition amplitudes of quantum mechanics. Anyway, in the usual framework we do not know what would be the quantum mechanics of the

Euclidian formulation of the theory — the usual quantum mechanics essentially uses the causal structure for the definition of commutation relations and definitions of initial and final states.

The formalism developed in this chapter gives us a hope for another option. We could formulate boundary quantum mechanics even for a Euclidian version of the theory and make the connection with the path integral already in the Euclidian formulation

$$(phys|pos : \mathrm{x}) = A_{pos}(\mathrm{x}) = \int\limits_{\substack{\mathrm{h}\in\boldsymbol{\mathcal{H}}\\ \mathbf{x}(\mathrm{h})=\mathrm{x}}} \mathfrak{M}^F(\mathrm{h}) \exp\bigl(-I(\mathrm{h})\bigr) \quad . \tag{10.20}$$

In the Lorentzian case this reduces to the relations (10.19) above. In the Euclidian case it 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. The form of boundary quantum mechanics formulated here in the Euclidian version does not correspond with the Euclidian path integral. The problem is hidden in the method of quantization we have used. The translation of Poisson brackets of the classical theory to the commutators of the quantum theory

$$\{\ ,\ \} \rightarrow i[\ ,\ ] \tag{10.21}$$

intrinsically contains reference to the Lorentzian signature. The imaginary unit in this translation causes the imaginary unit in the exponent of the transition amplitude (10.17) computed in boundary quantum mechanics independently of the version of the theory. For the Euclidian theory it would be more appropriate to construct a "Euclidian quantum mechanics" based on the commutation relation generated by the rule

$$\{\ ,\ \} \rightarrow [\ ,\ ] \quad , \tag{10.22}$$

with observables represented, probably, on a real Hilbert space. But 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 a Euclidian quantum mechanics.

Let us finally note that the rules above can be written uniformly using theEuclidian convention for Poisson brackets (see (D.10) in appendix D)

$$^{E}\{\ ,\ \} \rightarrow -[\ ,\ ] \quad . \tag{10.23}$$

11 Configuration and holomorphic representations

Introduction

In the previous part we have formulated the quantum theory of a non-interacting scalar field based on quantization of the covariant phase space. Now we build up boundary quantum mechanics for the scalar field — the quantum mechanics based on the quantization of the boundary phase space. First we apply a general method for the quantization of a linear phase space discussed in the chapters 5, 6 and 7, and we construct special bases in the quantum space $\mathcal{H}_{\boldsymbol{\mathcal{B}}}$ of boundary quantum mechanics. Than we formulate conditions for the physical state and compute the transition amplitudes. Finally we compare the results with the previous formulation.

Most of the first part can be again applied for a general linear phase space. This essentially gives a unified form for configuration and holomorphic representation following the similar coresspondence on the classical level where were able to deal with the real and complex boundary conditions using one formalism (see chapters 3, 4).

Quantization of the boundary phase space

In chapter 2 we have introduced the boundary phase space[12] $\boldsymbol{\mathcal{B}}[\partial\Omega]$ associated with the boundary $\partial\Omega$ of the investigated domain Ω. It is a linear phase space with the basic observable $\partial\Phi$, the Poisson brackets of which are given in (2.19). Similar what was done in chapter 6, we assume that the quantum version of the basic observable $\hat{\Phi} \in \boldsymbol{\mathcal{B}} \otimes \mathcal{O}_{\boldsymbol{\mathcal{B}}}$ has the commutation relations

$$[\hat{\Phi}, \hat{\Phi}] = -i\hbar\, \partial\mathcal{F}^{-1}\, \hat{\mathbb{1}} \quad . \tag{11.1}$$

As before, we drop the domain and boundary dependence in the notation where it cannot lead to confusion.

We have also introduced a constant $\hbar$ in the commutation relations. It can represent the usual Planck constant, but we use it mainly to trace the influence of the constant in the commutation relations on the transition amplitudes, motivated by comments at the end of the previous chapter. In comparison with the path integral approach (see chapter 16), we will find that we would need to set its value to $\frac{i}{n}$. But the reasoning in this chapter is consistent only for real positive value of $\hbar$, i.e. only for physical value of the signature factor n of the spacetime metric. In the Euclidian case further investigation is needed of how to generalize the quantization scheme to accommodate an imaginary value for $\hbar$. We also have to change definitions of some other quantities as, for example, the product $(\phi_1, \phi_2)_m = -\frac{i}{\hbar}\phi_1 \diamond \overleftrightarrow{d\mathcal{F}} \diamond \phi_2$, or the measure $d\Gamma = \operatorname{Det} \frac{\partial\mathcal{F}}{2\pi\hbar}^{\frac{1}{2}}$, etc..

We can define the displacement operator

$$\hat{\mathrm{W}}[\phi] = \exp\bigl(i\hbar\, \phi \diamond \partial\mathcal{F} \diamond \hat{\Phi}\bigr) \quad . \tag{11.2}$$

with the same properties as its counter-part in the covariant phase space quantization.

We can build up the same machinery of the particle and coherent states based on the choice of a complex structure J_p on the boundary phase space, which also determines complex boundary conditions on the boundary.

Now we define a similar construction for real boundary conditions characterized, for example, by the unit operator I_b as discussed in chapter 3. It is straightforward to generate the configuration (value) representation, but we will do it in a manner more close to the holomorphic representation.

Given real boundary conditions we can define $\boldsymbol{\mathcal{V}}$ and $\tilde{\boldsymbol{\mathcal{V}}}$-valued quantum observables of the field value and momentum on the boundary:

$$\begin{aligned} \hat{\varphi}_b &= \underline{\varphi}_b \diamond \hat{\Phi} \quad , \quad \hat{\varphi}_b^\dagger = \hat{\varphi}_b \quad , \\ \hat{\pi}_b &= \underline{\pi}_b \diamond \hat{\Phi} \quad , \quad \hat{\pi}_b^\dagger = \hat{\pi}_b \quad , \end{aligned} \tag{11.3}$$

with commutation relations

$$[\hat{\varphi}_b, \hat{\pi}_b] = i\hbar\delta_{\boldsymbol{\mathcal{V}}}\hat{\mathbb{1}} \quad , \quad [\hat{\varphi}_b, \hat{\varphi}_b] = 0 \quad , \quad [\hat{\pi}_b, \hat{\pi}_b] = 0 \quad . \tag{11.4}$$

These define value and momentum bases as discussed in chapter 5. Specifically we choose the following phase fixing and normalization[13]:

$$\begin{gathered} \hat{\varphi}_b|b\,val:\varphi) = \varphi|b\,val:\varphi) \quad , \quad \hat{\pi}_b|b\,val:\varphi) = i\hbar\,\mathrm{d}|b\,val:\varphi) \quad , \\ (b\,val:\varphi_1|b\,val:\varphi_2) = \big(\mathfrak{Q}_b^{-1}\delta\big)(\varphi_1|\varphi_2) \quad , \quad \hat{\mathbb{1}} = \int\limits_{\varphi\in\boldsymbol{\mathcal{V}}} \mathfrak{Q}_b(\varphi)|b\,val:\varphi)(b\,val:\varphi| \quad . \end{gathered} \tag{11.5}$$

$$\begin{gathered} \hat{\pi}_b|b\,mom:\pi) = \pi|b\,mom:\pi) \quad , \quad \hat{\varphi}_b|b\,mom:\pi) = -i\hbar\,\mathrm{d}|b\,mom:\pi) \quad , \\ (b\,mom:\pi_1|b\,mom:\pi_2) = \big(\mathfrak{Q}\delta\big)\Big(\frac{\pi_1}{2\pi\hbar}\Big|\frac{\pi_2}{2\pi\hbar}\Big) \quad , \quad \hat{\mathbb{1}} = \int\limits_{\varphi\in\boldsymbol{\mathcal{V}}} \mathfrak{Q}_b^{-1}\Big(\frac{\pi}{2\pi\hbar}\Big)|b\,mom:\pi)(b\,mom:\pi| \quad , \\ (b\,mom:\pi|b\,val:\varphi) \in \mathbb{R}^+ \quad . \end{gathered} \tag{11.6}$$

Here $\mathfrak{Q}_b$ is a constant measure on $\boldsymbol{\mathcal{V}}$ associated with the b-boundary conditions. It is easy to check that with this normalization we have

$$(b\,mom:\pi|b\,val:\varphi) = \exp(-\frac{i}{\hbar}\pi\diamond\varphi) \quad . \tag{11.7}$$

Next we define generators of the shift operators

$$\begin{aligned} \hat{\mathrm{a}}_b[\phi] &= (\phi,\hat{\Phi})_b = -\frac{i}{\hbar}\phi\diamond\overleftrightarrow{d\mathcal{F}}_b\diamond\hat{\Phi} = -\frac{i}{\hbar}\pi_b(\phi)\diamond\hat{\varphi}_b \quad , \\ \hat{\mathrm{c}}_b[\phi] &= (\hat{\Phi},\phi)_b = -\frac{i}{\hbar}\hat{\Phi}\diamond\overleftrightarrow{d\mathcal{F}}_b\diamond\phi = -\frac{i}{\hbar}\varphi_b(\phi)\diamond\hat{\pi}_b \quad , \end{aligned} \tag{11.8}$$

with properties

$$\begin{aligned} \exp\big(-\hat{\mathrm{c}}_b[\phi]\big)\,\hat{\varphi}_b\,\exp\big(\hat{\mathrm{c}}_b[\phi]\big) &= \hat{\varphi}_b + \varphi_b(\phi)\,\hat{\mathbb{1}} \quad , \\ \exp\big(\hat{\mathrm{a}}_b[\phi]\big)\,\hat{\pi}_b\,\exp\big(-\hat{\mathrm{a}}_b[\phi]\big) &= \hat{\pi}_b + \pi_b(\phi)\,\hat{\mathbb{1}} \quad , \end{aligned} \tag{11.9}$$

$$\begin{aligned} \exp\big(\hat{\mathrm{c}}_b[\phi]\big)\,|b\,val:\varphi) &= \big|b\,val:\varphi+\varphi_b(\phi)\big) \quad , \\ \exp\big(-\hat{\mathrm{a}}_b[\phi]\big)\,|b\,mom:\pi) &= \big|b\,mom:\pi+\pi_b(\phi)\big) \quad , \end{aligned} \tag{11.10}$$

$$\phi\diamond\partial\mathcal{F}\diamond\hat{\Phi} = i\hbar\big(\hat{\mathrm{a}}_b[\phi]+\hat{\mathrm{a}}_{\sim b}[\phi]\big) = -i\hbar\big(\hat{\mathrm{c}}_b[\phi]+\hat{\mathrm{c}}_{\sim b}[\phi]\big) \quad , \tag{11.11}$$

$$\hat{\mathrm{W}}[\phi] = \exp\big(\frac{1}{2}(\phi,\phi)_b\big)\exp\big(-\hat{\mathrm{a}}_b[\phi]\big)\exp\big(\hat{\mathrm{c}}_b[\phi]\big) = \exp\big(-\frac{1}{2}(\phi,\phi)_b\big)\exp\big(\hat{\mathrm{c}}_b[\phi]\big)\exp\big(-\hat{\mathrm{a}}_b[\phi]\big) \tag{11.12}$$

and the commutation relations

$$\begin{gathered}\big[\hat{a}_b[\phi_1], \hat{c}_b[\phi_2]\big] = (\phi_1, \phi_2)_b\, \hat{1} \quad , \\ \big[\hat{a}_b[\phi_1], \hat{a}_b[\phi_2]\big] = 0 \quad , \quad \big[\hat{c}_b[\phi_1], \hat{c}_b[\phi_2]\big] = 0 \quad .\end{gathered} \tag{11.13}$$

The definitions and commutation relations of these operators have a clear resemblance to annihilation and creation operators $\hat{a}_p[\phi]$ and $\hat{a}_p[\phi]^\dagger$ for the complex boundary conditions. However the similarity breaks down with operations based on complex conjugation. For example,

$$\begin{aligned}\hat{a}_b[\phi]^\dagger &= -\hat{a}_b[\phi] = \hat{c}_{\sim b}[\phi] \quad , \\ \hat{c}_b[\phi]^\dagger &= -\hat{c}_b[\phi] = \hat{a}_{\sim b}[\phi] \quad .\end{aligned} \tag{11.14}$$

But we will follow the resemblance with the case of complex boundary conditions further, so we can use the formalism developed for coherent states.

Generalized holomorphic representation

Let an m-index represents a real or complex boundary condition. We define an m-base as vectors in the quantum space $\mathcal{H}_{\boldsymbol{\mathcal{B}}}$ labeled by elements from $\boldsymbol{\mathcal{B}}$ in a way similar to (7.16) and (7.17)

$$\begin{aligned}\hat{a}_m[\phi]\,|m:\phi_1) &= (\phi, \phi_1)_m \quad , \\ \hat{c}_m[\phi]\,|m:\phi_1) &= \phi \diamond \mathrm{d}\,|m:\phi_1) \quad .\end{aligned} \tag{11.15}$$

Similarly we define a m-cobase as a base for covectors

$$\begin{aligned}(m\star:\phi_1|\,\hat{c}_m[\phi_2] &= (\phi_1, \phi_2)_m \quad , \\ (m\star:\phi_1|\,\hat{a}_m[\phi] &= \phi \diamond \mathrm{d}\,(m\star:\phi_1|\end{aligned} \tag{11.16}$$

with relative normalization

$$(m\star:0|m:0) = 1 \quad . \tag{11.17}$$

From the properties of the displacement operator, it follows that

$$\begin{aligned}|m:\phi) &= \exp\big(\tfrac{1}{2}(\phi,\phi)_m\big)\hat{W}[\phi]\,|m:0) = \exp\big(\hat{c}_m[\phi]\big)\,|m:0) \quad , \\ (m\star:\phi| &= \exp\big(\tfrac{1}{2}(\phi,\phi)_{\sim m}\big)\,(m\star:0|\,\hat{W}[\phi]^\dagger = (m\star:0|\,\exp\big(\hat{a}_{\sim m}[\phi]\big) \quad .\end{aligned} \tag{11.18}$$

For the real boundary conditions we have only reformulated previous definitions of the value and momentum bases

$$|b:\phi) = \alpha|b\,val:\varphi_b(\phi)) \quad , \quad (b\star:\phi| = \frac{1}{\alpha}(b\,mom:\pi_b(\phi)| \tag{11.19}$$

with some normalization factor $\alpha \in \mathbb{C}$. Using (11.7) and the completeness of the bases we get

$$(b\star:\phi_1|b:\phi_2) = \exp\big((\phi_1,\phi_2)_b\big) \quad , \tag{11.20}$$

$$\hat{1} = \int\limits_{\phi\in\boldsymbol{\mathcal{B}}} d\Gamma_{\boldsymbol{\mathcal{B}}}\, \exp\big(-(\phi,\phi)_b\big)\,|b:\phi)(b\star:\phi| \quad , \tag{11.21}$$

$$\mathsf{P}_b^- \diamond \mathrm{d}\,|b:.) = 0 \quad , \quad \mathsf{P}_b^+ \diamond \mathrm{d}\,(b\star:.| = 0 \quad . \tag{11.22}$$

Here $d\Gamma_{\boldsymbol{\mathcal{B}}}$ is a cannonical measure (B.8) on the phase space $\boldsymbol{\mathcal{B}}$.

For the complex boundary conditions the p-base and cobase reduces to the base of coherent states

$$|p:\phi) = |p\star:\phi) = |p\,coh:\phi) \quad , \tag{11.23}$$

and we have already proven relations (11.20-11.22) above for this case.

So we have found that the m-base and cobase share some properties of the coherent states. We can define a representation similar to the holomorphic representation and use formulas derived before, now in both real and complex cases.

$$\mathfrak{f}_m\left[|state)\right](\phi) = (m\star : \phi|state) \quad , \tag{11.24}$$

$$\mathfrak{f}_m\left[(state|\right](\phi) = (state|m : \phi) \quad , \tag{11.25}$$

$$\mathfrak{f}_m\left[\hat{\mathrm{A}}\right](\phi_1,\phi_2) = (m\star : \phi_1|\hat{\mathrm{A}}|m : \phi_2) \quad . \tag{11.26}$$

Thanks to the completeness relations derived above we have composition laws similar to (7.23) for this representation. We list some of the properties derived in chapter 7.

$$\begin{aligned}
\mathfrak{f}_m\left[\hat{\mathrm{c}}_m[\phi]|st)\right](\phi_1) &= (\phi_1,\phi)_m\,\mathfrak{f}_m\left[|st)\right](\phi_1) \quad ,\\
\mathfrak{f}_m\left[\hat{\mathrm{a}}_m[\phi]|st)\right](\phi_1) &= \phi\diamond\big(\mathrm{d}\,\mathfrak{f}_m\left[|st)\right]\big)(\phi_1) \quad ,\\
\mathfrak{f}_m\left[(st|\hat{\mathrm{a}}_m[\phi]\right](\phi_1) &= (\phi,\phi_1)_m\,\mathfrak{f}_m\left[(st|\right](\phi_1) \quad ,\\
\mathfrak{f}_m\left[(st|\hat{\mathrm{c}}_m[\phi]\right](\phi_1) &= \phi\diamond\big(\mathrm{d}\,\mathfrak{f}_m\left[(st|\right]\big)(\phi_1) \quad .
\end{aligned} \tag{11.27}$$

$$\mathfrak{f}_m\left[|m : \phi_2)\right](\phi_1) = \exp\big((\phi_1,\phi_2)_m\big) \quad , \tag{11.28}$$

$$\mathfrak{f}_m\left[(m\star : \phi_1)\right](\phi_2) = \exp\big((\phi_1,\phi_2)_m\big) \quad , \tag{11.29}$$

$$\mathfrak{f}_m\left[\hat{\mathrm{c}}_m[\phi]^n|m : \phi_2)\right](\phi_1) = {(\phi_1,\phi)_m}^n \exp\big((\phi_1,\phi_2)_m\big) \quad , \tag{11.30}$$

$$\mathfrak{f}_m\left[|m : \phi)(m\star : \phi|\right](\phi_1,\phi_2) = \exp\big((\phi_1,\phi)_m + (\phi,\phi_2)_m\big) \quad , \tag{11.31}$$

$$\mathfrak{f}_m\left[\hat{\mathbb{1}}\right](\phi_1,\phi_2) = \exp\big((\phi_1,\phi_2)_m\big) \quad , \tag{11.32}$$

$$\mathfrak{f}_m\left[\hat{\mathrm{W}}[\phi]\right](\phi_1,\phi_2) = \exp\big(-\frac{1}{2}(\phi,\phi)_m + (\phi_1,\phi)_m - (\phi,\phi_2)_m + (\phi_1,\phi_2)_m\big) \quad . \tag{11.33}$$

We can introduce also a normal ordering, which in the real case arranges all momenta observables to be to the left of the value observables and in the complex case coincides with the previously discussed normal ordering.

To summarize, we have introduced notation in which it is possible to treat on the same level both value and momentum representation for real boundary conditions and the coherent states representation for complex boundary conditions. We can use most of the formulas derived for the coherent states and holomorphic representation in chapter 7. We only have to be careful to distinguish the vectors and covectors because in the real case the elements of the base and cobase are not hermitian conjugates.

Specially related boundary conditions

It would be possible to develop the formalism for the comparison of two different real boundary conditions similarly to what we did for complex boundary conditions in chapter 8. We will do it explicitly only for specially related boundary conditions — for conditions which differ only in the value or momentum space. We cannot do something similar for complex boundary conditions, because in this case the spaces $\boldsymbol{\mathcal{B}}_p = \boldsymbol{\mathcal{B}}_p^-$ and $\boldsymbol{\mathcal{B}}_{\sim p} = \boldsymbol{\mathcal{B}}_p^+$ are not chosen independently but are complex conjugate.

First we investigate the dependence of a real b-base $|b : \phi)$ on the choice of the b-momentum. Let $|{\scriptstyle BB_1} : \phi)$ and $|{\scriptstyle BB_2} : \phi)$ be ${\scriptstyle BB_1}$ and ${\scriptstyle BB_2}$-bases for boundary conditions with the same value space $\boldsymbol{\mathcal{B}}_{\scriptscriptstyle B}$ and different momentum spaces $\boldsymbol{\mathcal{B}}_{\scriptscriptstyle B_1}$ and $\boldsymbol{\mathcal{B}}_{\scriptscriptstyle B_2}$. The first of the conditions of (11.15) says

$$\hat{\varphi}_{\scriptscriptstyle B}|{\scriptstyle BB_1} : 0) = 0 \quad , \quad \hat{\varphi}_{\scriptscriptstyle B}|{\scriptstyle BB_2} : 0) = 0 \quad , \tag{11.34}$$

so states $|_{BB_1}:0)$ and $|_{BB_2}:0)$ are proportional. The second of the conditions of (11.15) essentially fixes the relative phase between states of the base. But we have the freedom to choose a global normalization, i.e. we can choose

$$|_{BB_1}:0) = |_{BB_2}:0) \quad . \tag{11.35}$$

Using (3.61) we find

$$\overleftrightarrow{d}\mathcal{F}_{BB_2} - \overleftrightarrow{d}\mathcal{F}_{BB_1} = \mathcal{F}_{BB_2} - \mathcal{F}_{BB_1} = \bar{\mathcal{F}}_{BB_2} - \bar{\mathcal{F}}_{BB_1} \quad , \tag{11.36}$$

and therefore

$$(\phi,\phi)_{BB_2} = (\phi,\phi)_{BB_1} - \frac{i}{\hbar}\phi \diamond (\bar{\mathcal{F}}_{BB_2} - \bar{\mathcal{F}}_{BB_1}) \diamond \phi \quad . \tag{11.37}$$

Therefore from eq. (11.18) follows

$$|_{BB_2}:\phi) = \exp\Big(\frac{1}{2}\frac{i}{\hbar}\phi \diamond (\bar{\mathcal{F}}_{BB_1} - \bar{\mathcal{F}}_{BB_2}) \diamond \phi\Big)\, |_{BB_1}:\phi) \quad . \tag{11.38}$$

We see that $|_{BB_2}:\phi)$ and $|_{BB_1}:\phi)$ differ only by a phase factor.

We can write down also the relations of the shift operators,

$$\begin{aligned} \hat{\mathrm{a}}_{BB_2}[\phi] &= \hat{\mathrm{a}}_{BB_1}\big[\bar{G}_{BB_1} \diamond \bar{\mathcal{F}}_{BB_2} \diamond \phi\big] \quad , \\ \hat{\mathrm{c}}_{BB_2}[\phi] &= \hat{\mathrm{c}}_{BB_1}\big[\phi\big] + \hat{\mathrm{a}}_{BB_1}\big[(\bar{G}_{BB_1} \diamond \bar{\mathcal{F}}_{BB_2} - \delta_{\boldsymbol{\mathcal{B}}}) \diamond \phi\big] \quad . \end{aligned} \tag{11.39}$$

Next we turn to compare boundary conditions with different value space and the same momentum space. A similar calculation to the previous one gives

$$\begin{aligned} \hat{\mathrm{a}}_{B_2B}[\phi] &= \hat{\mathrm{a}}_{B_1B}\big[\phi\big] + \hat{\mathrm{c}}_{B_1B}\big[(\bar{G}_{BB_1} \diamond \overleftarrow{d}\mathcal{F}_{B_2B} - \delta_{\boldsymbol{\mathcal{B}}}) \diamond \phi\big] \quad , \\ \hat{\mathrm{c}}_{B_2B}[\phi] &= \hat{\mathrm{c}}_{B_1B}\big[\bar{G}_{BB_1} \diamond \overleftarrow{d}\mathcal{F}_{B_2B} \diamond \phi\big] \quad . \end{aligned} \tag{11.40}$$

We have different "annihilation" operators, so we get different states $|_{B_1B}:0)$ and $|_{B_2B}:0)$. The conditions

$$(_{B_1B\star}:\phi_1|\hat{\mathrm{a}}[\phi]|_{B_2B}:0) = 0 \quad , \tag{11.41}$$

using the properties of the generalized holomorphic representation, gives a variation equation for $(_{B_1B\star}:\phi|_{B_2B}:0)$. The solution is

$$(_{B_1B\star}:\phi|_{B_2B}:0) = \text{const}\ \exp\Big(\frac{1}{2}\frac{i}{\hbar}\,\phi \diamond (\bar{\mathcal{F}}_{BB_1} - \bar{\mathcal{F}}_{BB_2}) \diamond \phi\Big) \tag{11.42}$$

with

$$\text{const} = (_{B_1B\star}:0|_{B_2B}:0) \quad . \tag{11.43}$$

Thanks to the fact that

$$(\bar{\mathcal{F}}_{BB_1} - \bar{\mathcal{F}}_{BB_2}) = (\bar{\mathcal{F}}_{BB_1} - \bar{\mathcal{F}}_{BB_2}) \diamond D_B \quad , \tag{11.44}$$

and using the properties of the generalized holomorphic representation, we get

$$|_{B_2B}:0) = \text{const}\ \exp\Big(\frac{1}{2}\frac{i}{\hbar}\,\hat{\Phi} \diamond (\bar{\mathcal{F}}_{BB_1} - \bar{\mathcal{F}}_{BB_2}) \diamond \hat{\Phi}\Big)\ |_{B_1B}:0) \quad . \tag{11.45}$$

The physical state

As we have discussed at the general level, the dynamics of boundary quantum mechanics is described by the physical state. The conditions which characterize the relations of the physical observables to this state are quantum versions of the classical constraints given by the classical equation of motion. Now we apply this idea to scalar field theory and derive transition amplitudes.

The classical equation of motion reduced to the boundary is given by equation (3.42). This equation is formed from linear observables, so we can write down its quantum version. It can be expressed in any of the following equivalent forms:

$$\begin{aligned} \forall\phi \in \boldsymbol{\mathcal{S}} \quad \phi \diamond \partial\mathcal{F} \diamond \hat{\Phi}\, |phys) = \phi \bullet J\, |phys) \quad , \\ D_m \diamond \partial\mathcal{F} \diamond \hat{\Phi}\, |phys) = D_m \bullet\, J|phys) \quad , \\ \hat{\underline{\vartheta}}|phys) = \vartheta_m(J)\, |phys) \quad , \end{aligned} \tag{11.46}$$

where the quantum version of the generator of the physical phase space $\hat{\underline{\vartheta}}$ can be written for real boundary conditions as

$$\hat{\underline{\vartheta}} = \hat{\pi}_b \cdot \gamma_b - \hat{\varphi}_b \quad . \tag{11.47}$$

We are investigating theories with a generally non-zero external source. It will be useful to fix a phase of the bases introduced above relative to the physical state for different values of the external source. We will use the following choice

$$(phys|m:0) = \mathrm{o}_m \exp\big(\frac{i}{\hbar}\frac{1}{2}\, J \bullet G^F_m \bullet J\big) \quad , \tag{11.48}$$

with some complex number o_m.

Using these conditions we can derive the generalized holomorphic representation of the physical state — the transition amplitudes we are interested in. The holomorphic representation of the constraint equation (11.46) gives

$$\begin{aligned} &(phys|\big(D_m \diamond \partial\mathcal{F} \diamond \hat{\Phi} - D_m \bullet J\big)|m:\phi) = \\ &\quad = (phys|\big(-\hat{\Phi} \diamond \overleftrightarrow{d\mathcal{F}}_m \diamond D_m + D_m \diamond \overleftrightarrow{d\mathcal{F}}_m \diamond \hat{\Phi} - D_m \bullet J\big)|m:\phi) = \\ &\quad = -i\hbar D_m \diamond \mathrm{d}(phys|m:\phi) + \big(\phi \diamond \bar{\mathcal{F}}_m - J \bullet D_m\big)(phys|m:\phi) \quad , \end{aligned} \tag{11.49}$$

where we used the definition properties (11.15) of the m-base. This variation equation has a solution

$$\begin{aligned} &(phys|m:\phi) = \\ &\quad = \mathrm{o}_m \exp\Big(-\frac{1}{2}\frac{i}{\hbar}\phi \bullet \bar{\mathcal{F}}_m \bullet \phi + \frac{i}{\hbar} J \bullet D_m \bullet \phi + \frac{1}{2}\frac{i}{\hbar} J \bullet G^F_m \bullet J\Big) = \\ &\quad = \mathrm{o}_m \exp\Big(\frac{1}{2}\frac{i}{\hbar}\mathcal{J}_m(J,\phi) \bullet G_{\sim m} \bullet \mathcal{J}_m(J,\phi)\Big) = \\ &\quad = \mathrm{o}_m \exp\big(\frac{i}{\hbar}\bar{S}_m(J,\phi)\big) \quad , \end{aligned} \tag{11.50}$$

with the classical action associated with the m-boundary conditions given by (9.24).

This amplitude is interpreted as the transition amplitude between a state measured by an observer on the boundary and the physical state of the system. I.e., as the physical amplitude for an experiment performed on the system on the whole boundary — including both the initial and final measurements, if the notions of *initial* and *final* have sense.

Relation to usual quantum mechanics

We have computed the physical transition amplitudes in boundary quantum mechanics without reference to some causal structure, without distinguishing between initial and final states. Now we compare it with the previously derived results in the case of a sandwich domain in a globally hyperbolic spacetime.

As we discussed in the general introduction to boundary quantum mechanics in the case when we have well defined initial and final parts of the boundary which carry full sets of Cauchy data, we can represent the quantum space of the boundary quantum mechanics as a tensor product of quantum spaces build on canonical phase spaces. Precisely, for initial and final states $|\mathrm{i}\, st\rangle$, $|\mathrm{f}st\rangle$ we have the state from $\mathcal{H}_{\mathcal{B}}$ given by the tensor product

$$\langle \mathrm{f}st| \otimes |\mathrm{i}st\rangle \quad . \tag{11.51}$$

Similarily we can construct observables on $\mathcal{H}_{\mathcal{B}}$ using observables on $\mathcal{H}$.

In the case of the scalar field we have a clear correspondence between basic observables

$$\hat{\Phi}[\partial\Omega] = \partial\hat{\Phi}[-\Sigma_{\mathrm{f}}] \otimes \hat{\mathbb{1}} \oplus \hat{\mathbb{1}} \otimes \partial\hat{\Phi}[\Sigma_{\mathrm{i}}] = \underline{\partial\Phi}[-\Sigma_{\mathrm{f}}] \bullet \hat{\Phi} \otimes \hat{\mathbb{1}} \oplus \hat{\mathbb{1}} \otimes \underline{\partial\Phi}[\Sigma_{\mathrm{i}}] \bullet \hat{\Phi} \quad . \tag{11.52}$$

Next we will assume that the boundary conditions we are using are local for both parts of the boundary — it is possible to formulate them using independent conditions on the initial and final hypersurface. Then we can write for the real boundary conditions

$$\begin{aligned} \hat{\varphi}_b[\partial\Omega] &= \hat{\varphi}_b[\Sigma_{\mathrm{f}}] \otimes \hat{\mathbb{1}} \oplus \hat{\mathbb{1}} \otimes \hat{\varphi}_b[\Sigma_{\mathrm{i}}] \quad , \\ \hat{\pi}_b[\partial\Omega] &= -\hat{\pi}_b[\Sigma_{\mathrm{f}}] \otimes \hat{\mathbb{1}} \oplus \hat{\mathbb{1}} \otimes \hat{\pi}_b[\Sigma_{\mathrm{i}}] \quad . \end{aligned} \tag{11.53}$$

The value and momentum bases are related by

$$\begin{aligned} |b\, val : \varphi_{\mathrm{f}} \oplus \varphi_{\mathrm{i}}) &= \langle \mathrm{f}, b\, val : \varphi_{\mathrm{f}}| \otimes |\mathrm{i}, b\, val : \varphi_{\mathrm{i}}\rangle \quad , \\ |b\, mom : -\pi_{\mathrm{f}} \oplus \pi_{\mathrm{i}}) &= \langle \mathrm{f}, b\, mom : \pi_{\mathrm{f}}| \otimes |\mathrm{i}, b\, mom : \pi_{\mathrm{i}}\rangle \quad . \end{aligned} \tag{11.54}$$

From this follows that

$$(phys|b\, val : \varphi_{\mathrm{f}} \oplus \varphi_{\mathrm{i}}) = \langle \mathrm{f}, b\, val : \varphi_{\mathrm{f}}|\mathrm{i}, b\, val : \varphi_{\mathrm{i}}\rangle \quad . \tag{11.55}$$

For the complex boundary conditions we already discussed that the complex structures on the initial and final hypersurfaces induce the complex structure on the boundary phase space

$$\mathsf{J}_p = -\mathsf{J}_{p_{\mathrm{f}}} \oplus \mathsf{J}_{p_{\mathrm{i}}} \quad . \tag{11.56}$$

In this case we have the relationship

$$|p\, coh : \phi_{\mathrm{f}} \oplus \phi_{\mathrm{i}}) = \langle \mathrm{f}, p_{\mathrm{f}}\, coh : \phi_{\mathrm{f}}| \otimes |\mathrm{i}, p_{\mathrm{i}}\, coh : \phi_{\mathrm{i}}\rangle \quad , \tag{11.57}$$

and therefore

$$(phys|p\, coh : \phi_{\mathrm{f}} \oplus \phi_{\mathrm{i}}) = \langle \mathrm{f}, p_{\mathrm{f}}\, coh : \phi_{\mathrm{f}}|\mathrm{i}, p_{\mathrm{i}}\, coh : \phi_{\mathrm{i}}\rangle \quad . \tag{11.58}$$

Now we can compare the amplitude (9.21) computed in the previous part with the amplitude (11.50) and we see that we have obtained the same results, except that in the boundary quantum mechanics we do not derive the normalization constant o_m. We have also introduced the constant $\hbar$ to the commutation relations which is reflected in the transition amplitudes.

Part IV

Sum-over-Histories Formulation of a Particle-like Theory

12 General principles of the sum-over-histories formulation of quantum mechanics

Introduction

In this part we will discuss the particle-like theory using the sum-over-histories approach to quantum mechanics. Our goal is to show that such a theory leads to the same predictions of amplitudes as the field theory discussed in the previous parts. We want to establish a relation between particle interpretations of field theory and interactions of particles with space-like boundaries (i.e "measurement" of particles at initial and final time) in the particle theory.

The usual approach to a quantized relativistic particle is through field theory. But it would be nice to see that field theory is really equivalent to some kind of quantization of the classical particle theory. But the straightforward canonical quantization of the relativistic particle theory faces several well known problems. Therefore it is necessary to adopt some other approach for quantization.

Another reason for attempting to quantize a classical relativistic particle is that this theory is equivalent from the mathematical point of view to classical minisuperspace models for cosmology. It is well known that classical gravitation coupled with matter reduces to a particle-like theory in a Lorentzian manifold with a potential, when restricted to a finite number of degrees of freedom. And we would like to understand a quantum version of such a minisuperspace theory. Unfortunately the quantization using the field theory does not help us with this understanding — there is too big a gap in the interpretation of such a theory. We need a more straightforward way to quantize minisuperspace models.

A much more promising way to understand quantization of such theories is the sum-over-histories approach to quantum mechanics. The classical explanation of this approach for usual nonrelativistic physics can be found in [13] and more technically in [14–17]. An overview for a relativistic theory can be found in [18]. Beside these classical introductions, this approach has received considerable attention in recent years (see for example [8]). The new development has led to a generalization of this method called *generalized quantum mechanics* (see [8, 19–22]).

Space of histories and probabilistic interpretation

The sum-over-histories approach is based on emphasizing the role of amplitudes. In this approach the basic notions are histories and their amplitudes. For each theory we have to specify a space of *elementary histories* — the set of trajectories in spacetime in the case of particle theory, the spacetime field configurations in the case of field theory, etc.. These elementary histories can be gathered to sets of histories which represents physical questions we can ask about the system under investigation. I.e., a set of histories can be characterized by a condition that its elements possess some property, or have correlations of some properties — e.g. the set of all histories which cross a spacetime region in the case of a particle theory or all field configurations with some value at a initial time and another value at the final time for the field theory.

Next we need some mechanism which give us predictions about experimental questions. As usual in quantum mechanics we are looking for probabilistic predictions — the predictions which can be interpreted as a confidence to the expectation that correlations of properties represented by the set of histories is observed. We need a rule which tells us to which sets of histories we can assign probabilities and what are their values. The main weakness of the sum-over-histories approach is that this rule is stated very intuitively — it tells us that we can assign a probability to a set of histories which is "physically distinguishable" from its complement, or a bit more generally, we can assign probabilities to a sequence of mutually disjoint sets of histories, which together exhaust the whole space of histories, if they are "physically distinguishable". What exactly the phrase "physically distinguishable" means is a very delicate problem connected with a definition of a measurement situation. But it can be used very powerfully on the intuitive level as can be seen for example in [13]. Attempts to define this notion more precisely led to the mentioned generalized quantum mechanics and an introduction of a *decoherence functional*. But before discussing this point in more detail we assume for now that we know an algorithm which tells us for which sets of histories we have a probabilistic interpretation.

Quantum amplitudes

Now we would like to now what the probability is. Quantum mechanics tells us, that the probability (if it has meaning) is given by the square of the absolute value of a *quantum amplitude* — of a complex number associated with each set of histories. And the sum-over-histories approach is mainly an algorithm for how to calculate such amplitudes. It can be summarized in two main rules:

- The amplitude of a set of histories is given by the sum of amplitudes of all elementary histories in the set. (12.1)
- The amplitude of an elementary history composed from independent components is given by the multiplication of amplitudes of all these components. (12.2)

The second rule introduces the possibility that an elementary history has some inner structure. It is common to assume that an elementary history of a complex system can be viewed as a composition of several elementary histories of subsystems of the whole system. E.g., the elementary history of two-particle theory is composed from two elementary histories of two one-particle theories. Another common situation is that the elementary history is composed from a couple of consequent parts or events. For example an elementary history of a system which is composed from two subsystems which interact with each other can be represented by elementary histories of each subsystem and events of interactions.

To conclude the definition of the algorithm for the calculation of quantum amplitudes, values of amplitudes of basic components of elementary histories has to be given. The usual heuristic for the most systems is that the amplitude of an elementary history is proportional to the exponential of its classical action[14]

$$A(\mathrm{h}) = \mathfrak{M}(\mathrm{h}) \exp\bigl(-I(\mathrm{h})\bigr) \quad . \tag{12.3}$$

Here $\mathfrak{M}$ is a measure on the space of histories which has to be specify for each particular theory. Clearly, there is an ambiguity in the separation of the amplitude into the measure and action parts. Intuitively the most of the important physical information is contained in the action part. But the measure can also contain nontrivial information (as we will see below), and it would be nice to have some general prescription for it.

We can ask whether we need to investigate an inner structure of elementary histories. The answer is yes, we do. The reason is that the only "canonical" choice of histories without structure would be fully extended histories (i.e. for example not bounded in the time direction). However for such histories we expect that the amplitude given by the expression (12.3) is not well defined (the action is infinite). We need to work with histories bounded in time. But this makes it necessary to introduce some inner structure for elementary histories.

It can be noted that the exponential nature of the action part of the elementary amplitude and usual additivity of the action reflects the rule (12.2). This suggests that the elementary history can be viewed as a sequence of infinitesimal sub-histories and the amplitude can be determined using (12.2) from amplitudes of these pieces. Such an argument can impose a condition on the measure $\mathfrak{M}$ — it has to satisfy some kind of composition law similar to the rule (12.2). Such a condition can be used in the definition of the measure as we will see in the next chapter.

Relation to a generalized quantum mechanics

As mentioned above, a generalization of the sum-over-histories approach led to the formulation of generalized quantum mechanics. It is a much broader framework which mainly addresses the question of the probabilistic interpretation of a quantum theory. It introduces a tool for determination of which sets of histories (and associated questions about the system) can be assigned probabilities. The central object of the generalized quantum mechanics is a *decoherence functional* which is essentially a generalization of the quantum amplitude. Using this functional we can introduce a notion of *decoherent sets of histories* — physically distinguishable sets of histories in the sense discussed above.

The decoherence functional D assigns a complex number $\mathrm{D}(\mathrm{H}_1, \mathrm{H}_2)$ to a pair of sets of histories H_1 and H_2. The sequence of sets of mutually disjoint sets of histories $\{\mathrm{H}_k\}$ which together exhaust the whole space of histories is called *decoherent* if the decoherence functional of these sets is sufficiently diagonal, i.e.

$$\mathrm{D}(\mathrm{H}_k, \mathrm{H}_l) \approx p(\mathrm{H}_k)\delta_{kl} \quad . \tag{12.4}$$

The probabilities assigned to such decoherent histories then are given by the coefficients $p(\mathrm{H}_k)$. The exactness of diagonality give us a quantitative measure for the notion of physical distinguishability we were missing in the sum-over-histories approach.

The decoherence functional must satisfy the following conditions:

$$\text{Additivity:} \qquad \mathrm{D}(\mathrm{H}_1 \cup \mathrm{H}_2, \mathrm{H}) = \mathrm{D}(\mathrm{H}_1, \mathrm{H}) + \mathrm{D}(\mathrm{H}_2, \mathrm{H}) \quad \text{for} \quad \mathrm{H}_1 \cap \mathrm{H}_2 = \emptyset \quad , \tag{12.5}$$

$$\text{Hermiticity:} \qquad \mathrm{D}(\mathrm{H}_1, \mathrm{H}_2) = \mathrm{D}(\mathrm{H}_2, \mathrm{H}_1)^* \quad , \tag{12.6}$$

$$\text{Positivity:} \qquad \mathrm{D}(\mathrm{H}, \mathrm{H}) \geqslant 0 \quad , \tag{12.7}$$

$$\text{Normalization:} \qquad \mathrm{D}(\boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{H}}) = 1 \quad , \tag{12.8}$$

where $\boldsymbol{\mathcal{H}}$ is a set of all histories. The first condition is an analog of the rule (12.1) of the sum-over-histories approach and reflects the principle of superposition in the quantum mechanics. Using this property a value of the decoherence functional for general sets of histories can be determined from a knowledge of the decoherence functional for elementary histories. The second condition tells us about a relation of both arguments of the decoherence functional. The last two conditions are needed for the interpretation of coefficients in (12.4) as probabilities.

The sum-over-histories version of a quantum theory can be formulated as a generalized quantum mechanics if we define the decoherence functional using amplitudes. A general way how to do it is to define the decoherence functional for elementary histories as

$$\mathrm{D}(\mathrm{h}_1, \mathrm{h}_2) = A(\mathrm{h}_1)A(\mathrm{h}_2)^* = \mathfrak{M}(\mathrm{h}_1)\mathfrak{M}(\mathrm{h}_2)\exp\bigl(-I(\mathrm{h}_1) - I(\mathrm{h}_2)^*\bigr) \quad . \tag{12.9}$$

The problem with this definition is that the amplitude for a whole history is not usually well defined. For example the values of the action for unbounded particle trajectory or configuration of a field on whole spacetime are infinite. Therefore we restrict histories to some domain "bounded in the time direction". But in this case we have to include some additional terms in the definition of the decoherence functional which are localized on a "boundary" of restricted histories and which correspond to initial and final states of the system. Unfortunately these terms have different structures for different theories, and one of the main motivations of our work is the desire for a better understanding of an origin of these terms.

Beside this problem with the definition of the decoherence functional, the generalized quantum mechanics has another weakness. In distinction to the sum-over-histories approach it is missing an analog of the rule (12.2). We do not know the behavior of the decoherence functional under the decomposition of elementary histories to its components. This lack of knowledge is closely related to the previous problem — we need to know some composition law for the decoherence functional.

In the following we will use the sum-over-histories approach to quantize a particle-like theory instead of the other candidate — generalized quantum mechanics — mainly because the problems mentioned above. The price we are paying is that we do not have a clear definition of decoherent histories, and we will have to supply it by more intuitive arguments. But we hope that this approach gives us a better understanding of possible solutions of these problems.

13 Particle in a curved space without boundary

Space of histories and action

In this chapter we shortly repeat the classical formulation of a particle-like theory and formulate the quantum version of the theory using the sum-over-histories approach.

As usual in the sum-over-histories approach, the theory is characterized by a space of histories and an action. An elementary history in our case is a *trajectory* — an imbedding $\boldsymbol{X}$ of a 1-dimensional manifold N (called the *inner space*) with two one-point boundaries to a d-dimensional *target manifold* M — and an *inner space metric* h on the inner manifold N.

$$\boldsymbol{X} \;:\; N \;\to\; N \quad , \quad h \in \mathfrak{T}^0_2 N \quad . \tag{13.1}$$

M is equipped with a target space metric g and scalar potential V.

In the Euclidian version of the theory h is positive definite; in the physical version it is negative definite. For a non-relativistic particle g is positive definite; for a relativistic particle it is Lorentzian.

The Euclidian action[15] is given by

$$I(\boldsymbol{X}, h, N) = \frac{1}{2} \int\limits_N \Big(h^{\text{-}1\,\boldsymbol{ab}}\, \mathrm{D}^{\boldsymbol{\alpha}}_{\boldsymbol{a}} \boldsymbol{X}\; \mathrm{D}^{\boldsymbol{\beta}}_{\boldsymbol{b}} \boldsymbol{X}\; g_{\boldsymbol{\alpha\beta}}(\boldsymbol{X}) + V(\boldsymbol{X}) \Big)\, \mathfrak{h}^{\frac{1}{2}} \quad , \tag{13.2}$$

where $\mathfrak{h}^{\frac{1}{2}}$ is volume element associated with the inner metric h.

This is the simplest example of a σ-model theory. In the general case the inner space N can have a higher dimension. The case $dim N = 2$ leads to a string theory.

Clearly, the action is invariant under diffeomorphisms of the inner manifold N. For $\boldsymbol{f} \in \mathrm{Diff}(N, \tilde{N})$ we have

$$\begin{gathered} [\boldsymbol{X}, h, N] \quad \to \quad [\tilde{\boldsymbol{X}}, \tilde{h}, \tilde{N}] \quad , \\ \boldsymbol{f} : N \to \tilde{N} \quad , \quad \tilde{\boldsymbol{X}} = \boldsymbol{f}^\star \boldsymbol{X} \quad , \quad \tilde{h} = \boldsymbol{f}^\star h \quad , \\ I(\tilde{\boldsymbol{X}}, \tilde{h}, \tilde{N}) = I(\boldsymbol{X}, h, N) \end{gathered} \tag{13.3}$$

We can use this fact for a parametrization of the space of histories. Let $\tilde{N}$ be a fixed "canonical" copy of the inner space with a fixed coordinate $\eta : \tilde{N} \to \langle 0, 1 \rangle$. For any history $[\boldsymbol{X}, h, N]$ we can always find an equivalent history $[\tilde{\boldsymbol{X}}, \tilde{h}, \tilde{N}]$ related by a diffeomorphism $\boldsymbol{f} : \tilde{N} \to N$ and using a diffeomorphism of $\tilde{N}$ itself we can choose a history for which

$$\tilde{h}_{\boldsymbol{ab}} = \nu^2 \tau^2\, \mathrm{d}_{\boldsymbol{a}} \eta\, \mathrm{d}_{\boldsymbol{b}} \eta \quad , \quad \tilde{\mathfrak{h}}^{\frac{1}{2}} = \nu \tau\, d\eta \quad , \quad \tau \in \mathbb{R}^+ \tag{13.4}$$

where τ is an *inner length* or *inner time* of the space N in the metric h which is diffeomorphism invariant. ν is a constant signature factor distinguishing Euclidian and physical versions of the theory (see appendix D). In the former case ν is real, in the later one it is imaginary. We use it also to fix a proper numerical factor in the action in front of the kinetic term. We set $\nu = m^{\text{-}1}$ in the case of nonrelativistic particle and $\nu = 2$ for relativistic particle in the Euclidian version of the theory. In the physical version of the theory these values are multiplied by i.

Moreover, we can use for simplicity maps $\boldsymbol{x}, f$

$$\begin{array}{llll} \boldsymbol{x} : \langle 0,1\rangle & \rightarrow & M \quad , & \boldsymbol{x}(\eta) = \tilde{\boldsymbol{X}} \quad , \\ f : \langle 0,1\rangle & \rightarrow & N \quad , & f(\eta) = \boldsymbol{f} \end{array} \tag{13.5}$$

instead of the imbedding $\boldsymbol{X}$ and diffeomorphism $\boldsymbol{f}$. The conditions above fix $\boldsymbol{x}, \tau, f$ uniquely, and therefore a general history $[\boldsymbol{X}, h, N]$ can be parametrized by $\boldsymbol{x}, \tau, f$.

The action in these variables has the form

$$I(\tau, \boldsymbol{x}) = I(\tau, \boldsymbol{x}, f) = \frac{1}{2} \int\limits_{\langle 0,1\rangle} \left(\frac{1}{\nu\tau} \dot{\boldsymbol{x}}^\alpha \dot{\boldsymbol{x}}^\beta g_{\alpha\beta}(\boldsymbol{x}) + \nu\tau\, V(\boldsymbol{x}) \right) d\eta \quad . \tag{13.6}$$

As we expected, it is independent of the diffeomorphism parameter f.

Amplitudes

The sum-over-histories approach to quantum theory is based on the notion of quantum amplitudes. For a set of histories H we can define an amplitude $A(\mathrm{H})$ by "summing" over amplitudes of elementary histories in the set,

$$A(H) = \int\limits_{\mathrm{h}\in\mathrm{H}} \mathfrak{M}(\mathrm{h})\ \exp\bigl(-I(\mathrm{h})\bigr) \quad . \tag{13.7}$$

Here $\mathfrak{M}$ is a measure on the space of histories. We will assume that it has the same symmetry as the action. It is well known that there are severe technical problems in defining such a measure, at least in the case of Lorentzian theory, but we will ignore them now.

The quantum amplitude is not directly a physical measurable quantity. As we said, we need an additional notion of *distinguishable* or *decoherent* histories to give a probabilistic interpretation to the square of amplitudes. We expect that this notion has the same symmetry as the action and the measure. This means that we will be always interested in amplitudes of sets of histories which are invariant under the action of the diffeomorphism group. For such sets we can factorize the path integral and eliminate the reference to the diffeomorphism:

$$\begin{aligned} A(\mathrm{H}) = \int\limits_{\mathrm{h}\in\mathrm{H}} \mathfrak{M}(\mathrm{h})\ \exp\bigl(-I(\mathrm{h})\bigr) &= \int\limits_{\substack{\boldsymbol{f}\in\mathrm{Diff} \\ [\mathrm{h}]\in\mathrm{H}/\mathrm{Diff}}} [\mathfrak{M}]([\mathrm{h}])\mathfrak{D}(\boldsymbol{f})\ \exp\bigl(-I([\mathrm{h}])\bigr) = \\ &= \int\limits_{[\mathrm{h}]\in\mathrm{H}/\mathrm{Diff}} \mathfrak{M}_{red}([\mathrm{h}])\ \exp\bigl(-I([\mathrm{h}])\bigr) \quad , \end{aligned} \tag{13.8}$$

where a reduced measure $\mathfrak{M}_{red} = (\mathfrak{M}/\mathfrak{D}) \int_{\mathrm{Diff}} \mathfrak{D}$ contains all factors given by change of variables (Fadeev-Popov determinant) and an integral over symmetry orbits (here $\mathfrak{D}$ is an invariant measure on the diffeomorphism group). We assume such a normalization of $\mathfrak{M}$ that $\mathfrak{M}_{red}$ is "well" defined. It, of course, implies some kind of regularization of the infinite normalization factors which we will escape by a characterization of the measure $\mathfrak{M}_{red}$ instead of the original measure. But see [23] for a discussion of this question.

If we rewrite the last equation in variables $\mathrm{h} = [\tau, \boldsymbol{x}]$ we get

$$A(\mathrm{H}) = \int\limits_{[\tau,\boldsymbol{x}]\in\mathrm{H}} \mathfrak{M}_{red}(\tau, \boldsymbol{x})\ \exp\bigl(-I(\tau, \boldsymbol{x})\bigr) \quad . \tag{13.9}$$

Propagator

It is useful to compute an amplitude $\frac{1}{n}K(\tau, x_f|x_i)$ – called the *propagator* or *heat kernel* – for the set of histories restricted only by positions of end points of the trajectory x_f and x_i in the target manifold M and by fixing an inner time to a particular value τ:

$$\frac{1}{n}K(\tau, x_f|x_i) = \int\limits_{\boldsymbol{x}\in\boldsymbol{\mathcal{T}}(x_f|x_i)} \mathfrak{M}^F(\tau, x_f|x_i)[\boldsymbol{x}]\ \exp\bigl(-I(\tau,\boldsymbol{x})\bigr) \quad , \tag{13.10}$$

where $\boldsymbol{\mathcal{T}}(x_f|x_i)$ is a set of trajectories $\boldsymbol{x} : \langle 0,1\rangle \to M$ with $\boldsymbol{x}(1) = x_f$ and $\boldsymbol{x}(0) = x_i$. Because the set of histories $[\tau, \boldsymbol{\mathcal{T}}(x_f|x_i)] = \{\tau\} \times \boldsymbol{\mathcal{T}}(x_f|x_i)$ is a lower dimensional subset of the space of all histories, $K(\tau, x_f|x_i)$ is essentially an amplitude "density" on the space $\mathbb{R}^+ \times M \times M$ of values $[\tau, x_f, x_i]$. Therefore we have to expect that the restriction $\mathfrak{M}^F(\tau, x_f|x_i)$ of the measure $\mathfrak{M}_{red}$ to the space $[\tau, \boldsymbol{\mathcal{T}}(x_f|x_i)]$, which we call the *Feynman measure*, depends on τ and end points x_f and x_i; maybe only in a "trivial" way. The factor n governs the signature of the spacetime metric[16] (see appendix D).

In other words, an amplitude density of an elementary history on the space $[\tau, \boldsymbol{\mathcal{T}}(x_f|x_i)]$ is

$$A(\tau,\boldsymbol{x}) = \mathfrak{M}^F(\tau, x_f|x_i)[\boldsymbol{x}]\ \exp\bigl(-I(\tau,\boldsymbol{x})\bigr) \quad . \tag{13.11}$$

It is well known [7,8,14,24] that with the right choice of the measure $\mathfrak{M}^F(\tau, x_f|x_i)$ the propagator satisfies the equation

$$-\dot{K}(\tau) = \frac{\nu}{2}\mathrm{F} \bullet K(\tau) \quad , \quad K(0) = \mathcal{G}^{-1} \quad , \tag{13.12}$$

where F is a wave operator fixed by the action and the measure, $\mathcal{G} = \mathfrak{g}^{\frac{1}{2}}\delta$ is as before a delta distribution on M normalized to the volume element $\mathfrak{g}^{\frac{1}{2}}$. (See appendix A for more details on notation.) In other words, K is the exponential of F

$$K(\tau) = \exp\Bigl(-\frac{\nu\tau}{2}\mathrm{F}\Bigr) \bullet \mathcal{G}^{-1} \quad . \tag{13.13}$$

We have not specified the "right choice" of the measure yet. As mentioned, it can be a very problematic task from the pure mathematical point of view. Instead of trying to develop a measure theory on infinite dimensional spaces for oscillatory integrals (where the main problem lies), we take the usual approach of formal manipulations, and we define the measure by its decomposition properties and approximation for small time intervals. The former is given in equation (13.19), and the latter is given in equation (13.30).

The idea of the proof of the relations (13.12) is in proving key properties of the exponential,

$$K(\tau_f) \bullet \mathcal{G} \bullet K(\tau_i) \;=\; K(\tau_f + \tau_i) \quad , \tag{13.14}$$

$$\mathcal{G} \bullet K(\tau) \bullet \mathcal{G} \;=\; \mathcal{G} - \frac{\nu\tau}{2}\mathcal{F} + \mathcal{O}(\tau^2) \quad , \tag{13.15}$$

where $\mathcal{F} = \mathcal{G} \bullet \mathrm{F}$ is the quadratic form of the differential operator F.

Composition law

The first condition (13.14) is a composition law for the amplitude K. This law reflects the possibility to decompose a history $[\tau, \boldsymbol{x}]$ into histories $[\tau_i, \boldsymbol{x}_i]$ during an initial amount of inner time τ_i and $[\tau_f, \boldsymbol{x}_f]$ during a final amount of inner time τ_f. We say that a history $[\tau, \boldsymbol{x}]$ is given by *joining* of histories $[\tau_f, \boldsymbol{x}_f]$ and $[\tau_i, \boldsymbol{x}_i]$ if

$$\begin{gathered}[\tau, \boldsymbol{x}] = [\tau_f, \boldsymbol{x}_f] \odot [\tau_i, \boldsymbol{x}_i] \qquad \text{iff} \\ \tau = \tau_f + \tau_i \quad , \quad \boldsymbol{x}_f(0) = \boldsymbol{x}_i(1) \quad , \quad \boldsymbol{x}_f = \boldsymbol{x}\Bigl(\frac{\tau_i + \eta\tau_f}{\tau}\Bigr) \quad , \quad \boldsymbol{x}_i = \boldsymbol{x}\Bigl(\frac{\eta\tau_i}{\tau}\Bigr) \quad .\end{gathered} \tag{13.16}$$

The actions of such histories are related by

$$I(\tau,\boldsymbol{x}) = I(\tau_{\mathrm{f}},\boldsymbol{x}_{\mathrm{f}}) + I(\tau_{\mathrm{i}},\boldsymbol{x}_{\mathrm{i}}) \quad . \tag{13.17}$$

This induces a decomposition of the set of histories $[\tau, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})]$ which defines the propagator $K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ to disjoint sets $[\tau_{\mathrm{f}}, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{o}})] \times [\tau_{\mathrm{i}}, \boldsymbol{\mathcal{T}}(x_{\mathrm{o}}|x_{\mathrm{i}})]$

$$[\tau, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})] = \bigcup_{x_{\mathrm{o}}\in M} [\tau_{\mathrm{f}}, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{o}})] \times [\tau_{\mathrm{i}}, \boldsymbol{\mathcal{T}}(x_{\mathrm{o}}|x_{\mathrm{i}})] \quad . \tag{13.18}$$

If the measures on these sets are related by

$$\mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}] = \mathfrak{M}^F(\tau_{\mathrm{f}}, x_{\mathrm{f}}|x_{\mathrm{o}})[\boldsymbol{x}_{\mathrm{f}}]\; n\mathfrak{g}^{\frac{1}{2}}(x_{\mathrm{o}})\; \mathfrak{M}^F(\tau_{\mathrm{i}}, x_{\mathrm{o}}|x_{\mathrm{i}})[\boldsymbol{x}_{\mathrm{i}}] \quad , \tag{13.19}$$

for $[\tau,\boldsymbol{x}] = [\tau_{\mathrm{f}},\boldsymbol{x}_{\mathrm{f}}] \odot [\tau_{\mathrm{i}},\boldsymbol{x}_{\mathrm{i}}]$ it follows that

$$\begin{aligned} K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}}) &= \int\limits_{\boldsymbol{x}\in\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})} n\, \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}]\; \exp\bigl(-I(\tau,\boldsymbol{x})\bigr) = \\ &= \int\limits_{x_{\mathrm{o}}\in M} \mathfrak{g}^{\frac{1}{2}}(x_{\mathrm{o}}) \int\limits_{\boldsymbol{x}_{\mathrm{f}}\in\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{o}})} n\, \mathfrak{M}^F(\tau_{\mathrm{f}}, x_{\mathrm{f}}|x_{\mathrm{o}})[\boldsymbol{x}_{\mathrm{f}}]\; \exp\bigl(-I(\tau_{\mathrm{f}},\boldsymbol{x}_{\mathrm{f}})\bigr)\times \\ &\qquad\qquad \times \int\limits_{\boldsymbol{x}_{\mathrm{i}}\in\boldsymbol{\mathcal{T}}(x_{\mathrm{o}}|x_{\mathrm{i}})} n\, \mathfrak{M}^F(\tau_{\mathrm{i}}, x_{\mathrm{o}}|x_{\mathrm{i}})[\boldsymbol{x}_{\mathrm{i}}]\; \exp\bigl(-I(\tau_{\mathrm{i}},\boldsymbol{x}_{\mathrm{i}})\bigr) = \\ &= \bigl[K(\tau_{\mathrm{f}}) \bullet \mathcal{G} \bullet K(\tau_{\mathrm{i}})\bigr](x_{\mathrm{f}}|x_{\mathrm{i}}) \quad , \end{aligned} \tag{13.20}$$

which is what we wanted to prove.

The condition (13.19) represents a reasonable assumption of the locality of the measure $\mathfrak{M}^F$. Together with the additivity of the action it reflects the rule (12.2) of the sum-over-histories approach to quantum mechanics — that the amplitude of independent (here consequent) events is given by multiplication of individual amplitudes. This condition is the first part of our definition of the measure. Now we know how to construct the measure $\mathfrak{M}^F(\tau)$ for some time τ from measures for shorter time intervals. To conclude the definition of the measure, we need to specify it for an infinitesimally short inner time interval. This moves us to an investigation of the short time behavior of the heat kernel.

Short time amplitude

Now we turn to prove equation (13.15). It can be found in the literature (e.g. [7,24]), but we present it here to show how the measure is actually determined and how the operator $\mathcal{F}$ depends on this choice.

As we said, we ignore technical difficulties in the definition of the path integral, and we assume that this integral has most of the properties of a usual integral in a finite-dimensional manifold. This allows us to find the short time behavior for the propagator.

First we write an expansion of the action for small τ

$$I(\tau,\boldsymbol{x}) = \frac{1}{\tau}\, I_{-1}(\boldsymbol{x}) + I_0(\boldsymbol{x}) + \tau\, I_1(\boldsymbol{x}) + \dots \quad . \tag{13.21}$$

For the simplest action we are using we have

$$I_{-1}(\boldsymbol{x}) = \frac{1}{2\nu} \int\limits_{\eta\in\langle 0,1\rangle} \dot{\boldsymbol{x}}^{\alpha}\dot{\boldsymbol{x}}^{\beta} g_{\alpha\beta}(\boldsymbol{x}) d\eta \quad , \tag{13.22}$$

$$I_0(\boldsymbol{x}) = 0 \quad , \tag{13.23}$$

$$I_1(\boldsymbol{x}) = \frac{\nu}{2} \int\limits_{\eta\in\langle 0,1\rangle} V(\boldsymbol{x}) d\eta \quad . \tag{13.24}$$

We assume that the measure is slowly changing in τ compared to the leading term in the action.

The dominant contribution to the integral (13.10) comes from an extremum $\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})$ of the leading term I_{-1} in the exponent. But the extremum of the functional (13.22) is clearly a geodesic of the metric g. We expand all expressions around this extremum

$$\boldsymbol{x} = \bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}}) + \sqrt{\tau}\vec{\boldsymbol{x}} \quad , \tag{13.25}$$

where $\vec{\boldsymbol{x}}$ is a tangent vector to the space $\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})$ at the extremum $\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})$. We actually need to specify what the addition in the last equation means. It will be done more carefully in a similar situation in appendix F (see eq. (F.5)). But now we are interested more in a qualitative answer, so we skip these details here. The expanded integral (13.10) has the structure

$$\begin{aligned}\frac{1}{n} K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}}) = \exp\Big(-I\big(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})\big)\Big) \int\limits_{\vec{\boldsymbol{x}}\in \mathbf{T}_{\bar{\boldsymbol{x}}}\boldsymbol{\mathcal{T}}} \mathfrak{M}^{F}{}_{*}(\tau, x_{\mathrm{f}}|x_{\mathrm{i}}) \exp\left(-\frac{1}{2}\vec{\boldsymbol{x}}\cdot\delta^2 I_{-1}(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}}))\cdot\vec{\boldsymbol{x}}\right) \times \\ \times \Big(1 + \sqrt{\tau}\,(\vec{\boldsymbol{x}}^{\mathrm{odd}}\text{- terms}) + \tau\,(\vec{\boldsymbol{x}}^{\mathrm{even}}\text{- terms}) + \dots\Big) \quad .\end{aligned} \tag{13.26}$$

Here $\mathfrak{M}^{F}{}_{*}(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ is a leading term in τ and the $\vec{\boldsymbol{x}}$-expansion of the measure $\mathfrak{M}^{F}(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ after change of variables $\boldsymbol{x} \to \vec{\boldsymbol{x}}$. $\mathfrak{M}^{F}{}_{*}$ is a constant measure on the vector space $\mathbf{T}_{\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})}\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})$ (a tangent space to the space of trajectories $\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})$). The actual dependence on $\vec{\boldsymbol{x}}$ is hidden in higher terms of the $\vec{\boldsymbol{x}}$-expansion. As a leading term in the τ-expansion, $\mathfrak{M}^{F}{}_{*}$ depends on τ in a trivial way — it is proportional to a power of τ. Of course, this statement is formal — the exponent of τ in $\mathfrak{M}^{F}{}_{*}$ is of the order of the dimension of the space $\vec{\boldsymbol{\mathcal{T}}}$, which is infinite.

"$\vec{\boldsymbol{x}}$-terms" in the last equation represents terms resulting from the expansion of the action and the measure; $\vec{\boldsymbol{x}}^{\mathrm{odd}}$ or $\vec{\boldsymbol{x}}^{\mathrm{even}}$ suggest that $\vec{\boldsymbol{x}}$ occurs in these terms in odd or even power. For convenience we combined the term τI_1 into the prefactor despite the fact that it could be included among terms proportional to τ.

The value $\nu I_{-1}(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}}))$ is a well-known quantity called the world function, or half the squared geodesic distance,

$$\sigma(x_{\mathrm{f}}|x_{\mathrm{i}}) = \nu I_{-1}(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})) = \frac{1}{2} \int\limits_{\langle 0,1\rangle} \dot{\bar{\boldsymbol{x}}}(x_{\mathrm{f}}|x_{\mathrm{i}}) \cdot g(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})) \cdot \dot{\bar{\boldsymbol{x}}}(x_{\mathrm{f}}|x_{\mathrm{i}})\, d\eta \quad . \tag{13.27}$$

We also use the notation

$$\bar{V}(x_{\mathrm{f}}|x_{\mathrm{i}}) = \frac{2}{\nu} I_1(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}})) = \int\limits_{\langle 0,1\rangle} V(\bar{\boldsymbol{x}}(x_{\mathrm{f}}|x_{\mathrm{i}}))\, d\eta \quad . \tag{13.28}$$

The integral (13.26) is a simple Gaussian integration. (In fact, one approach to defining infinite-dimensional integrals is through the definition of a "Gaussian" measure which in our case would be

$\mathfrak{M}^F{}_* \exp(-\frac{1}{2}\,\vec{\boldsymbol{x}}\cdot\delta^2 I_{-1}\cdot\vec{\boldsymbol{x}}))$. The integration can be performed, at least formally, to give

$$\begin{aligned}\frac{1}{n}K(\tau,x_{\rm f}|x_{\rm i}) = \exp\big(-\frac{1}{\nu\tau}\sigma(x_{\rm f}|x_{\rm i}) - \frac{\nu\tau}{2}\bar{V}(x_{\rm f}|x_{\rm i})\big)\times\\ \times\,\mathfrak{M}^F{}_*(\tau,x_{\rm f}|x_{\rm i})\,{\rm Det}\left(\frac{\delta^2 I_{-1}(\bar{\boldsymbol{x}}(x_{\rm f}|x_{\rm i}))}{2\pi\nu\tau}\right)^{-\frac{1}{2}}\Big(1+\tau(\dots)+\dots\Big)\quad.\end{aligned}\tag{13.29}$$

The terms proportional to $\sqrt{\tau}$ disappear during integration, thanks to the odd power of $\vec{\boldsymbol{x}}$. Coefficients in front of powers of τ could be expressed in terms of variations of the action and the measure. But because we did not specify the measure precisely yet, we can do it now by fixing this short time amplitude. I.e., we can define the measure $\mathfrak{M}^F$ by choosing functions $\alpha_0(x_{\rm f}|x_{\rm i})$ and $\alpha_1(x_{\rm f}|x_{\rm i})$ in a slightly rearranged version of the last equation,

$$\begin{aligned}K(\tau,x_{\rm f}|x_{\rm i}) \;=\; \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\Delta(x_{\rm f}|x_{\rm i})\,\Big(\alpha_0(x_{\rm f}|x_{\rm i}) - \tau\frac{\nu}{2}\,\alpha_1(x_{\rm f}|x_{\rm i}) + \mathcal{O}(\tau^2)\Big)\times\\ \times\exp\left(-\frac{1}{\nu\tau}\sigma(x_{\rm f}|x_{\rm i}) - \frac{\nu\tau}{2}\bar{V}(x_{\rm f}|x_{\rm i})\right)\quad,\end{aligned}\tag{13.30}$$

where $\alpha_0(x_{\rm f}|x_{\rm i})$ satisfies

$$\alpha_0(x|x) = 1\quad.\tag{13.31}$$

Here $\Delta(x_{\rm f}|x_{\rm i})$ is Van Vleck-Morette determinant (see (G.13)). This ansatz together with equation (13.31) gives us a condition

$$\mathfrak{M}^F{}_*(\tau,x|x)\,{\rm Det}\left(\frac{\delta^2 I_{-1}(\bar{\boldsymbol{x}}(x|x))}{2\pi\nu\tau}\right)^{-\frac{1}{2}} = \frac{1}{(2\pi\nu\tau)^{\frac{d}{2}}}\quad.\tag{13.32}$$

As we will see, this τ-dependence of the measure is necessary for further proof of equation (13.15), and the particular choice a coincidence limit of the coefficient α_0 is needed for a proper normalization in (13.12).

In the following we will prove that a form of the operator $\mathcal{F}$ in (13.15) depends only on the coincidence limits of α_1 and the first two derivatives of α_0. So we can ignore terms with higher power of τ in eq. (13.30). As discussed before, equations (13.15) together with composition law (13.14) determines the propagator K, i.e. also all important information hidden in the measure $\mathfrak{M}^F$. This means that a knowledge of the mentioned coincidence limits concludes our definition of the measure and path integral itself.

Let us note that this section is some kind of justification of the usual time-discretization of the path integral and on a priori choice of the short time amplitude in the form (13.30). But in principle it would be possible to define the measure $\mathfrak{M}^F$ in some more compact way and compute exactly the form of the functions α_0 and α_1 in terms of variation of the action and the measure. This would be a hard task because variations of I_{-1} up to the fourth order are important for α_1. Also some kind of regularization would be needed because of the infinite dimension of the space of trajectories. It probably does not make sense to attempt to do this before we have a better understanding of a definition of the measure $\mathfrak{M}^F$ in general.

As equation (13.32) suggests, the leading term $\mathfrak{M}^F{}_*$ should be "almost" the same as ${\rm Det}(\frac{\delta^2 I_{-1}}{2\pi\nu\tau})^{\frac{1}{2}}$, and our guess is that the full measure has this structure but with some specific boundary conditions needed for the definitions of $\delta^2 I_{-1}$ and for the functional determinant Det which are different from Dirichlet conditions used for these definitions in (13.29). The difference will cause the extra factor $(2\pi\nu\tau)^{-\frac{d}{2}}\Delta\alpha_0$ in our ansatz (13.30). But this is more-or-less a speculation at this moment.

Short time behavior of the heat kernel

Now we continue with the proof of equation (13.15). We show that for small τ the amplitude (13.30) has the desired behavior in a distributional sense. Most of the technical work is done in appendix F where it is shown that for small τ the following expansion holds (equation (F.8))

$$\begin{aligned} \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{x,z\in M} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\, \Delta(x|z)\, \exp\Big(-\frac{1}{\nu\tau}\sigma(x|z)\Big)\varphi(x)\psi(z) = \\ = \varphi \bullet \mathcal{G} \bullet \psi \;-\; \tau\frac{\nu}{2}\,\varphi \bullet \mathcal{L} \bullet \psi \;+\; \mathcal{O}(\tau^2) \quad , \end{aligned} \tag{13.33}$$

where φ and ψ are smooth test functions and $\mathcal{L}$ is the Laplace operator quadratic form

$$\begin{aligned} \varphi \bullet \mathcal{L} \bullet \psi = \int\limits_M \mathfrak{g}^{\frac{1}{2}}\, (\mathrm{d}\varphi) \cdot g^{-1} \cdot (\mathrm{d}\psi) = \\ = -\int\limits_M \mathfrak{g}^{\frac{1}{2}} \varphi\, (\nabla^2 \psi) \;=\; -\int\limits_M \mathfrak{g}^{\frac{1}{2}} \psi\, (\nabla^2 \varphi) \quad . \end{aligned} \tag{13.34}$$

Let us remember that now we are discussing the case of a manifold without boundary, and therefore we do not have to worry about boundary conditions for the Laplace operator and integration by parts.

Using this result it is easy to show that

$$\begin{aligned} &\varphi \bullet \mathcal{G} \bullet K(\tau) \bullet \mathcal{G} \bullet \psi \;= \\ &\quad = \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{x,z\in M} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z) \Big(\alpha_0(x|z) - \tau\frac{\nu}{2}\,\alpha_1(x|z) + \mathcal{O}(\tau^2)\Big) \times \\ &\qquad\qquad \times \exp\Big(-\frac{1}{\nu\tau}\sigma(x|z) - \frac{\nu\tau}{2}\bar{V}(x|z)\Big)\, \varphi(x)\psi(z) = \\ &\quad = \int\limits_{x,z\in M} \Big(\mathcal{G}(x|z) - \tau\frac{\nu}{2}\mathcal{L}(x|z)\Big)\, \varphi(x)\psi(z) \Big(\alpha_0(x|z) - \tau\frac{\nu}{2}\,\alpha_1(x|z)\Big) \times \\ &\qquad\qquad \times \exp\Big(-\frac{\nu\tau}{2}\bar{V}(x|z)\Big)\, \big(1 + \mathcal{O}(\tau^2)\big) = \\ &\quad = \;\varphi \bullet \mathcal{G} \bullet \psi - \\ &\qquad - \tau\frac{\nu}{2}\,\varphi \bullet \Big(\mathcal{L} + \big(V\,\mathcal{G}\big) + \big(g^{-1\,\mu\nu}[\mathrm{d}_{\mathbf{l}\mu}\mathrm{d}_{\mathbf{r}\nu}\alpha_0]\mathcal{G}\big) + \big([\alpha_1]\mathcal{G}\big)\Big) \bullet \psi - \\ &\qquad - \tau\frac{\nu}{2}\,\varphi \bullet \Big(\big(\overleftarrow{\mathrm{d}} \cdot g^{-1} \cdot [\mathrm{d}_{\mathbf{l}}\alpha_0]\big) \bullet \mathcal{G} + \mathcal{G} \bullet \big([\mathrm{d}_{\mathbf{r}}\alpha_0] \cdot g^{-1} \cdot \overrightarrow{\mathrm{d}}\big)\Big) \bullet \psi + \\ &\qquad + \mathcal{O}(\tau^2) \quad , \end{aligned} \tag{13.35}$$

where we used $[\bar{V}] = V$ and $[\alpha_0] = 1$. Here the $[A]$ denotes a coincidence limit of a bitensor A, $\mathrm{d}_{\mathbf{r}}A$ and $\mathrm{d}_{\mathbf{l}}A$ are derivatives with respect of the right and left arguments and the bi-distributions $\big(f\mathcal{G}\big)$, $\overleftarrow{\mathrm{d}}$ and $\overrightarrow{\mathrm{d}}$ are defined as in (A.6), (A.7).

If the condition

$$[\mathrm{d}_{\mathbf{r}}\alpha_0] = [\mathrm{d}_{\mathbf{l}}\alpha_0] = 0 \tag{13.36}$$

is satisfied, we see that the propagator $K(\tau)$ has really the form (13.15) with

$$\mathcal{F} = \mathcal{L} + \mathcal{V} \quad , \tag{13.37}$$

$$\mathcal{V} = \big(V + [\alpha_1] + g^{-1\,\mu\nu}[\mathrm{d}_{\mathbf{l}\mu}\mathrm{d}_{\mathbf{r}\nu}\alpha_0]\big)\mathcal{G} \quad . \tag{13.38}$$

I.e., $\mathcal{F}$ is a Laplace operator with a potential term which include the original potential V from the action and additional parts depending on the choice of the measure.

A common choice for α_0 is a power of the Van Vleck-Morette determinant

$$\alpha_0 = \Delta^{-p} \quad , \tag{13.39}$$

which satisfies the condition (13.36). It leads to an additional part in the potential,

$$g^{-1\,\mu\nu}[\mathrm{d}_{1\mu}\mathrm{d}_{\mathrm{r}\nu}\Delta^{-p}] = \frac{p}{3}R \quad , \tag{13.40}$$

where R is a scalar curvature of the metric g.

The condition (13.36) is actually a consequence of (13.31) and an assumption of the symmetry of α_0

$$\alpha_0(x|z) = \alpha_0(z|x) \quad . \tag{13.41}$$

It is a natural assumption in the case when the theory is symmetric under trajectory reversal. However this condition does not have to be satisfied if there is a preferred path direction as for example in the case of interaction with an electromagnetic field. (In this case the operator $\mathcal{F}$ is Laplace-like operator with the covariant derivative containing an EM vector potential and corrections from a measure.) But we will not discuss such a situation, and in the following we will assume that the conditions (13.41) and (13.36) are satisfied.

This concludes our proof of the relation (13.15). In summary, we have seen that for small τ the propagator $K(\tau)$ has the behavior given by (13.15) where the operator $\mathcal{F}$ is the Laplace-like operator associated with the metric g and is fixed by the action and the measure. If the measure is defined using the decomposition property (13.14) and the short time amplitude (13.30), the operator $\mathcal{F}$ is fixed by knowledge of the coincidence limits of α_1 and the first two derivatives of α_0.

Interacting theory

Now we introduce an *interacting theory* — a many particle theory in which particles can be created or annihilated and can interact with each other. This theory can be build from the free theory using general ideas of the sum-over-histories approach to quantum mechanics as discussed in the introduction of this part.

The space of histories of such an interacting theory is the set of an arbitrary number of copies of one-particle free histories, endpoints of which can be glued in interaction vertices. An example of an elementary history is shown in the figure 13.1. Next we have to specify the amplitude (density) associated with such an elementary history. According to the general principle, the amplitude of a history composed from several one-particle histories is given by a product of amplitudes of all these histories. If interactions are present, the amplitude has to be additionally multiplied by amplitudes associated with each interaction. Finally, the amplitude of a set of histories is, as usual, given by the sum of amplitudes of elementary histories in the set.

The simplest interaction are *sources* (one-leg vertices — e.g. J-vertex in the figure) and a *potential interaction* (two-leg vertices — e.g. V-vertex in the figure). Non-trivial interaction is introduced using vertices of higher order.

In the next chapter we encounter also an interaction of particles with a boundary.

Dynamical origin of the potential

We have started with the action in the form (13.6) with a general potential V. But it is actually possible to derive the form of this action using an action without a potential and an assumption of a simple potential interaction.

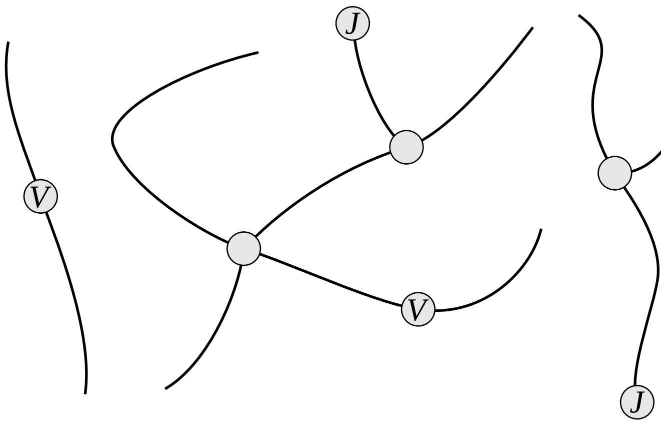


Figure 13.1: An example of the elementary history of the interacting theory.
The elementary history of the many particle interacting theory is formed by one-particle histories which can be glued in interaction vertices. The simplest interaction are sources — one-leg J-vertices in the figure — and a potential interaction — two-leg V-vertices in the figure.

We start with a free particle with the action

$$I_{\text{free}}(\tau,\boldsymbol{x}) = \frac{1}{2}\int\limits_{\langle 0,1\rangle} \frac{1}{\nu\tau}\dot{\boldsymbol{x}}^{\boldsymbol{\alpha}}\dot{\boldsymbol{x}}^{\boldsymbol{\beta}} g_{\boldsymbol{\alpha\beta}}(\boldsymbol{x})d\eta \quad . \tag{13.42}$$

and we assume that such particle can interact through an interaction which conserves the number of particles, i.e., the interaction represented by a two-leg vertex. The amplitude associated with this interaction can be generally a space-dependent function, more precisely a density, which we denote $-n\mathfrak{g}^{\frac{1}{2}}\,V$.

Thanks to the conservation of the number of particles through the interaction we can restrict ourself again to the one-particle theory. An elementary history of such one-particle interacting theory can be parametrized by its components between interactions, i.e.

$$\mathrm{h} = \big[[\tau_N,\boldsymbol{x}_N],\dots,[\tau_1,\boldsymbol{x}_1],[\tau_0,\boldsymbol{x}_0]\big] \quad \text{where} \quad \boldsymbol{x}_k(0)=\boldsymbol{x}_{k-1}(1) \quad \text{for} \quad k=1,\dots,N \quad , \tag{13.43}$$

or by joining these components to a single trajectory and specifying when the interactions occur

$$\mathrm{h} = \big[[\tau,\boldsymbol{x}]\,;\eta_N,\dots,\eta_1\big] \quad , \tag{13.44}$$

where

$$\begin{gathered} 1=\eta_{N+1}\geqslant\eta_N\geqslant\dots\geqslant\eta_1\geqslant\eta_0=0 \quad , \\ \tau_k=\tau\lambda_k \quad , \quad \lambda_k=\eta_{k+1}-\eta_k \quad \text{for} \quad k=0,\dots,N \quad , \\ [\tau,\boldsymbol{x}] = \bigodot_{k=1,\dots,N} [\tau_k,\boldsymbol{x}_k] \quad . \end{gathered} \tag{13.45}$$

τ and $\boldsymbol{x}$ are called an *inner time* and a *trajectory* of the elementary history of the one-particle interacting theory.

Now, let us compute the amplitude associated with a set of histories which includes all elementary histories with common inner time τ and trajectory $\boldsymbol{x}$ but with an arbitrary number of interaction.

It is given by

$$A(\tau,\boldsymbol{x}) = \sum_{N\in\mathbb{N}_0} \int\limits_{\substack{\eta_k\in\langle 0,1\rangle,\ k=1,\dots,N\\ 1\geqslant\eta_N\geqslant\cdots\geqslant\eta_1\geqslant 0}} \Big(\prod_{k=1,\dots,N} \Big(-\big(n\mathfrak{g}^{\frac{1}{2}}\,V\big)(\boldsymbol{x}(\eta_k))\ \frac{\nu\tau}{2} d\eta_{\,k}\Big)\Big) \times \\ \times \prod_{k=0,\dots,N} A_{\mathrm{free}}(\tau_k,\boldsymbol{x}_k) \quad . \tag{13.46}$$

Here we used the fact that the amplitude of an elementary history is given by the product of amplitudes of its free components and amplitudes of all interactions. And then we summed over all possible numbers of interactions and all times when interactions occurred. We chose the measure for summing over all possible times of interactions to be

$$\frac{\nu}{2} d\tau = \frac{\nu\tau}{2} d\eta \quad . \tag{13.47}$$

Next we substitute the free amplitude given by eq. (13.11) with the action I_{free}, use the additivity of the action $I_{\mathrm{free}}(\tau,\boldsymbol{x}) = \sum_{k=0,\dots,N} I_{\mathrm{free}}(\tau_k,\boldsymbol{x}_k)$ and the composition law (13.19) for the measure and relable times η_k in such way that we relax the condition $1 \geqslant \eta_N \geqslant \cdots \geqslant \eta_1 \geqslant 0$, and we get

$$\begin{aligned} A(\tau,\boldsymbol{x}) &= \\ &= \sum_{N\in\mathbb{N}_0} \frac{1}{N!} \int\limits_{\substack{\eta_k\in\langle 0,1\rangle\\ k=1,\dots,N}} \Big(\prod_{k=1,\dots,N} \big(-\frac{\nu\tau}{2}\big)\, V\big(\boldsymbol{x}(\eta_k)\big)\, d\eta_{\,k}\Big)\ \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}]\ \exp\big(-I_{\mathrm{free}}(\tau,\boldsymbol{x})\big) = \\ &= \Big(\sum_{N\in\mathbb{N}_0} \frac{1}{N!} \Big(-\int\limits_{\langle 0,1\rangle} \frac{\nu\tau}{2}\ V(\boldsymbol{x})\, d\eta\ \Big)^N\Big)\ \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}]\ \exp\big(-I_{\mathrm{free}}(\tau,\boldsymbol{x})\big) = \\ &= \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}]\ \exp\Big(-I_{\mathrm{free}}(\tau,\boldsymbol{x}) - \frac{\nu\tau}{2} \int\limits_{\langle 0,1\rangle} V(\boldsymbol{x})\, d\eta\Big) = \\ &= \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}]\ \exp\big(-I(\tau,\boldsymbol{x})\big) \quad , \end{aligned} \tag{13.48}$$

where I is given by eq. (13.6). This shows that the non-interacting theory with the action I is equivalent to the simple interacting theory with the free action I_{free} in the sense that the amplitude of an elementary history $[\tau,\boldsymbol{x}]$ of the former theory is the same as the amplitude of the set of histories of the latter theory composed of histories with common inner time τ and trajectory $\boldsymbol{x}$.

Feynman Green Function

There are other amplitudes we can be interested in beside the heat kernel $\frac{1}{n}K(\tau)$. Especially for the relativistic particle the inner time is physically undetectable and therefore any physical set of histories will include elementary histories with all possible inner times. Therefore we are interested in the amplitude $\frac{1}{n}G^F(x_{\mathrm{f}}|x_{\mathrm{i}})$ associated with the set of histories restricted only by the initial and final points $x_{\mathrm{f}}, x_{\mathrm{i}}$. This amplitude is called the *Feynman Green function*. We can obtain it from the propagator $\frac{1}{n}K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ by summing over all possible inner times τ using the measure (13.47)[16]

$$\frac{1}{n} G^F(x_{\mathrm{f}}|x_{\mathrm{i}}) = \int\limits_{\mathbb{R}+} \frac{1}{n} K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})\ \frac{\nu}{2} d\tau \quad . \tag{13.49}$$

Using eq. (13.13) we immediately get that the Feynman Green function is the inverse of the wave operator $\mathcal{F}$,

$$G^F(x|z) = \mathcal{F}^{-1}(x|z) \qquad \text{i.e.} \qquad \mathcal{F}\bullet G^F = \delta \quad . \tag{13.50}$$

Finally, let us note that we do not have an immediate generalization of the composition law for the Feynman Green function similar to (13.14).

Boundary conditions

In this chapter we completely ignored the question of boundary conditions using as excuse that we are working in a manifold without boundary. Certainly this is correct, if the manifold M is compact. But it is also correct in the case of a non-compact manifold with a sufficiently “nice” metric g at infinities. In such cases there exists a canonical choice of boundary conditions for differential operators used above, and these boundary conditions usually allow us to integrate by parts. Problem can arise for the relativistic particle when the manifold M is Lorentzian and operators as $\mathcal{L}$, $\mathcal{F}$ are hyperbolic. In this case the choice of boundary conditions at the temporal infinities plays an important physical role, and it is worth further investigation. First let us note that in a special situations (e.g. existence of a time-like Killing vector in the distant past and future) a canonical choice of boundary conditions still exists. But *canonical* here essentially means the most natural physical choice. In a general spacetime we do not have this special choice, and we have to address the question of the boundary conditions. To deal with this problem we will investigate our theory in a bounded domain Ω of the manifold M in the next chapter.

14 Particle in a curved space with boundary

General consideration

Now we want to generalize the theory described in the previous chapter to manifolds with boundaries. Our goal is a better understanding of the physical meaning of boundary conditions for the differential operators in the Schrödinger or Klein-Gordon equation. Therefore we restrict ourselves to a domain Ω in the manifold M which is bounded "in all physically interesting directions". This means that we will investigate the boundary conditions on boundaries which are not at infinity. But we allow the domain Ω be unbounded if we know that its infinity is "safe".

The main situation we have in the mind is the Lorentzian globally hyperbolic manifold with asymptotically flat spatial infinity. In this case we can ignore spatial infinity because it makes a sense to restrict ourselves to situations in which spacetime is "empty" sufficiently far in space directions. (Let us note that in non-asymptotically flat space the notion "empty" may not have a clear definition.) But because of the hyperbolic nature of the evolution equation we cannot ignore boundary conditions in the time directions. They represent "initial" and "final" conditions of the system. And we want to understand exactly this relationship.

Therefore in the case of a Lorentzian globally hyperbolic manifold, the typical choice of the domain will be a sandwich domain between two Cauchy surfaces. Such a domain is unbounded in spatial directions, but this "boundary in infinity" does not create important problems. Physically interesting boundary conditions are in the time directions which we restrict by boundary Cauchy surfaces.

Restriction to a domain — naive approach

Let us start with a straighforward restriction to a domain Ω in the target space M. We want to compute an amplitude $K_{\mathrm{o}}(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ which corresponds to a set of histories with inner time τ, endpoints x_{i}, x_{f} and which wholly belong to the domain Ω. We can repeat the derivation of the short time amplitude (13.30), at least for x_{f}, x_{i} sufficiently far from the boundary, because for small τ only trajectories near to the geodesic between x_{f} and x_{i} contribute to the amplitude.

If we compute the asymptotic expansion of the short time amplitude (13.30) in the domain with boundary, we find that there is a new term in the expansion. As can be seen in eq. (F.7), the smoothed short time amplitude leads to a Gauss integration in a variable Z from a tangent space at a point x, and in the case of a space without boundary the integration of odd powers of Z disappears. But in the case of a domain with a boundary for a point x near the boundary the Gauss integration is not always over the whole tangent space and therefore the integral of odd powers of Z does not disappear. As shown in appendix F (equation (F.26)), the correct asymptotic expansion of the leading term of the short time amplitude (equivalent of (13.33)) is given by[16]

$$
\begin{aligned}
&\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{x,z\in M} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z)\exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right)\varphi(x)\psi(z) = \\
&\qquad = \varphi\bullet\left(\mathcal{G} + \sqrt{\tau}\Big(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\Big)\mathcal{Q} - \tau\frac{\nu}{2}\overset{\leftrightsquigarrow}{\mathcal{L}} + \mathcal{O}(\tau^{\frac{3}{2}})\right)\bullet\psi \quad ,
\end{aligned}
\tag{14.1}
$$

where $\mathcal{Q}[\partial\Omega]$ is a delta bi-distribution localized on the boundary normalized to the boundary volume element $\mathfrak{q}^{\frac{1}{2}}$ understood as a distribution on spacetime,

$$\varphi \bullet \mathcal{Q} \bullet \psi = \int\limits_{\partial\Omega} \varphi\psi\, \mathfrak{q}^{\frac{1}{2}} \quad , \tag{14.2}$$

and $\overset{\leftrightsquigarrow}{\mathcal{L}}$ is a particular ordering of the Laplace operator given by

$$\overset{\leftrightsquigarrow}{\mathcal{L}} = \frac{1}{2}\left(\overleftarrow{\mathcal{L}} + \overrightarrow{\mathcal{L}}\right) \quad , \tag{14.3}$$

$$\varphi \bullet \overrightarrow{\mathcal{L}} \bullet \psi = -\int\limits_{\Omega} \varphi(\nabla^2\psi)\,\mathfrak{g}^{\frac{1}{2}} \quad . \tag{14.4}$$

Using this result it is easy to show that the expansion of the propagator K_{o} is

$$\mathcal{G} \bullet K_{\mathrm{o}}(\tau) \bullet \mathcal{G} = \mathcal{G} + \sqrt{\tau}\Big(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\Big)\mathcal{Q} \,-\, \tau\frac{\nu}{2}\overset{\leftrightsquigarrow}{\mathcal{F}} \,+\, \mathcal{O}(\tau^{\frac{3}{2}}) \tag{14.5}$$

and $\overset{\leftrightsquigarrow}{\mathcal{F}}$ is a Laplace-like quadratic form with potential,

$$\overset{\leftrightsquigarrow}{\mathcal{F}} = \frac{1}{2}(\overleftarrow{\mathcal{F}} + \overrightarrow{\mathcal{F}}) = \overset{\leftrightsquigarrow}{\mathcal{L}} + \mathcal{V} \quad , \tag{14.6}$$

$$\overleftarrow{\mathcal{F}}^{\top} = \overrightarrow{\mathcal{F}} = \overrightarrow{\mathcal{L}} + \mathcal{V} \quad . \tag{14.7}$$

The corrected potential $\mathcal{V}$ is given again by the expression (13.38) and we have assumed the condition (13.36) is satisfied.

We see that the expansion of the propagator has an additional term localized on the boundary $\partial\Omega$ proportional to $\sqrt{\tau}$. This τ-dependence causes a problem because $\dot{K}_{\mathrm{o}}(0)$ is singular on the boundary. An origin of the singular term on the boundary lies in our careless approximation of the propagator by the short time amplitude (13.30). This approximation is correct only for endpoints sufficiently far from the boundary. For points near the boundary we have to investigate the structure of the propagator more thoroughly.

Boundary correction term

The short time amplitude (13.30) represents the dominant contribution to the heat kernel from trajectories near the geodesic joining endpoints x_{f} and x_{i}. But in the case of a sum over trajectories restricted to the domain Ω there are other dominant terms given by contributions of trajectories near extremal paths which reflect on the boundary.

In general we should take into account trajectories with an arbitrary number of reflections on the boundary and compute the dominant contributions from all of them. However, for endpoints sufficiently far from the boundary the contributions from the reflected paths are negligible compared to the straight geodesic — for small τ only short paths contribute to the sum (therefore the leading term is non-trivial only for close endpoints), and any trajectory with a reflection on the boundary is too long (see figure 14.1)

But for endpoints near to the boundary the contributions from the reflected trajectories can be comparable with the leading term. For the endpoints near a smooth boundary there exists exactly one extreme trajectory $\bar{\boldsymbol{x}}_{\mathrm{b}}(x|z))$ with one reflection which gives a contribution comparable to the contribution from the straight geodesic $\bar{\boldsymbol{x}}(x|z))$ (see figure 14.1). Let us note that for boundary with "corners" we would have other non-trivial terms corresponding to trajectories with multiple reflections.

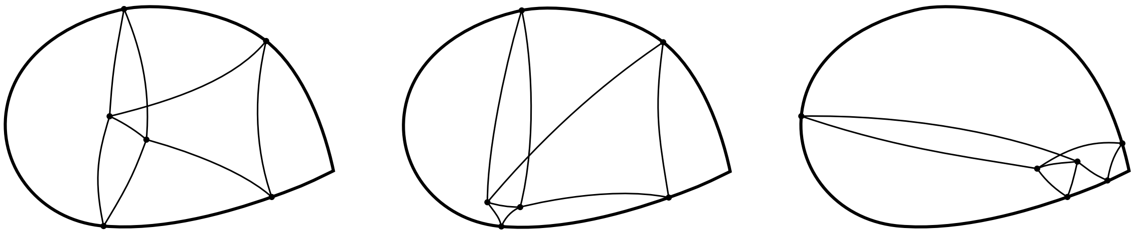


Figure 14.1: Example of extremal trajectories.

Dominant terms to sum over trajectories are given by trajectories near to extreme trajectories, possibly reflected from the boundary. If close endpoints are sufficiently far from the boundary, the reflected geodesics are longer then the straight geodesic. If the endpoints are near the boundary, there is a reflected geodesic with the length comparable to the length of straight one. Near the corner there is more reflected geodesics with comparable length.

Now we will write down conditions on the *reflected extreme trajectory* $\bar{\boldsymbol{x}}_{\mathrm{b}}(x|z))$. It is an extremum of the leading term of the action (13.22) with the additional condition that the trajectory reflects on the boundary. Let's denote the *point of the reflection* $b(x|z)$ and the *parameter for which the reflection occurs* $\lambda_{\mathrm{r}}(x|z)$ and its complement $\lambda_{\mathrm{l}}(x|z)$

$$\begin{aligned} b(x|z) = \bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)|_{\lambda_{\mathrm{r}}(x|z)} \in \partial\Omega \quad , \\ 1 = \lambda_{\mathrm{l}}(x|z) + \lambda_{\mathrm{r}}(x|z) \quad . \end{aligned} \tag{14.8}$$

The extremum condition implies that the trajectory is a joining of two geodesics

$$[\tau, \bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)] = [\lambda_{\mathrm{l}}(x|z)\tau, \bar{\boldsymbol{x}}(x|b(x|z))] \odot [\lambda_{\mathrm{r}}(x|z)\tau, \bar{\boldsymbol{x}}(b(x|z)|z)] \quad . \tag{14.9}$$

Using additivity of the action we get the value of its leading term

$$\sigma_{\mathrm{b}}(x|z) \overset{\mathrm{def}}{=} \nu I_{-1}(\bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)) = \frac{\sigma_{\mathrm{l}}(x|z)}{\lambda_{\mathrm{l}}(x|z)} + \frac{\sigma_{\mathrm{r}}(x|z)}{\lambda_{\mathrm{r}}(x|z)} \quad , \tag{14.10}$$

where, following the convention (G.77),

$$\sigma_{\mathrm{l}}(x|z) = \sigma(x|b(x|z)) \quad , \quad \sigma_{\mathrm{r}}(x|z) = \sigma(b(x|z)|z) \quad . \tag{14.11}$$

The extremum requirement gives us conditions on b and λ_{l}, λ_{l},

$$\frac{\mathrm{D}\sigma(x|b(x|z))}{\lambda_{\mathrm{l}}(x|z)} + \frac{\mathrm{D}\sigma(b(x|z)|z)}{\lambda_{\mathrm{r}}(x|z)} = 0 \quad , \tag{14.12}$$

$$\frac{\sigma_{\mathrm{l}}}{\lambda_{\mathrm{l}}^2} = \frac{\sigma_{\mathrm{r}}}{\lambda_{\mathrm{r}}^2} \quad , \tag{14.13}$$

where D denotes the orthogonal projection of the gradient on the boundary

$$\mathrm{D}_{\boldsymbol{\alpha}} f = \mathfrak{d}^{\boldsymbol{\beta}}_{\boldsymbol{\alpha}} \, \mathrm{d}_{\boldsymbol{\beta}} f \quad , \quad \mathfrak{d}^{\boldsymbol{\beta}}_{\boldsymbol{\alpha}} = \delta^{\boldsymbol{\beta}}_{\boldsymbol{\alpha}} - \vec{n}^{\boldsymbol{\beta}} n_{\boldsymbol{\alpha}} \quad . \tag{14.14}$$

See appendix G for more details and other quantities defined on the boundary.

Now we can estimate the contribution from the trajectories near to the reflected geodesic $\bar{\boldsymbol{x}}_{\mathrm{b}}(x|z))$. Using reasoning similar to that used for deriving (13.30), we can write an approximation of the short time amplitude associated with the reflected geodesic as

$$K_{\mathrm{b}}(\tau, x_{\mathrm{f}}|x_{\mathrm{i}}) \;=\; \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \Delta_{\mathrm{b}}^{1-p}(x_{\mathrm{f}}|x_{\mathrm{i}})\, \beta(\tau, x_{\mathrm{f}}|x_{\mathrm{i}}) \exp\Big(-\frac{1}{\nu\tau}\sigma_{\mathrm{b}}(x_{\mathrm{f}}|x_{\mathrm{i}})\Big) \quad , \tag{14.15}$$

where $\Delta_{\rm b}$ is Van Vleck-Morette determinant associated with the reflected geodesic (see (G.89)). The coefficient β is an analog of the coefficients α_0, α_1, only in this case we have to expect an expansion in powers of $\sqrt{\tau}$:

$$\beta(\tau, x|z) = \beta_0(x|z) + \sqrt{\tau}\beta_{\frac{1}{2}}(x|z) + \mathcal{O}(\tau) \quad . \tag{14.16}$$

As we will see, the right normalization relative to the leading term $K_{\rm o}$ requires

$$\beta_0(x|x) = 1 \quad . \tag{14.17}$$

We did not bother to write down a potential term, because terms of order $\mathcal{O}(\tau)$ are negligible in the approximation we need, as can be seen in the calculation in appendix F. We also already anticipated an arbitrary power of the Van Vleck-Morette determinant, similarly to the choice (13.39).

Fixing this short time amplitude (i.e. specification of coefficients p and β, or more precisely its coincidence limits as we will see below) together with amplitude (13.30) concludes the definition of the path integral in the domain with a smooth boundary.

Short time behavior of the heat kernel

Next we proceed to derive the short time behavior of the propagator. Again, the technical work is done in appendix F, where it is shown that for small τ we have the expansion (see eq. (F.46))

$$\begin{aligned} &\varphi \bullet \mathcal{G} \bullet K_{\rm b}(\tau) \bullet \mathcal{G} \bullet \psi = \\ &\quad = \sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\,\varphi \bullet \mathcal{Q} \bullet \psi - \\ &\quad - \tau\frac{\nu}{2}\frac{1}{2}\varphi \bullet (d\overleftrightarrow{\mathcal{F}}_d + d\overleftrightarrow{\mathcal{F}}_d) \bullet \psi - \\ &\quad - \tau\frac{\nu}{2}\,\varphi \bullet \Big(\frac{1+p}{3}k + \beta\text{-terms}\Big)\mathcal{Q} \bullet \psi + \mathcal{O}(\tau^{\frac{3}{2}}) \quad . \end{aligned} \tag{14.18}$$

The β-terms contains coincidence limits of the first two derivatives of the coefficient β on the boundary, and the exact form can be found in (F.56). k is the trace of the external curvature (see equation (G.50)). Here we already have used the normalization (14.17), otherwise the first term would contain a coincidence limit $[\beta_0]$ on the boundary. Our normalization ensure that the $\sqrt{\tau}$ term in $K_{\rm b}$ cancels exactly with such a term in $K_{\rm o}$.

So, if we add both dominant terms we get

$$K_k(\tau) = K_{\rm o}(\tau) + K_{\rm b}(\tau) \quad , \tag{14.19}$$

$$\mathcal{G} \bullet K_k(\tau) \bullet \mathcal{G} = \mathcal{G} - \tau\frac{\nu}{2}\mathcal{F}_{\sim k} + \mathcal{O}(\tau^{\frac{3}{2}}) \quad , \tag{14.20}$$

where $\mathcal{F}_{\sim k}$ is the quadratic form of Laplace-like operator with the boundary conditions given by the choice of β coefficients

$$\mathcal{F}_{\sim k} = \mathcal{F}_d - \Theta_k \tag{14.21}$$

with $\mathcal{F}_d$ corresponding to the Dirichlet boundary condition (defined in (2.3)) with a potential term in the form (13.38), and

$$\Theta_k \overset{\rm def}{=} \underset{\sim}{\varphi} \cdot {}^{\eta}\theta_k \cdot \underset{\sim}{\varphi} \overset{\rm def}{=} -\Big(\frac{1+p}{3}k + \beta\text{-terms}\Big)\mathcal{Q} \quad . \tag{14.22}$$

$\mathcal{F}_{\sim k}$ identifies what kind of boundary conditions the propagator K_k satisfies. If we compare $\mathcal{F}_{\sim k}$ with the operator $\overrightarrow{\mathcal{F}}$, equation (3.61) gives us

$$d\overrightarrow{\mathcal{F}}_{\sim k} = d\overrightarrow{\mathcal{F}}_d - \Theta_k = \underset{\sim}{\varphi} \cdot (\underline{\pi} - {}^{\eta}\theta_k \cdot \underset{\sim}{\varphi}) \quad . \tag{14.23}$$

We see that $\sim k$-boundary conditions have the same generalized value as the Dirichlet boundary conditions but different generalized momentum,

$$\underline{\varphi}_{\sim k} = \underline{\varphi} \quad , \quad \underline{\pi}_{\sim k} = \underline{\pi} - {}^{r}\theta_k \cdot \underline{\varphi} \quad . \tag{14.24}$$

I.e., these boundary conditions have the structure $k = \kappa D$. Equation (3.57) and the normalization condition (3.15) give similar expressions for $\underline{\varphi}_k$ and $\underline{\pi}_k$:

$$\begin{gathered} \underline{\varphi}_k = \gamma^{-1}_{\sim k} \cdot (\underline{\pi} - {}^{r}\theta_k \cdot \underline{\varphi}) \quad , \quad \underline{\pi}_k = -\gamma_{\sim k} \cdot \underline{\varphi} \quad , \\ \gamma_{\sim k} = \gamma - {}^{r}\theta_k \quad , \end{gathered} \tag{14.25}$$

$$\overset{\rightsquigarrow}{d\mathcal{F}}_k = \overset{\rightsquigarrow}{d\mathcal{F}}_n + \Theta_k \quad . \tag{14.26}$$

The short time behavior (14.20) together with the composition law again prove the heat equation for the propagator:

$$-\mathcal{G} \bullet \dot{K}_k(\tau) = \frac{\nu}{2} \mathcal{F}_{\sim k} \bullet K_k(\tau) \tag{14.27}$$

The solution of the heat equation is smooth for non-zero time τ. To see clearly what kind of boundary conditions it satisfies, we write the heat equation in the following way

$$-\mathcal{G} \bullet \dot{K}_k(\tau) = \frac{\nu}{2} \overset{\rightsquigarrow}{\mathcal{F}} \bullet K_k(\tau) + \frac{\nu}{2} \overset{\rightsquigarrow}{d\mathcal{F}}_{\sim k} \bullet K_k(\tau) \quad . \tag{14.28}$$

The left-hand side is smooth, as well as the first term on the right-hand side. The second term is localized on the boundary and therefore it has to vanish. So we find

$$\overset{\rightsquigarrow}{d\mathcal{F}}_{\sim k} \bullet K_k(\tau) = -\overset{\leftrightsquigarrow}{d\mathcal{F}}_k \bullet K_k = 0 \qquad \text{i.e.} \qquad \underline{\varphi}_k \bullet K_k(\tau) = 0 \tag{14.29}$$

or, in terms of value and momentum on the boundary,

$$(\underline{\pi} - {}^{r}\theta_k \cdot \underline{\varphi}) \bullet K_k(\tau) = 0 \quad . \tag{14.30}$$

Let us summarize. We have found that the propagator given by the sum of amplitudes over histories in the domain Ω with fixed endpoints and inner time τ is a solution of the heat equation with specific boundary conditions. The boundary conditions depend on the definition of the path integral through the coincidence limits of derivatives of coefficients β in the short time amplitude (14.15). In general, they are Robin-like conditions with a non-degenerate coefficient in front of momentum.

Green function

In the case of a relativistic particle the inner time is an unphysical quantity, and all physically distinguishable sets of histories should contain histories with all possible inner times. Therefore we will compute the amplitude associated with the set of histories with fixed endpoints but without a restriction on the inner time. As before, we will call this amplitude the Feynman Green function[16]

$$\frac{1}{n} G_{\sim k}(x|z) = \int\limits_{\tau \in \mathbb{R}^+} \frac{1}{n} K_k(\tau, x|z) \frac{\nu}{2} d\tau \quad . \tag{14.31}$$

The name is consistent with the usage in chapter 3 in the spirit of equation (3.71). Using the heat equation and initial conditions for the heat kernel, the integration gives

$$\mathcal{F}_{\sim k} \bullet G_{\sim k} = \delta \quad , \tag{14.32}$$

and thanks to the boundary conditions for K_k we have

$$D_k \bullet G_{\sim k} \bullet J = 0 \quad \text{for} \quad J \in \tilde{\boldsymbol{\mathcal{P}}} \quad . \tag{14.33}$$

So, $G_{\sim k}$ is the inverse of $\mathcal{F}_{\sim k}$ and restricted to smooth sources it satisfies the same boundary conditions as the propagator K_k — it is an extension of the Feynman Green function.

Amplitude of particles emitted by a source

Let us compute the amplitude $Z_k^{(1)}(J)$ of a set of histories which end at a given point x and are emitted by a source described by a spacetime dependent amplitude[17] nJ. We will call it the one-particle amplitude. It is clearly given by

$$Z_k^{(1)}(J) = G_{\sim k} \bullet J = \bar{\phi}_k(J) \quad . \tag{14.34}$$

It satisfies the same boundary conditions as the Feynman Green function.

We will interpret these boundary conditions as a consequence of the fact that we have not allowed particles to start on the boundary. More precisely, we have allowed the smooth source to be non-zero up to the boundary, but we have not allowed an emission of particles from the boundary comparable to an emission from a finite volume.

We can ask why some particular boundary conditions means that no particles are emitted from the boundary. What about different boundary conditions? Why is the choice of the conditions above special? We are touching a question of what kind of particles we are dealing with. What does it mean that no particles are emitted (or absorbed — for scalar particle the meanings are interchangeable, if we do not distinguish initial and final parts of the boundary).

First we have to realize that the statement "no particles on the boundary" has to be interpreted as a result of a measurement on the boundary. We have to arrange apparatuses on the whole boundary which are sensitive to particles, and when all these devices measure no particle we can speak about no emission or absorption. Clearly this is very complicated global measurement. It depends on an exact arrangement of experimental devices on the whole boundary and on an interaction of particles with devices. We have hidden this dependence in the definition of the path integral through the non-specified β-terms. Therefore we see that we cannot expect a unique canonical meaning for the statement "no particles on the boundary". Only if we specify the kind of measurement we are performing do we have a meaning for this statement. And information about experimental devices can be phenomenologically characterized by the choice of boundary conditions of the type we encountered above.

Emission from the boundary

Of course, we can ask what the amplitude is to find a particle at a point x if we allow an emission from the boundary. Let us assume that the amplitude of the emission from the boundary is given by a density $nj \in \tilde{\boldsymbol{\mathcal{V}}}[\partial\Omega]$ on the boundary manifold, which we call the *boundary source*. The amplitude $Z_k^{(1)}(\tau; j)$ associated with the set of one-particle histories which are emitted by this boundary source and end in time τ at a point x, can be written using the *boundary propagator* $K_k^{\dashv}$

$$Z_k^{(1)}(\tau; j) = K_k^{\dashv}(\tau) \cdot j \quad . \tag{14.35}$$

The boundary propagator propagates between points inside of the domain and boundary sources. It has the character of a function on the domain Ω in the left argument and the function on the boundary manifold $\partial\Omega$ in the right argument.

Clearly, the boundary propagator satisfies a composition law similar to (13.14)

$$K_k^{\dashv}(\tau) = K_k(\tau - \epsilon) \bullet \mathcal{G} \bullet K_k^{\dashv}(\epsilon) \quad . \tag{14.36}$$

We can take a limit $\epsilon \to 0$ and get

$$K_k^{\dashv}(\tau) = K_k(\tau) \bullet \overleftarrow{\widetilde{K}}_k \quad , \tag{14.37}$$

$$\overleftarrow{\widetilde{K}}_k \stackrel{\text{def}}{=} \mathcal{G} \bullet K_k^{\dashv}(0) \quad . \tag{14.38}$$

We see that the amplitude is given by the propagator $K_k(\tau)$ with no emission from the boundary, and by the boundary term $\overleftrightarrow{K}_k$ which "translates" between the space of sources on the boundary and amplitudes in the domain. Similarly, if we sum over all possible inner times we get

$$Z_k^{(1)}(j) = G_{\sim k} \bullet \overleftrightarrow{K}_k \cdot j \quad . \tag{14.39}$$

The boundary term $\overleftrightarrow{K}_k$ is a zero-time amplitude, so it is straightforward to estimate it. The short time amplitude approximation similar to (13.30) for the boundary propagator is

$$\begin{aligned}
&\phi \bullet \mathcal{G} \bullet K_k^{\dashv}(\tau) \cdot j = \\
&\quad = \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{\substack{x\in\Omega \\ \hat{y}\in\partial\Omega}} \mathfrak{g}^{\frac{1}{2}}(x)\phi(x)j(\hat{y})\,\Delta(x|\hat{y})\ \exp\Bigl(-\frac{1}{\nu\tau}\sigma(x|\hat{y})\Bigr)\bigl(1+\mathcal{O}(\sqrt{\tau})\bigr) = \\
&\quad \int\limits_{\hat{y}\in\partial\Omega} \phi(\hat{y})j(\hat{y})\ \bigl(1+\mathcal{O}(\sqrt{\tau})\bigr) = \\
&\quad \phi \bullet \underline{\varphi} \cdot j\ \bigl(1+\mathcal{O}(\sqrt{\tau})\bigr) \quad .
\end{aligned} \tag{14.40}$$

Therefore, for zero inner time we get

$$\overleftrightarrow{K}_k = \underline{\varphi} \quad . \tag{14.41}$$

We have found that the emission from the boundary is equivalent to the emission of particles inside of the domain but with a distributional source with support on the boundary

$$\partial J = j \cdot \underline{\varphi} \in \partial\tilde{\boldsymbol{\mathcal{J}}}_{\sim k} \subset \tilde{\boldsymbol{\mathcal{J}}}_{\sim k} \quad . \tag{14.42}$$

It is consistent with the fact that K_k is exponential and $G_{\sim k}$ is the inverse of $\mathcal{F}_{\sim k}$ in the space $\tilde{\boldsymbol{\mathcal{J}}}_{\sim k}$, so they can be coupled to such a source. We will use both representations of boundary sources ∂J or j as will be convenient.

Thanks to the property (3.66) of the Green function, we find

$$Z_k^{(1)}(j) = G_{\sim k} \bullet \underline{\varphi} \cdot j = \underline{D} \cdot \gamma_k^{-1} \cdot j \quad , \tag{14.43}$$

or

$$Z_k^{(1)}(\partial J) = G_{\sim k} \bullet \partial J = \bar{G}_{\sim k} \bullet \partial J = \bar{\phi}_k(\partial J) \qquad \text{for} \qquad \partial J \in \partial\tilde{\boldsymbol{\mathcal{J}}}_{\sim k} \quad . \tag{14.44}$$

I.e. the one-particle amplitude with sources only on the boundary is a solution of the free field equation.

Allowing both boundary sources and sources inside of the domain, we find that the one-particle amplitude is

$$Z_k^{(1)}(J, \partial J) = G_{\sim k} \bullet (J + \partial J) = \bar{\phi}_k(J + \partial J) \quad . \tag{14.45}$$

It satisfies the full equation of motion in the form

$$\mathcal{F}_{\sim k} \bullet \bar{\phi}_k(J + \partial J) = J + \partial J \quad . \tag{14.46}$$

We can represent boundary sources also in a different way — we can use the one-particle amplitude near to the boundary to identify the boundary source. Substituting the decomposition of the operator $\mathcal{F}_{\sim k} = \overrightarrow{\overleftarrow{\mathcal{F}}} - \overleftrightarrow{d\mathcal{F}}_k$ into the field equation gives

$$\partial J = -\overleftrightarrow{d\mathcal{F}}_k \bullet \bar{\phi}_k(J + \partial J) \quad . \tag{14.47}$$

Therefore the restriction of the one-particle amplitude to the boundary phase space determines the boundary source. Actually, only the projection to the subspace $\boldsymbol{\mathcal{B}}_k$ is important for determination of the boundary sources. It is consistent with what we said before — the part of the amplitude with zero k-value originates from sources with no emission on the boundary. If we use the restriction of the one-particle amplitude to the boundary phase space for the representation of the boundary sources, we get

$$Z_k^{(1)}(J, \partial\phi) = G_k^F \bullet \big(J - \overleftrightarrow{d}\mathcal{F}_k \bullet \partial\phi\big) = \bar{\phi}_k(J, \partial\phi) \tag{14.48}$$

with $\bar{\phi}_k$ introduced in eq. (9.23).

15 Many-particle theory and transition amplitudes

Multi-particle histories

Now we turn to the many-particle theory. We will investigate amplitudes of sets of multi-particle histories, i.e. histories which are composed from elementary one-particle histories, perhaps interacting. First we realize what consequences the rules (12.1) and (12.2) have for computations of amplitudes in this case.

As we discussed in chapter 13, multi-particle histories can be represented by elementary one-particle histories with endpoints possibly joined in interaction vertices. I.e. we can associate with each multi-particle history a graph with vertices given by free endpoints and interactions, and lines given by one-particle trajectories. We say that two histories have the same structure if they are associated with the same graph. We can also speak about connected components of multi-particle histories — subhistories with connected graphs.

Let's assume that we have a set of multi-particle histories. We can divide it into disjunct subsets, each of them which is composed of histories with the same structure. Rule (12.1) tells us that the amplitude of the whole set is given by the sum of amplitudes of these subsets.

If the set of histories with the same structure is characterized only by fixing endpoints and specifying interactions, we can always sum over all possible one-particle components with fixed endpoints — which gives the propagator computed in the previous chapter — and after that multiply these one-particle amplitudes by the amplitudes of interactions and sum over all possible connection points of the interaction and the one-particle histories. This mean that the amplitude of the set of histories of this type is given by product of amplitudes (propagators) corresponding to the lines of the associated graph, and amplitudes of interactions corresponding to vertices, summed over all possible connections of these lines and vertices at the end.

But this structure is in exact correspondence with the diagrammatic notation (see appendix I) for the algebra of multi-argument functions and distributions which we use for writing down transition amplitudes. Therefore it will be very useful to use this notation. Diagrams for the amplitudes which we will use, will have two meanings. They first suggest an amplitude of which set of histories we compute — the set of histories restricted only by the requirement that they are associated with a given graph. But they also represent the exact expression for the amplitude in the sense of the diagrammatic notation.

Before we define and compute some concrete multi-particle amplitudes, we make one more general comment. Let us again assume that we have a set of histories H composed of all possible histories with the same structure. I.e., all have the same graph. Such a set of histories can be represented as the Cartesian product $\mathrm{H} = \mathrm{H}_1 \times \mathrm{H}_2 \times \dots$ where each of set of subhistories H_1, H_2, $\dots$, contains all subhistories with the same connected graph and product is over all connected components of the graph of the whole set H. Thanks to rule (12.2), the amplitude of each history is given by the product of amplitudes of its connected components, and therefore the amplitude of the set H also factorizes to the product

$$A(\mathrm{H}) = \prod_k A(\mathrm{H}_k) \quad . \tag{15.1}$$

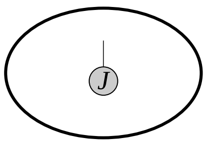
Diagrammatic dictionary

As we said, it will be easier to remember the meaning of the amplitudes if we use a diagrammatic notation for them. See appendix I for some details on diagrammatic notation in general. We can use this notation because the multi-argument functions (and distributions) on the spacatime domain can be understood as tensors from spaces $\boldsymbol{\mathcal{P}}^l_k$. Tensor indices are essentially arguments of these functions, and contraction is the integration over the domain (or application of distributions on test functions). The diagrammatic notation can be viewed as only a convenient representation of such tensors. But it remains slightly a mystery that this representation is intuitively so close to the interpretation of the theory.

So we represent amplitudes using diagrams. We enclose each diagram in a bounded area to suggest the fact that we are working in a domain with boundary. Because we will not distinguish initial and final boundaries, we use only one boundary in our diagrams, in contrast to chapters 8 and 9. The boundary of the diagrams will serve to emphasize that we work also with tensors which have a distributional character with "the support of the tensor indices localized on the boundary". Usually, legs of diagrams representing such tensor indices will originate from the boundary of the diagram, as e.g. in the case of boundary sources (15.3) below.

As before, we represents the smooth source J by the diagram

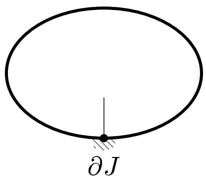
$$nJ \quad \leftrightarrow$$



, (15.2)

and boundary sources ∂J by

$$n\partial J \quad \leftrightarrow$$

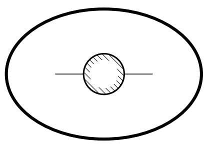


, (15.3)

where hatching labels the boundary phase space to which ∂J belongs. If it cannot lead to confusion, we use also elements of the boundary phase space for labeling of boundary sources as discussed at the end of the previous chapter. But we have to be careful with this convention if we deal with different boundary conditions, because in this case the same element of boundary phase space can represent different boundary sources.

The propagator between two points computed in the last chapter will be represent as

$$\frac{1}{n} G_{\sim k} \quad \leftrightarrow$$

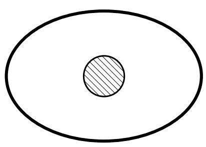


, (15.4)

where again, hatching labels boundary conditions.

Next we introduce the simplest amplitude — the *vacuum amplitude*

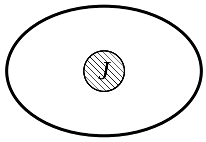
$$A^{(0)}_k \quad \leftrightarrow$$



. (15.5)

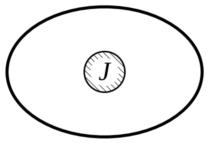
It is the amplitude that no particle is emitted or absorbed from any source inside or on the boundary of the domain. It corresponds to multi-particle histories without endpoints. We do not compute this amplitude in sum-over-histories formalism — it would need an additional discussion of the path integral over closed paths (but see [23] for some details). The vacuum amplitude is usually a prefactor of other amplitudes, and we can factor it out. We call amplitudes not including this global prefactor *relative amplitudes*. But let us note that the vacuum amplitude has a physical meaning. As we will see in the last chapter, it corresponds to the vacuum–vacuum amplitude of canonical quantized scalar field theory.

If sources nJ inside of the domain are present, we denote the amplitude that no particle is detected anywhere as

$A_k^{(0)}(J) \quad \leftrightarrow$ 

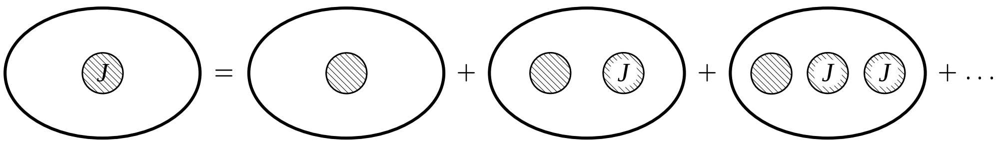
. (15.6)

More precisely this amplitude is associated with the set of multiple-particle histories which are composed of arbitrary number of one-particle histories emitted and absorbed by the source nJ. The corresponding graphs have the structure of all possible combinations of connected pieces which contains the source, and vacuum amplitude. I.e., if we denote the *relative connected vacuum amplitude* as

$Z_k^{(0)}(J) \quad \leftrightarrow$ 

, (15.7)

we have

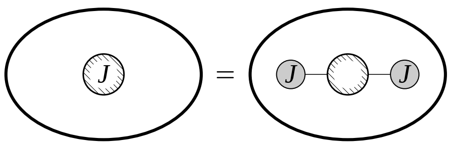


. (15.8)

In other words

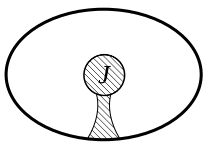
$$A_k^{(0)}(J) = A_k^{(0)} \exp\left(Z_k^{(0)}\right) \quad . \tag{15.9}$$

Clearly, the only connected component which contains sources is



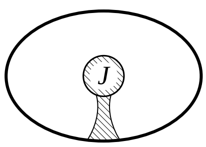
. (15.10)

Similarly we define the vacuum amplitude in the presence of boundary sources

$A_k^{(0)}(J, \partial J) \quad \leftrightarrow$ 

, (15.11)

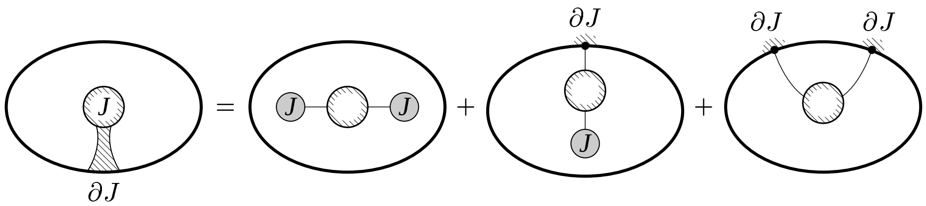
∂J

$Z_k^{(0)}(J, \partial J) \quad \leftrightarrow$ 

. (15.12)

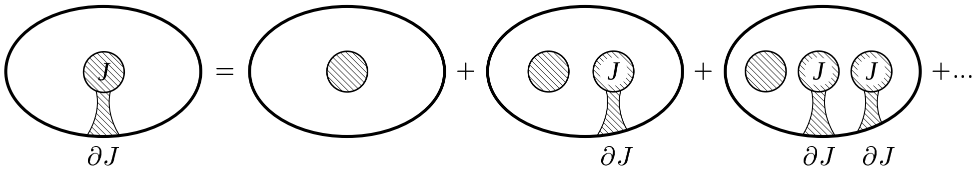
∂J

The connected relative amplitudes are



, (15.13)

and again



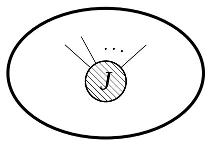
. (15.14)

This means

$$A_k^{(0)}(J,\partial J) = A_k^{(0)}\ \exp\Big(n\frac{1}{2}(J+\partial J)\bullet G_k^F\bullet(J+\partial J)\Big) \quad . \tag{15.15}$$

Next we define amplitudes associated with the set of histories with given endpoints. I.e. the corresponding set of histories contains multi-particle histories with given endpoints which can be emitted from the source J. In general, for m endpoints we have amplitude $A_k^{(m)\boldsymbol{x}_1\ldots\boldsymbol{x}_m}(J)$ which are represented by graphs with m free legs

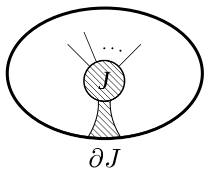
$A_k^{(m)}(J) \quad \leftrightarrow$



. (15.16)

Similarly, if the boundary sources are present

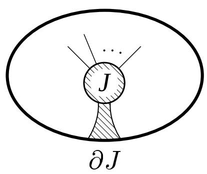
$A_k^{(m)}(J,\partial J) \quad \leftrightarrow$



. (15.17)

Relative connected amplitudes correspond to connected histories which contain a source or an end-point. The notation is obvious, e.g.

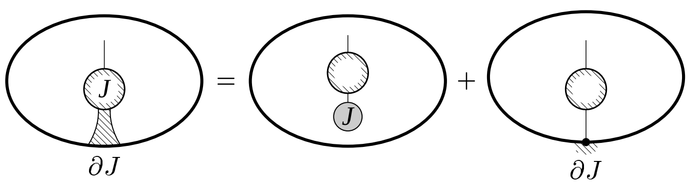
$Z_k^{(m)}(J,\partial J) \quad \leftrightarrow$



. (15.18)

We have already encountered two examples of such amplitudes — the one-particle amplitude

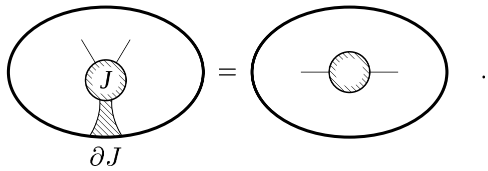
$Z_k^{(1)}(J,\partial J) \quad \leftrightarrow$



, (15.19)

and the propagator

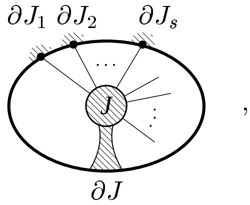
$$Z_k^{(2)}(J, \partial J) \quad \leftrightarrow$$



(15.20)

Finally, we define amplitudes associated with the set of histories for which a fixed number of particles is additionally emitted from the boundary sources with prescribed source amplitudes,

$$A_k^{(m)}[\partial J_1, \partial J_2, \ldots, \partial J_s](J, \partial J) \quad \leftrightarrow$$



(15.21)

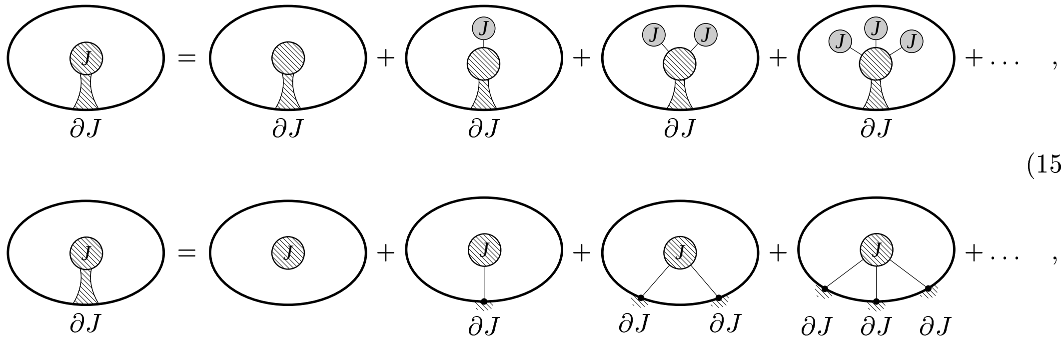
and similarly for the relative connected amplitude.

All these amplitudes can be derived from the basic vacuum amplitude (15.15) by variation with respect of sources nJ and $n\partial J$. Specifically

$$A_k^{(m)}(J, j) = \frac{1}{n^m} \underbrace{\mathrm{d} \ldots \mathrm{d}}_{m} A_k^{(0)}(J, j) \quad , \tag{15.22}$$

$$A_k^{(m)}[j_1, j_2, \ldots](J, j) = j_1 \cdot \mathrm{d}_\partial \, j_2 \cdot \mathrm{d}_\partial \ldots A_k^{(m)}(J, j) \quad , \tag{15.23}$$

where d is the variation with respect to J and d_∂ with respect to j. Therefore we will call the vacuum amplitude the *generating functional*. The proof follows from the structure of amplitudes — they are associated with set of histories composed of all possible connections of the given sources and endpoints. But endpoints can be created by "tearing out" the source J. As discussed in appendix I, this operation is essentially the variation with respect to J. Similarly for boundary sources. The fact that $A_k^{(0)}(J, \partial J)$ is the generating functional of other amplitudes can be also represented by the identities



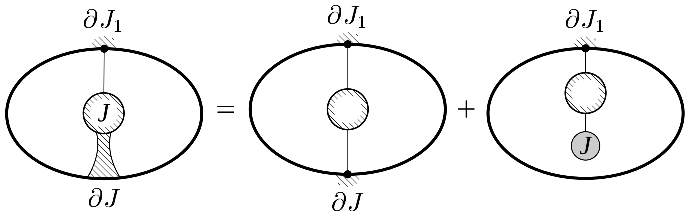
(15.24)

Summarizing, we have introduced a number of physically interesting amplitudes which are derivable from the vacuum amplitude (15.15), also called the generating functional. Similarly, we have a generating functional for connected relative amplitudes

$$Z_k^{(0)}(J, \partial j) = n\frac{1}{2}(J + \partial J) \bullet G_k^F \bullet (J + \partial J) \quad . \tag{15.25}$$

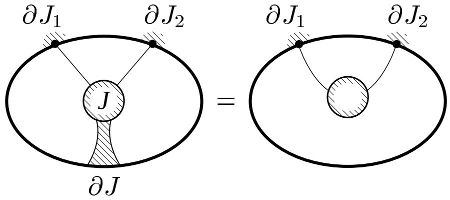
By varying this functional we get elementary connected amplitudes. As expected for the non-interacting theory, there are only a few of them. Additionally to $Z_k^{(0)}(J,\partial J)$ (eq. (15.13)), $Z_k^{(1)}(J,\partial J)$ (eq. (15.19)), and $Z_k^{(2)}(J,\partial J)$ (eq. (15.20)), we have

$Z_k^{(0)}[\partial J_1](J,\partial J) \quad \leftrightarrow$



, (15.26)

$Z_k^{(0)}[\partial J_1,\partial J_2](J,\partial J) \quad \leftrightarrow$



. (15.27)

Interaction with the boundary

Now we return to investigate the meaning of boundary conditions on the propagator. We have derived that the propagator is given by the Green function $G_{\sim k}$ and boundary sources live in the space $\partial\tilde{\mathcal{J}}_{\sim k}$ with k-boundary conditions given by (14.25). We said that the choice of these boundary conditions is given by the particular choice of measurement devices on the boundary. But we admitted that we could have different experimental apparatuses on the boundary, and they can lead to different boundary conditions. Now we demonstrate this on the phenomenological level.

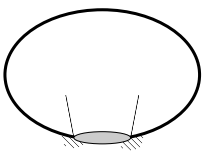
For simplicity of notation let's assume we have made such a choice of experimental setup which leads to Neumann boundary conditions[18], i.e. $\Theta_n = 0$ in (14.21). Now we would like to investigate some another experimental setup from this point of view. I.e. let us have some different set of measurement devices which can be used for the definition of no emission from the boundary, one-particle emission, etc.. But a different measurement of particles means a different interaction of particles with apparatuses on the boundary. Therefore we have to expect that the new devices on the boundary emit and absorb particles in our original sense, even if they themselves do not measure any particles. Let us use this fact for the phenomenological description of the new experimental devices — we characterize them by their interaction with our particles. We will investigate some of the simplest examples of such interactions.

We have already discussed sources on the boundary — they correspond to emission by our original devices from the boundary. To describe different devices we need to go behind the sources. The next simplest choice is an interaction which can emit or absorb particles on the boundary in pairs. I.e. let us study the situation when we have additionally to sources nJ and $n\partial J$ also the possibility of pair emission on the boundary described by an interaction vertex $n\Theta_k$. In general, it is a symmetric two-point distribution with arguments which have the character of boundary sources

$$\Theta_k = \underset{\sim}{\varphi} \cdot {}^r\theta_k \cdot \underset{\sim}{\varphi} \quad . \tag{15.28}$$

If we allow some more complicated global measurements, it can even be non-local. We use the following diagram for this interaction vertex

$n\Theta_k \quad \leftrightarrow$

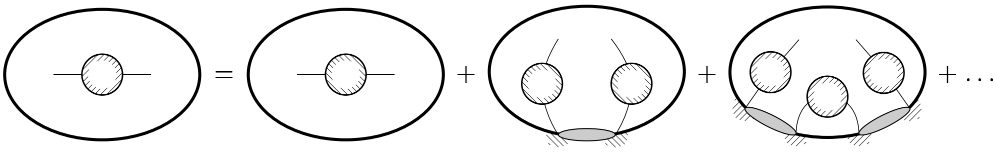


. (15.29)

Now we want to know what description an observer who does not see this interaction has to use, an observer who is using different experimental devices (which cause this interaction from our point of view) for the definition of his notion of particles. We are looking for a description in which he has only a free propagator (maybe different from ours) and sources as basic elements, which produce the same amplitudes for the set of histories as our description (which includes additional interactions). Of course, it is not clear that such a description exists.

But it does. We can give a prescription for the new propagator and show that the amplitudes defined in the previous section computed using this new propagator are equivalent to the amplitudes computed using our original propagator, including the additional interaction. I.e., a different measurement of particles with no additional interaction is equivalent to our measurement of particles with a possible interaction caused by another measurement process.

The new propagator must clearly contain the cumulative effect of an arbitrary number of interactions with the boundary, i.e.



. (15.30)

This means

$$G_{\sim k} = G_{\sim n} + G_{\sim n} \bullet \Theta_k \bullet G_{\sim n} + G_{\sim n} \bullet \Theta_k \bullet G_{\sim n} \bullet \Theta_k \bullet G_{\sim n} + \cdots = \\ = (G_{\sim n}^{-1} - \Theta_k)^{-1} = \mathcal{F}_{\sim k}^{-1} \quad , \tag{15.31}$$

where

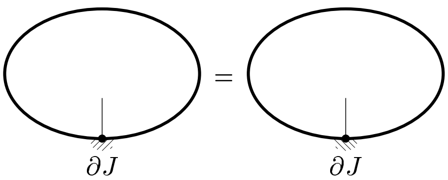
$$\mathcal{F}_{\sim k} = \mathcal{F}_{\sim n} - \Theta_k \quad . \tag{15.32}$$

So, the new propagator is again a Green function, but with different boundary conditions. Moreover, thanks to (15.28), we have boundary conditions exactly of the kind obtained from the path integral in the previous chapter (at least for local ${}^{r}\theta_k$).

The change of the propagator does not affect the source space — both the original and new boundary conditions have the same space of boundary sources,

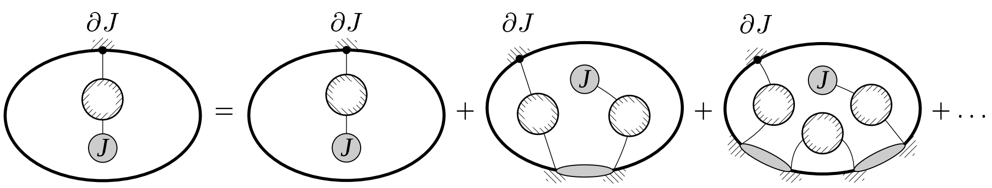
$$\partial\tilde{\mathcal{J}}_{\sim k} = \partial\tilde{\mathcal{J}}_{\sim n} = \partial\tilde{\mathcal{J}}_{D} \quad . \tag{15.33}$$

In diagrammatic notation this means



. (15.34)

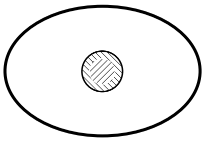
It is straightforward to see that in the description with the new propagator without an interaction is equivalent to the description with the old propagator and the interaction. For example we have



. (15.35)

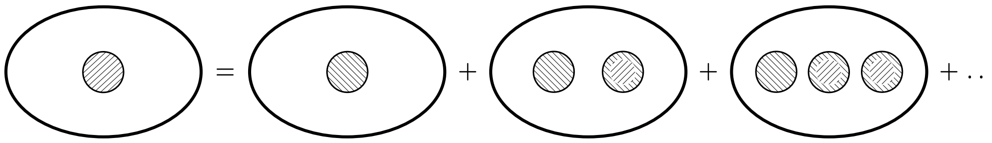
More non-trivial is the relation between vacuum amplitudes. If we define the relative connected amplitude $Z^{(0)}_{kn}$ as

$$Z^{(0)}_{kn} = \ln \frac{A^{(0)}_k}{A^{(0)}_n} \quad \leftrightarrow$$

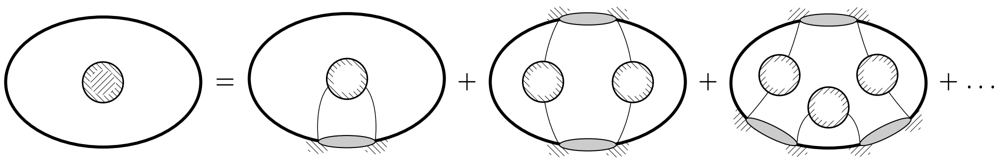


,

(15.36)

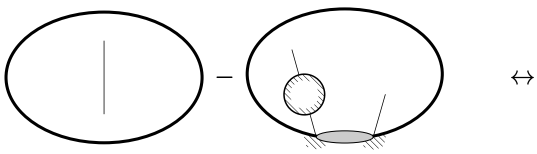


we have



. (15.37)

Comparing with (I.9) we see that the right hand side is minus half of the trace of the logarithm of the operator



(15.38)

$$\begin{aligned}\delta - G_{\sim n} \bullet \Theta_k &= \Delta_{\sim k} + D_{\sim k} - \bar{G}_{\sim n} \bullet \Theta_k = \Delta_{\sim k} + \underline{D} \cdot (\delta_{\mathcal{V}} - \gamma^{-1} \cdot {}^{r}\theta_k) \cdot \underline{\varphi} = \\ &= \Delta_{\sim k} + \underline{D} \cdot \gamma^{-1} \cdot \gamma_{\sim k} \cdot \underline{\varphi} \quad ,\end{aligned}$$

with $\gamma_{\sim k}$ given by relation (14.25). Here the first graph represents the delta distribution. Therefore, exponentiating back to full amplitudes, we find

$$A^{(0)}_k = A^{(0)}_n \Big(\det\nolimits_{\mathcal{B}_n} \bar{G}_{\sim n} \bullet \bar{\mathcal{F}}_{\sim k}\Big)^{-\frac{1}{2}} = A^{(0)}_n \Big(\det\nolimits_{\mathcal{V}} \gamma^{-1}_{\sim k} \cdot \gamma\Big)^{\frac{1}{2}} \quad . \tag{15.39}$$

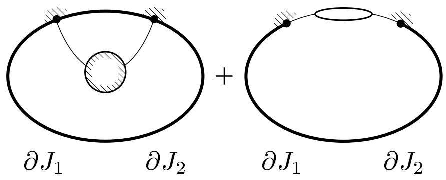
To recapitulate, we have found that the phenomenological description of different measurement devices by pair creation on the boundary leads to the notion of particles with a different propagator and the same boundary source space. The new propagator corresponds to different boundary conditions. The new and old boundary conditions differ in their value space, but they have the same momentum space.

Therefore conversely, we can use the boundary conditions $k = \kappa D$ for a phenomenological specification of the measurement devices on the boundary. We know that any such boundary conditions can be realized by a suitable interaction localized on the boundary.

Interaction of boundary sources

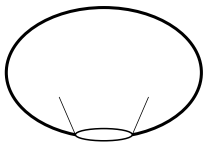
Now we turn to a different possibility of changing the experimental setup. In the sense of our original meaning of particles, the particles emitted from the boundary and absorbed again on the boundary propagate only through the interior of the domain. This propagation is described by the propagator $G_{\sim n}$. But let us investigate a situation when we allow additional propagation between boundary sources caused by an additional experimental devices on the boundary. We would like to interpret such a situation in a similar way as we did with pair creation in the previous section. I.e. we would like to find a new propagator and new sources which give the same predictions for amplitudes as the old propagator and sources in the presence of the additional propagation between boundary sources.

The additional propagation "inside boundary" does not affect any propagation inside the domain, it affects only amplitudes which contains a propagation between two boundary sources, i.e. the elementary amplitude now is



, (15.40)

where the additional propagator

$$-\frac{1}{n}\Xi_{n'} \qquad \leftrightarrow$$  (15.41)

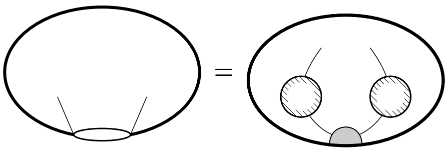
is sensitive only to the boundary sources. Therefore it can be represented as

$$\Xi_{n'} = G_{\sim n} \bullet \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} \bullet G_{\sim n} \quad , \tag{15.42}$$

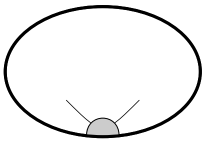
because for smooth J

$$J \bullet G_{\sim n} \bullet \underline{\pi} = 0 \quad . \tag{15.43}$$

Diagrammatically



,

$$n \ \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} \qquad \leftrightarrow$$  . (15.44)

The additional propagation can be also written using quantities living on value space only,

$$j_1 \cdot \underline{\varphi} \bullet \Xi_{n'} \bullet \underline{\varphi} \cdot j_2 = j_1 \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot j_2 \quad . \tag{15.45}$$

The definition of the new propagator is not so straightforward as it would seem. If we would define the new propagator as $G_{\sim n} - \Xi_{n'}$, it would correspond to the wave operator

$$\begin{aligned}(G_{\sim n} - \Xi_{n'})^{-1} &= \mathcal{F}_{\sim n} + \mathcal{F}_{\sim n} \bullet \Xi_{n'} \bullet \mathcal{F}_{\sim n} + \mathcal{F}_{\sim n} \bullet \Xi_{n'} \bullet \mathcal{F}_{\sim n} \bullet \Xi_{n'} \bullet \mathcal{F}_{\sim n} + \cdots = \\ &= \mathcal{F}_{\sim n} + \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} \quad .\end{aligned} \tag{15.46}$$

The associated boundary conditions have the same value space as n-boundary conditions but a different momentum space. Therefore the boundary source spaces differ, and we need to find the right correspondence between sources.

This is possible to do, if we define the new propagator in a different way and rearrange all amplitudes in specific way. The key observation is the identity

$$G_{\sim n} - \Xi_{n'} = \big(\delta - G_{\sim n} \bullet \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}\big) \bullet G_{\sim n'} \bullet \big(\delta - \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} \bullet G_{\sim n}\big) \quad , \tag{15.47}$$

where the new propagator is

$$G_{\sim n'} = \big(G^{-1}_{\sim n} - \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}\big)^{-1} \quad . \tag{15.48}$$

Now, if we substitute for the term $G_{\sim n} - \Xi_{n'}$ using this identity in any amplitude composed from the old propagator $\frac{1}{n} G_{\sim n}$, additional propagator $-\frac{1}{n}\Xi_{n'}$, and sources, and absorb the term $(\delta - G_{\sim n} \bullet \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi})$ into the definition of sources, we get the desired result — the description with the new propagator $G_{\sim n'}$, sources nJ inside the domain, and new boundary sources $n\partial J_{n'}$, which predict the same amplitudes as the old description.

First we find the boundary conditions of the new propagator. From the definition of the propagator we get

$$\mathcal{F}_{\sim n'} = \mathcal{F}_{\sim n} - \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} \quad , \tag{15.49}$$

$$\overset{\leftrightarrow}{d}\mathcal{F}_{\sim n'} = \overset{\leftrightarrow}{d}\mathcal{F}_{\sim n} - \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} = (\underline{\varphi} - \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'}) \cdot \underline{\pi} \quad . \tag{15.50}$$

I.e., the n'-boundary conditions have the same value space $\boldsymbol{\mathcal{P}}_{N}$ as Neumann boundary conditions and different momentum space $\boldsymbol{\mathcal{P}}_{D'}$. A calculation similar to the one in the case of k-boundary condition gives

$$\begin{gathered} \underline{\varphi}_{D'} = \gamma_{\sim n'} \cdot \gamma \cdot (\underline{\varphi} - {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}) \quad , \\ \underline{\varphi}_{n'} = \gamma \cdot \underline{\pi} \quad , \quad \underline{\pi}_{n'} = \gamma \cdot (\underline{\varphi} - {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}) \quad , \\ \gamma_{\sim n'} = \gamma - \gamma \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \gamma \quad . \end{gathered} \tag{15.51}$$

Next we can check what the new sources are. The sources inside of the domain do not change,

$$J \bullet \big(\delta - G_{\sim n} \bullet \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}\big) = J \quad , \tag{15.52}$$

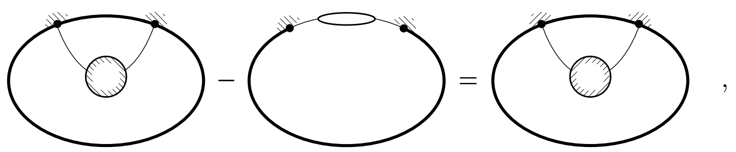
but boundary sources do change

$$\begin{aligned} \partial J_{n'} &= \partial J_n \bullet \big(\delta - G_{\sim n} \bullet \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}\big) = \\ &= \partial J_n \bullet \underline{D} \cdot (\underline{\varphi} - {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi}) = \\ &= \partial J_n \bullet \underline{D} \cdot \gamma^{-1} \cdot \gamma_{\sim n'} \cdot \underline{\varphi}_{D'} \quad , \end{aligned} \tag{15.53}$$

and we see that they belong to the boundary source space, which is consistent with the boundary conditions of the propagator,

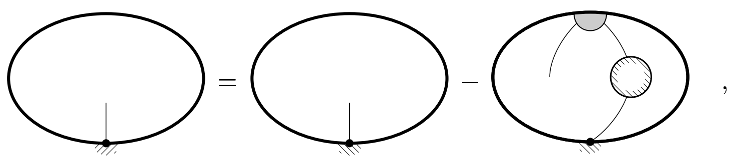
$$\partial J_{n'} \in \partial\tilde{\boldsymbol{\mathcal{J}}}_{\sim n'} \quad . \tag{15.54}$$

Diagrammatically we can summarize

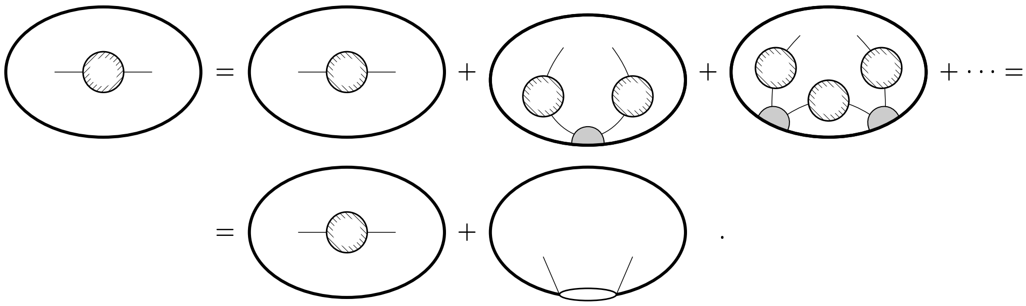


(15.55)

where



(15.56)



(15.57)

The last equality follows from

$$\underline{\pi} \bullet G_{\sim n} \bullet \underline{\pi} = 0 \quad ; \tag{15.58}$$

i.e., the new propagator is

$$G_{\sim n'} = G_{\sim n} + \Xi_{n'} \tag{15.59}$$

instead of the first guess $G_{\sim n} - \Xi_{n'}$.

We finally can conclude that the additional propagation between boundary sources from the point of view of the original experimental setup can be interpreted as no additional propagation in the new description which uses the new propagator and different sources. The new description corresponds to boundary conditions $n' = \mathrm{ND}'$. This means that we have the same notion of no-particle emission (the value spaces do not change), but we have a different description of boundary sources and different propagators.

Note that the one-particle amplitudes computed from the sources $\partial J_{n'}$ and ∂J_n related by relation (15.53) are the same,

$$Z^{(1)}_{n'}(J, \partial J_{n'}) = Z^{(1)}_{n}(J, \partial J_n) \quad . \tag{15.60}$$

Therefore, in comparing amplitudes for these two different boundary conditions, it will be useful to represent the boundary sources by one-particle amplitudes restricted to the boundary phase space as we discussed in the previous chapter. This is so, because if we compute generalized sources from $J \in \tilde{\boldsymbol{\mathcal{P}}}$ and $\partial\phi \in \boldsymbol{\mathcal{B}}$ as

$$J + \partial J_{n'} = \mathcal{J}_{n'}(J, \partial\phi) \quad , \quad J + \partial J_n = \mathcal{J}_n(J, \partial\phi) \quad , \tag{15.61}$$

$\partial J_{n'}$ and ∂J_n are related by (15.53).

Finally we compare the generating functionals. Substituting into (15.15), we get

$$A^{(0)}_{n'}(J, \partial\phi) = \exp\Big(-n\frac{1}{2}\,\partial\phi \bullet \underline{\pi} \cdot {}^{r}\theta^{-1}_{\sim n'} \cdot \underline{\pi} \bullet \partial\phi\Big)\, A^{(0)}_{n}(J, \partial\phi) \quad , \tag{15.62}$$

what is exactly what we have expected — an additional propagation between boundary sources.

Other boundary conditions

In the previous two sections we have interpreted the boundary conditions of the type $n' = \mathrm{ND}'$ and $k = \mathrm{KD}$ as introducing some additional interaction on the boundary in the original setup (which we have chosen to be given by Neumann boundary conditions $n = \mathrm{ND}$). Clearly, a combination of these two methods subsequently can interpret any boundary conditions $b = \mathrm{KD}'$.

This means that the theory in which amplitudes are computed using the propagator $\frac{1}{n}G_{\sim b}$ and sources $nJ \in \tilde{\boldsymbol{\mathcal{P}}}$ and $\partial J_{\sim b} \in \partial\tilde{\boldsymbol{\mathcal{J}}}_{\sim b}$ for b-boundary conditions can be interpreted as the theory where amplitudes are computed using the propagator $\frac{1}{n}G_{\sim k}$ obtained from the path integral, translated sources nJ and $\partial\tilde{\boldsymbol{\mathcal{J}}}_{\sim k}$, and additional pair creation on the boundary, and an additional propagation between boundary sources. These can be understood as an influence of some more complicated experimental devices on the boundary than was originally assumed in the definition of the path integral. I.e., the theory based on any boundary conditions can be interpreted in the sum-over-histories framework.

In closing, let us comment on the case of complex boundary conditions. It seems that there should be no problem to choose such additional interactions and propagation that we could reach complex boundary conditions. But in this case it is necessary to choose both kinds of discussed interaction simultaneously, because for complex boundary conditions the value and momentum spaces are not independent. It would be worth investigating the relation to complex boundary conditions in more detail to clarify all possible problems which could be hidden here.

16 Comparison with scalar field theory

Translation between theories

Finally we can compare the sum-over-histories quantization of relativistic particle theory (RPT) with scalar field theory (SFT). These two theories start from completely different backgrounds, and it seems they deal with completely different objects. But we can make a translation of some notions in these theories which allow us to compare the amplitudes computed in these theories, and we find that these amplitudes coincide.

After a detailed study of particle aspects in both theories the translation dictionary is obvious. We will identify the spacetime, identify external sources J, and identify the spacetime potential $V\mathcal{G}$ of SFT with the corrected potential $\mathcal{V}$ (eq. (13.38)) of the RPT. Next we identify the *pseudo-particles* in the SFT and particles emitted from the boundary in RPT, both corresponding to the same boundary conditions. By pseudo-particles associated with b-boundary conditions we means states

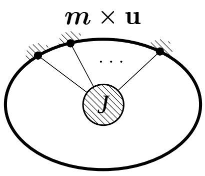
$$\hat{\mathrm{c}}_b[\mathbf{u}]^{\boldsymbol{m}}|b:0) \tag{16.1}$$

with a set of modes $\mathbf{u} = \{u_\mathrm{k}; \mathrm{k} \in \mathcal{I}\}$ in boundary phase space, and a multiindex[8] $\boldsymbol{m}$.

This means that we can speak in both theories about transition amplitudes between specified particle modes on the boundary — in the case of SFT modes they label pseudo-particle states, in the case of RPT they label boundary sources.

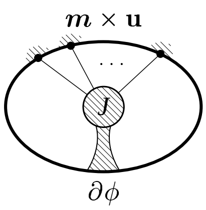
Transition amplitudes

Now we are prepared to compare the physical predictions of both theories — transition amplitudes. We claim that both theories give the same predictions. Specifically the following amplitudes coincide



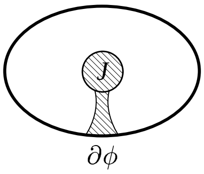
$$\leftrightarrow \qquad (phys|\hat{\mathrm{c}}_b[\mathbf{u}]^{\boldsymbol{m}}|b:0) = A_b^{(0)}[\boldsymbol{m} \times \mathbf{u}](J) \quad . \tag{16.2}$$

Here we have represented boundary sources of RPT by one-particle amplitudes given by modes $\boldsymbol{m} \times \mathbf{u}$. We can even write a more general relation



$$\leftrightarrow \qquad (phys|\hat{\mathrm{c}}_b[\mathbf{u}]^{\boldsymbol{m}}|b:\partial\phi) = A_b^{(0)}[\boldsymbol{m} \times \mathbf{u}](J, \partial\phi) \quad . \tag{16.3}$$

All these identities follows from the equivalence of generating functionals



$$\leftrightarrow \qquad \begin{aligned}(phys|b:\partial\phi) &= A_b^{(0)}(J,\partial\phi) = \\ &= \mathrm{o}_b \ \exp\bigl(n\frac{1}{2}\,\mathcal{J}_b(J,\partial\phi)\bullet G_{\sim b}\bullet \mathcal{J}_b(J,\partial\phi)\bigr) \quad .\end{aligned}$$

For the SFT it is given by equation (11.50), for RPT by equation (15.15), and we have identified

$$\mathrm{o}_b = A_b^{(0)} \quad . \tag{16.5}$$

To conclude the proof of (16.2) and (16.3) we note that in both theories these multi-particle amplitudes are obtained from the generating functional in an identical way — by variation with respect to the argument which describes the particle mode in SFT or the boundary source in RPT.

Let us note that the equivalence is true for the physical signature of the spacetime metric $n = i$. For Euclidian signature $n = 1$ we would need to choose $\hbar = i$ in equation (11.50). But for imaginary $\hbar$ the canonical quantization is not consistent. As we have discussed in chapter 5, this is connected with application of usual the quantization procedure on Euclidian theory. We have already suggested it could be solved by generalization of quantization scheme which would employ the quantization rule (10.22).

It seems plausible that a similar correspondence holds for the particle notion of SFT based on complex boundary conditions (usual particle states which form a Fock base) and particles in RPT defined by the same boundary conditions. But as we said in the previous chapter, particles in RPT corresponding to complex boundary conditions need further investigation.

Summary

We have found that SFT and RPT theories are equivalent on the level of transition amplitudes. The bridge between the two theories is the notion of particles. In both theories we can formulate experimental statements of the type "particles are emitted or absorbed from the boundary in given modes". Amplitudes predicted for such experimental statements computed in both theories coincide. In the SFT particle modes are realized by pseudo-particle states associated with a real boundary conditions, in the RPT particle modes represent boundary sources. Boundary conditions are phenomenological descriptions of the measurement setup on the boundary used for the definitions of the particles.

Conclusion

Recapitulation

The main goal of this work was to compare two quantum theories of a relativistic particle — the usual scalar field theory and the sum-over-histories quantization. It was accomplished in two steps. In the first three parts we investigated scalar field theory (SFT) and in the last part we quantized the sigma model action of a relativistic particle using the sum-over-histories approach.

First, we have looked at the classical level of SFT with special attention to the restriction of the theory to a bounded domain. We have introduced the notion of a boundary phase space which carries information about the value and momentum on the whole boundary with a natural symplectic structure derivable from the action. We have classified a wide class of boundary conditions which depend linearly on the value and momentum on the boundary of the domain. The boundary conditions were characterized using a subspace of the boundary phase space. We have studied the wave operator and its inverse — Green functions — for different boundary conditions, especially their extension on the space of generalized sources with distributional terms localized on the boundary. Finally we have studied the necessity of the causal structure for the theory, and we showed that it is not needed for structures on the boundary phase space but is needed for the definition of covariant and canonical phase spaces.

The content of the first part is mainly a review of the known classical formalism but some new ideas were used. The definition of the boundary phase space and the covariant phase space and the derivation of their symplectic structures from the action is new. Also the classification of the boundary conditions using a distributional representation of the wave operator is a slightly different approach from the one usually taken in mathematics.

The second part has been devoted to canonical quantization of SFT. The quantum Hilbert space of a free scalar field has been built using Fock quantization based on a choice of a particle interpretation — a generalized positive–negative frequency splitting. The classification of all possible particle interpretations has been done using a complex structure on the covariant phase space. The association with boundary conditions has been studied. It has been also shown that the condition of diagonalization of the Hamiltonian picks up a unique particle interpretation. This material is mainly a reformulation of known facts using the formalism based on the covariant phase space. But the explicit form of the dependence on the boundary conditions cannot be found elsewhere, to the author's knowledge.

Beside the particle representation, the holomorphic representation (the representation using coherent states) has been introduced. The formalism of covariantly labeled coherent states has been built. This formulation is original but is mostly equivalent to the usual coherent states defined using some special choice of value and momentum spaces.

Next, the relation between two particle interpretations has been studied. The covariant form of Bogoljubov coefficients has been defined, and the S-matrix has been computed. The in-out holomorphic representation has been introduced, and the generating functional for transition amplitudes has been found. It has been also shown that initial and final particle interpretations can be found from the knowledge of in-out Hadamard Green function. The covariant definition of the Bogoljubov operator is original, as well as the derivation of a number of properties of in-out Green functions (e.g., the composition law for Green functions, etc.), and the covariant form of the transition amplitude between coherent states.

Finally, the canonical formalism has been generalized to the case with non-zero external source.

In the third part we have introduced boundary quantum mechanics. It is essentially quantization of the boundary phase space. An advantage of this approach is that one does not need a causal structure. It treats the initial and final boundary of the investigated domain in a unique way, which simplifies the formalism, and it opens doors to a connection with the path integral formulation and the quantization of the Euclidian form of the theory.

We have generalized the value, particle and holomorphic representations to boundary quantum mechanics and have found a clear connection with boundary conditions of the wave operator. Finally we have found the transition amplitudes in this formalism.

The material of this part is entirely new. But the idea of treating initial and final states on the same level, but developed in different manner, can be found, for example in [25].

Simultaneously with the study of scalar field theory we investigated similar approaches on a general level. In chapter 1 we have built the full classical formalism for a very wide class of theories, defined boundary, covariant and canonical phase spaces and studied their relation. In chapter 5 we have studied canonical quantization of phase space with a cotangent bundle structure. It is essentially a generalization of the usual quantum mechanics to the case of a general curved configuration space. The covariant formulation of this material is original. In chapter 10 we have formulated the boundary quantum mechanics on a general level.

In the last part we have turned to investigate the sum-over-histories approach to the quantization of a relativistic particle. In chapter 12 the general ideas of this approach have been reviewed as well as the relation to generalized quantum mechanics. Some advantages and disadvantages of both methods have been discussed.

Applying the general method to the particle theory, we have computed the propagator for such a theory. The computation in spacetime without boundary is mostly a review of known material, but the generalization to a domain with boundary is new. Appendix F contains most of the technically non-trivial original computation.

Next, we have derived transition amplitudes for the multi-particle theory with sources of particles localized on the boundary. We have studied the influence of boundary conditions and interpreted different boundary conditions using phenomenological descriptions of a measurement process on the boundary. These ideas are original.

Finally we have compared scalar field theory and relativistic particle theory quantized using the sum-over-histories approach. We have shown that both theories are equivalent at the level of transition amplitudes. This comparison clarifies the relation of both theories, the nature of which was not completely clear before (see [21]). This is also a main result of this work.

Acknowledgments

This work was written to be as self-contained as possible. A consequence is that a lot of material used here was already known. Here we list the main influences on the material presented.

The general formalism of the first part is mainly motivated by the covariant approach to physical theories [1]. The 3+1 splitting can be found, for example, in [2]. A discussion of boundary conditions can be found in almost any book on differential operators, but author does not know any reference devoted mainly to the characterization of boundary conditions using distributional terms on the boundary. However such a reference probably exists — this approach is not new.

The quantization of a scalar field using a particle interpretation characterized by a complex structure in the second part is mainly a further development of the formalism introduced in [9]. The possibility of the diagonalization of the Hamiltonian is a well known fact (see [6,9,10]). The part on holomorphic representation and coherent states was motivated by a lectures by Prof. V. P. Frolov given in 1995 at the University of Alberta, where similar concepts were introduced in the case of a two dimensional phase space. The ideas of the reconstruction of initial and final particle interpretations from the Green function can be found also in [11]. The existence of canonical Bogoljubov coefficients is discussed for example in [12].

The introductory material of the last part is based on various material cited in chapter 12. The computation of the propagator of the particle theory in a space without boundary can be found in [24]. General ideas connected with the definition of the path integral can be found in [14,23]. A computation partially similar to the calculation of the propagator in the space with boundary (but in slightly different context) can be found in [26].

Finally, the author would like to thank Dr. Tomáš Kopf for a large number of useful discussions and Prof. Don Page for his support, help and inspiring comments during the preparation of this

work.

Open problems

Despite the fact that we have tried to cover thoroughly the investigated area, some open problems remain. Now we would like to mention some of them.

Both scalar field theory and quantization of a relativistic particle were studied in the absence of self-interaction. The generalization to the interacting theory would be desirable. The methods for such generalization are well known. In the case of SFT theory it is perturbation theory and in the case of RPT we have to add interaction vertices in calculations of multi-particle transition amplitudes. Most of the discussion about definitions of the boundary states and the boundary sources remains the same as in the non-interacting case.

In the third part we have encountered the problem of quantization of the Euclidian version of the theory. We have suggested that the "right" quantization should be based on a realization of the quantization rule (10.22) for commutation relations on a (real) Hilbert space. This idea needs further development.

It would be also worthwhile to investigate more thoroughly the dynamical equation of boundary quantum mechanics and to find its more explicit form on a general level.

Another interesting question is the relation of boundary quantum mechanics for different domains. It should be possible to develop a formalism which relates boundary quantum mechanics of the domain composed of two subdomains with boundary quantum mechanics of both subdomains. Some kind of infinitesimal foliation of the spacetime to small domains and boundary quantum mechanics on these small domains could lead to an interesting relation with the path integral over field configurations.

As discussed in the overview of the sum-over-histories approach to quantum mechanics and its relation to generalized quantum mechanics, the notion of the decoherence functional needs further investigation of its dependence on the spacetime domain. The lack of this knowledge is a main disadvantage of generalized boundary mechanics compared with the sum-over-histories approach, although otherwise generalized quantum mechanics seems to be the best foundation for consistent formulation of quantum mechanics.

We have devoted part of chapter 13 to gathering properties of the path-integral measure. But the definition of this object needs further clarification which would open the way for a more complete derivation of the amplitudes, particularly of the propagators. More explicit knowledge of the dependence of the measure on the choice of the spacetime domain would be also desirable.

In chapter 15 we have studied the interaction of particles with devices on the boundary of the domain described in a phenomenological way, using a new interaction vertex or a new propagation on the boundary. It would be very instructive to have an explicit realization of such interactions on the boundary. Such realization would give a more clear physical interpretation for different boundary conditions and the notion of particles itself.

Particularly a further investigation of interactions leading to complex boundary conditions would be very useful, because the usual particle states of scalar field theory are associated precisely with such boundary conditions.

Appendices

A Notation

Vector spaces

We often encounter vector spaces and tensor algebras over them. If V is a vector space we denote its dual as $V^\star$. Then we can form the tensor space V^k_l

$$V^k_l = \underbrace{V \otimes V \otimes \ldots}_{k} \underbrace{V^\star \otimes V^\star \otimes \ldots}_{l} \quad . \tag{A.1}$$

We use *abstract indices* to denote a tensor structure of objects from these spaces (see e.g. [27]). They tell from which space the object is, and allow us to write down a contraction in the tensor algebra by the usual repetition of the indices. We use bold letters for the abstract indices.

Of course, abstract indices are a generalization of coordinate indices and in most cases could be understood as such. But it is a question of a personal taste to distinguish covariant notions independent of the choice of a base, and the representation in a particular base. Therefore we distinguish tensors with abstract indices from their coordinate representation. We use normal letters for coordinate indices (but you can hardly find them here). I.e. choosing a base $e^{\boldsymbol{a}}_a$ and dual base $\epsilon^a_{\boldsymbol{a}}$, $a = 1, 2, \ldots$ we can write

$$\begin{aligned} A^{\boldsymbol{a}_1 \boldsymbol{a}_2 \ldots}_{\boldsymbol{b}_1 \boldsymbol{b}_2 \ldots} &= A^{a_1 a_2 \ldots}_{b_1 b_2 \ldots} \, e^{\boldsymbol{a}_1}_{a_1} e^{\boldsymbol{a}_2}_{a_2} \ldots \, \epsilon^{b_1}_{\boldsymbol{b}_1} \epsilon^{b_2}_{\boldsymbol{b}_2} \ldots \quad , \\ A^{a_1 a_2 \ldots}_{b_1 b_2 \ldots} &= A^{\boldsymbol{a}_1 \boldsymbol{a}_2 \ldots}_{\boldsymbol{b}_1 \boldsymbol{b}_2 \ldots} \, \epsilon^{a_1}_{\boldsymbol{a}_1} \epsilon^{a_2}_{\boldsymbol{a}_2} \ldots \, e^{\boldsymbol{b}_1}_{b_1} e^{\boldsymbol{b}_2}_{b_2} \ldots \quad . \end{aligned} \tag{A.2}$$

Here $A^{\boldsymbol{a}_1 \boldsymbol{a}_2 \ldots}_{\boldsymbol{b}_1 \boldsymbol{b}_2 \ldots}$ is a tensor object and $A^{a_1 a_2 \ldots}_{b_1 b_2 \ldots}$ is a bunch of numbers depending on the base.

Because it can be tiresome to write always indices (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 "dress" for the object serving for the denotation of tensor operations.) We also use an alternative notation for contraction using an infix operator *dot* (we use different dots for different spaces). The usage of the dot copies the index notation. It can be sometimes a bit tricky, especially when multiplying operators — i.e contracting tensors from V^1_1. To clarify our convention we give an example. Let $A, B \in V^1_1$ and $k \in V^0_2$. Now we can can write

$$B \cdot k \cdot k^{-1} \cdot A = A \cdot B \qquad \text{because} \qquad B^{\boldsymbol{m}}_{\boldsymbol{a}} k_{\boldsymbol{mp}} k^{-1\,\boldsymbol{pn}} A^{\boldsymbol{b}}_{\boldsymbol{n}} = A^{\boldsymbol{b}}_{\boldsymbol{p}} B^{\boldsymbol{p}}_{\boldsymbol{a}} \quad . \tag{A.3}$$

Or

$$B \cdot A \cdot k = (A \cdot B) \cdot k \qquad \text{because} \qquad B^{\boldsymbol{m}}_{\boldsymbol{a}} A^{\boldsymbol{n}}_{\boldsymbol{m}} k_{\boldsymbol{nb}} = (A \cdot B)^{\boldsymbol{m}}_{\boldsymbol{a}} k_{\boldsymbol{mb}} \quad , \tag{A.4}$$

where $(A \cdot B)^{\boldsymbol{a}}_{\boldsymbol{b}} = A^{\boldsymbol{a}}_{\boldsymbol{p}} B^{\boldsymbol{p}}_{\boldsymbol{b}}$. I.e. the order of multiplication of operators is given by the tensor structure of surrounding contracting objects. If there is no surrounding object which would determine an order of multiplication, the usual left to right order is used. See also note 5 for other examples.

Tensor bundles

We denote by $\mathbf{E}\, M$ a fiber bundle over base manifold M with standard fiber $\mathbf{E}$, and by $\mathbf{E}_x\, M$ the fiber at point x. If $\mathbf{E}$ is a vector space, $\mathbf{E}^k_l\, M$ denotes a fiber bundle with standard fiber the tensor space $\mathbf{E}^k_l$. $\mathrm{Sect}\, \mathbf{E}\, M$ denotes the space of sections of the bundle.

In particular we use the following fiber bundles: $\mathbb{R}M$ and $\mathbb{C}M$ are trivial bundles of real and complex numbers over M, $\mathfrak{F}M$ is the space of the sections of either of them (i.e. the space of functions on the manifold M). $\tilde{\mathbb{R}}^\alpha M$ and $\tilde{\mathbb{C}}^\alpha M$ are bundles of densities[6] of weight α on M and $\tilde{\mathfrak{F}}^\alpha M$ is the space of their sections. If the weight α is omitted, $\alpha = 1$ is assumed. $\mathbf{T}M$ denotes the tangent vector bundle, $\mathbf{T}^\star M = \mathbf{T}^0_1 M$ the bundle of tangent covectors and $\mathfrak{T}^k_l M$ is the space of sections of the tangent tensor bundle $\mathbf{T}^k_l M$.

Functional spaces

We often work with spaces of functions over a manifold (for example $\boldsymbol{\mathcal{P}}$ or $\boldsymbol{\mathcal{V}}[\Sigma]$) and we deal with them almost as with finite-dimensional spaces. It is, of course, dangerous — in the case of infinite-dimensional spaces attention has to be paid to the topology. There are two main methods which are used for handling this problem (not necessarily contradictory) — to work with distributional spaces, or to work with Hilbert spaces. See, for example, [28–30]. We use mainly the first method. It forces us to be careful with the notion of the dual space. The problem (or an advantage?) is that the functional dual to the space of test (sufficiently nice) functions is a bigger space which contains singular functions — distributions. (The advantage of the Hilbert space approach is that the dual space of a Hilbert space has "the same size", similarly to finite-dimensional vector spaces.)

Therefore for vector functions on a manifold M we introduce an additional notation. Let $\boldsymbol{\mathcal{E}} = \mathrm{Sect}\,\mathbf{E}M$ be the space of test sections of a vector bundle on the manifold M. We denote by $\tilde{\boldsymbol{\mathcal{E}}} = \mathrm{Sect}\,\tilde{\mathbf{E}}^\star M = \mathrm{Sect}\big(\tilde{\mathbb{R}} \otimes \mathbf{E}^\star\big) M$ the space of test densities with the dual vector structure (i.e., if elements of $\mathbf{E}M$ are vectors, elements of $\mathbf{E}^\star M$ are covectors, etc.). The space of vector distributions than is $\boldsymbol{\mathcal{E}}' = \tilde{\boldsymbol{\mathcal{E}}}^\star$ — the functional dual to the space $\tilde{\boldsymbol{\mathcal{E}}}$. The space of test vector functions can be identified as subspace of distributions $\boldsymbol{\mathcal{E}} \subset \tilde{\boldsymbol{\mathcal{E}}}$. Let us also note that we will use the word *smooth* in the sense of smoothness of manifold dependence, not in the sense of topology of functional spaces.

In chapter 1 we speak about the space of histories $\boldsymbol{\mathcal{H}}$ which can be represented as sections of a fiber bundle $\boldsymbol{\mathcal{H}} = \mathrm{Sect}\,\mathbf{H}M$ (it is not necessarily a vector bundle). We represent its tangent fiber[19] $\mathbf{T}_\mathrm{h}\boldsymbol{\mathcal{H}}$ as $\mathbf{T}_\mathrm{h}\boldsymbol{\mathcal{H}} = \big(\mathbf{T}_\mathrm{h}\,\mathbf{H}\big) M$ and by distributions $(\mathbf{T}_\mathrm{h}\boldsymbol{\mathcal{H}})'$ we mean a functional dual to $\mathbf{T}_{\mathrm{h}}{}^0_1\,\boldsymbol{\mathcal{H}} = \big(\tilde{\mathbf{T}}_{\mathrm{h}}{}^0_1\,\mathbf{H}\big) M$ following the definition above.

The space of test functions is always the space of infinitely differentiable functions with a compact support. But in the case of a manifold with boundary we have to identify the space of test functions more precisely. We define it as the space of functions with compact support which have all derivatives bounded up to the boundary. Let us note that there is another possibility for the choice of the space of test functions (see e.g. [30]), which requires compact support inside the interior of the manifold (and a carefully chosen topology). These two definitions differ in the notion of distributions on the boundary. Our choice allows us to identify distributions on the domain Ω with a subspace of distributions on the surrounding manifold M with support on Ω.

Finally, we use abstract indices notation also for functional spaces. The vector index here represents a cumulative index for local vector indices and manifold dependence. The contraction can have different meanings in this case — it can be an integration of test functions or an application of a distribution on a test function. It has always to be checked that we do not attempt to contract two distributions that are too singular. They have to be sufficiently smooth that the operation is well-defined.

Differential operators and quadratic forms

First we note that a volume element $\mathfrak{g}^{\frac{1}{2}}$ on spacetime defines a bi-distribution $\mathcal{G}$ — a delta function normalized to the volume element — as

$$\mathcal{G} = \mathfrak{g}^{\frac{1}{2}}\delta \quad , \quad \varphi \bullet \mathcal{G} \bullet \psi = \int \phi\psi\,\mathfrak{g}^{\frac{1}{2}} \quad . \tag{A.5}$$

For a smooth function f we can define the distribution $f\mathcal{G}$

$$\varphi \bullet (f\mathcal{G}) \bullet \psi = \int \mathfrak{g}^{\frac{1}{2}}\, f\varphi\psi \quad . \tag{A.6}$$

It is often convenient to represent differential operators on the manifold M as bi-distributions. We use arrows $\leftsquigarrow$ and $\rightsquigarrow$ to indicate direction of derivatives. So, for example,

$$\psi \bullet \big(\overleftarrow{\mathrm{d}}_{\boldsymbol{\alpha}} a^{\boldsymbol{\alpha}}\big) \bullet \omega = \omega \bullet \big(a^{\boldsymbol{\alpha}} \overrightarrow{\mathrm{d}}_{\boldsymbol{\alpha}}\big) \bullet \psi = \int \omega\, a^{\boldsymbol{\alpha}} \mathrm{d}_{\boldsymbol{\alpha}} \psi \tag{A.7}$$

for a test function ψ, a test density ω, and a vector field a.

In general, if D is a differential operator and $\overrightarrow{\mathrm{D}}$ its distributional representation, we can define a distribution $f\overrightarrow{\mathrm{D}}$ for sufficiently smooth f as

$$\omega \bullet \big(f\overrightarrow{\mathrm{D}}\big) \bullet \psi = \int \omega f\, (\mathrm{D}\psi) \quad . \tag{A.8}$$

For second order operators we will mostly use an associated quadratic form (in the presence of a volume element). For an operator A represented by bi-distribution $\overrightarrow{\mathrm{A}}$ we define

$$\overrightarrow{\mathcal{A}} = \mathcal{G} \bullet \overrightarrow{\mathrm{A}} \quad , \quad \varphi \bullet \overrightarrow{\mathcal{A}} \bullet \psi = \int \varphi \mathfrak{g}^{\frac{1}{2}}\, (\mathrm{A}\psi) \quad . \tag{A.9}$$

We also write

$$\overleftrightarrow{\mathcal{A}} = \frac{1}{2}(\overleftarrow{\mathcal{A}} + \overrightarrow{\mathcal{A}}) \quad , \tag{A.10}$$

and

$$\begin{gathered} \partial\mathcal{A}[\partial\Omega] = \chi[\Omega]\, \overrightarrow{\mathcal{A}} - \overleftarrow{\mathcal{A}}\, \chi[\Omega] \quad , \\ \varphi \bullet \partial\mathcal{A}[\partial\Omega] \bullet \psi = \int_{\Omega} \big(\varphi\, (\mathrm{A}\psi) - \psi\, (\mathrm{A}\varphi)\big)\, \mathfrak{g}^{\frac{1}{2}} \quad . \end{gathered} \tag{A.11}$$

Here $\chi[\Omega]$ is the characteristic function of the domain Ω defined below. $\partial\mathcal{A}[\partial\Omega]$ is the distribution localized on the boundary.

Delta distributions localized on a submanifold

We define the characteristic function of a domain Ω as

$$\chi[\Omega] = \begin{cases} 1 & \text{on } \Omega \quad , \\ 0 & \text{outside of } \Omega \quad . \end{cases} \tag{A.12}$$

The delta function localized on the boundary of the domain Ω can be defined as a gradient of the characteristic function

$$\delta_{\boldsymbol{\alpha}}[\partial\Omega] = \mathrm{d}_{\boldsymbol{\alpha}} \chi[\Omega] \quad . \tag{A.13}$$

It is possible to generalize this distribution to any oriented hypersurface Σ. We will say that a non-tangent non-degenerate vector on Σ has a direction in the sense of the hypersurface if

$$\delta_{\vec{n}}[\Sigma] \overset{\text{def}}{=} \vec{n}^{\boldsymbol{\alpha}}\, \delta_{\boldsymbol{\alpha}}[\Sigma] \tag{A.14}$$

is a positive delta function on the hypersurface. From this definition it follows that we have chosen the inside orientation for a hypersurface $\partial\Omega$ given as the boundary of the domain Ω.

Lorentzian signature convention

Here we list the conventions for spacetime quantities in the physical (Lorentzian) version of the theory. See appendix D for the case of Euclidian theory.

In general, we use the MTW sign convention ([2]) with the possible exception of the definition of the extrinsic curvature where the sign depends on the orientation of the hypersurface. Specifically

$$\begin{aligned}
&g_{\alpha\beta} = -n_\alpha n_\beta + q_{\alpha\beta} \quad , \quad q \text{ positive definite} \quad , \\
&\nabla g = 0 \quad , \\
&\mathrm{R}_{\alpha\beta}{}^{\mu}{}_{\nu} a^\nu = \nabla_{[\alpha}\nabla_{\beta]} a^\mu \quad , \\
&\mathrm{Ric}_{\alpha\beta} = \mathrm{R}_{\mu\alpha}{}^{\mu}{}_{\beta} \quad , \\
&R = \mathrm{Ric}_{\alpha\beta}\, g^{-1\,\alpha\beta} \quad , \\
&\mathrm{K}[\Sigma]_{\alpha\beta} = \mathfrak{d}^\mu_\alpha \mathfrak{d}^\nu_\beta\, \nabla_\mu n_\nu \quad , \quad n \text{ has the orientation of the hypersurface } \Sigma \quad , \\
&k[\sigma] = \mathrm{K}[\Sigma]_{\alpha\beta}\, g^{-1\,\alpha\beta} \quad , \\
&\mathfrak{d}^\beta_\alpha = \delta^\beta_\alpha - \vec{n}^\beta\, n_\alpha \quad , \quad \vec{n}^\alpha = -n_\mu g^{-1\,\mu\alpha} \quad .
\end{aligned} \tag{A.15}$$

For two connections $\bar{\nabla}$, ∇ we write

$$\bar{\nabla} = \nabla \oplus \Gamma \qquad \text{iff} \qquad \bar{\nabla}_\mu a^\alpha = \nabla_\mu a^\alpha + \Gamma^{\alpha}_{\mu\nu} a^\nu \quad . \tag{A.16}$$

It induces the relation for derivatives of a tensor density $A \in \tilde{\mathfrak{T}}^{\alpha}{}^{k}_{l}\, M$

$$\bar{\nabla}_\gamma A^{\alpha\dots}_{\beta\dots} = \nabla_\gamma A^{\alpha\dots}_{\beta\dots} + \Gamma^{\alpha}_{\gamma\mu} A^{\mu\dots}_{\beta\dots} + \dots - \Gamma^{\mu}_{\gamma\beta} A^{\alpha\dots}_{\mu\dots} - \dots - \alpha\Gamma^{\mu}_{\gamma\mu} A^{\alpha\dots}_{\beta\dots} \quad . \tag{A.17}$$

Abstract indices dictionary

Here we list what abstract indices and contraction operators we are using for different spaces.

space	**indices**	**dot**	**description**
$\mathbf{T}\,M$	$\alpha, \beta, \dots$	$\cdot$	tangent spaces of spacetime (inner manifold in the first three parts and target manifold in the last part)
$\mathbf{T}\,\Sigma$			tangent spaces of a part of boundary manifold (a hypersurface)
$\mathbf{T}\,N$	$a, b, \dots$		tangent spaces of inner manifold in the last part
$\mathbf{T}\,\mathcal{H}$	$\boldsymbol{x}, \boldsymbol{y}, \dots$	$\bullet$	tangent spaces of the space of histories in chapters 1, 2 and 10
$\mathbf{T}\,\mathcal{V}[\Sigma]$	$\mathrm{x}, \mathrm{y}, \dots$	$\centerdot$	tangent spaces of the value space in chapters 1, 2 and 10
$\mathbf{T}\,\mathcal{B}[\Sigma]$	$\mathrm{A}, \mathrm{B}, \dots$	$\diamond$	tangent spaces of the boundary or canonical phase space in chapters 1, 2 and 10
$\mathbf{T}\,\mathcal{S}$	$A, B, \dots$	$\circ$	tangent spaces of the covariant phase space in chapters 1, 2 and 10
$\mathcal{P}$	$\boldsymbol{x}, \boldsymbol{y}, \dots$	$\bullet$	space of scalar field histories
$\mathcal{V}[\Sigma]$	$\mathrm{x}, \mathrm{y}, \dots$	$\centerdot$	space of values of scalar field on hypersurface Σ
$\mathcal{B}[\Sigma]$	$\mathrm{A}, \mathrm{B}, \dots$	$\diamond$	boundary or canonical phase space of scalar field
$\mathcal{S}$	$A, B, \dots$	$\circ$	covariant phase space of scalar field

B Symplectic geometry

The phase space is a manifold $\boldsymbol{\mathcal{G}}$ of even dimension $2n$ with a *symplectic form* $\overleftrightarrow{\omega}$ which satisfies

$$\begin{aligned} &\overleftrightarrow{\omega}^{\top} = -\overleftrightarrow{\omega} \quad , \quad \overleftrightarrow{\omega} \in \mathfrak{T}^0_2 \boldsymbol{\mathcal{G}} \quad , \\ &\overleftrightarrow{\omega} \qquad \text{is non-degenerate} \quad , \\ &\overleftrightarrow{\omega} \qquad \text{is closed (i.e. } \mathrm{d}\overleftrightarrow{\omega} = 0) \quad . \end{aligned} \tag{B.1}$$

We can invert it

$$\overleftrightarrow{\omega}^{-1} \circ \overleftrightarrow{\omega} = -\delta_{\boldsymbol{\mathcal{G}}} \tag{B.2}$$

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

$$X_H = (\mathrm{d}H) \circ \overleftrightarrow{\omega}^{-1} \quad . \tag{B.3}$$

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

$$\mathcal{L}_{X_H} \overleftrightarrow{\omega} = 0 \quad . \tag{B.4}$$

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

$$\{A, B\} = X_A \circ \mathrm{d}B = X_A \circ \overleftrightarrow{\omega} \circ X_B = (\mathrm{d}A) \circ \overleftrightarrow{\omega}^{-1} \circ (\mathrm{d}B) \quad . \tag{B.5}$$

We have

$$\frac{d}{dt} B \stackrel{\text{def}}{=} \mathcal{L}_{X_H} B = \{H, B\} \quad , \tag{B.6}$$

$$[X_A, X_B] = X_{\{A,B\}} \quad , \tag{B.7}$$

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

$$d\Gamma = (2\pi)^{-n} \frac{1}{n!} \underbrace{|\,\overleftrightarrow{\omega} \wedge \overleftrightarrow{\omega} \wedge \cdots \wedge \overleftrightarrow{\omega}\,|}_{n \text{ times}} = \left(\mathrm{Det}\, \frac{\overleftrightarrow{\omega}}{2\pi}\right)^{\frac{1}{2}} \quad . \tag{B.8}$$

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

$$\overleftrightarrow{\omega} = \mathrm{d}p_a \wedge \mathrm{d}x^a \quad , \tag{B.9}$$

we get

$$\{x^a, p_b\} = -\delta^a_b \tag{B.10}$$

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

C Tangent and cotangent bundle geometry

In this appendix we discuss the geometry of tangent bundles to some manifold $\boldsymbol{\mathcal{V}}$. 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 will use $\mathsf{a}, \mathsf{b}, \dots$ as indices for tensors on the manifold $\boldsymbol{\mathcal{V}}$ and the dot $\cdot$ for contraction of this type, and $\mathsf{A}, \mathsf{B}, \dots$ as indices for tensors from tangent spaces to the cotangent bundle $\boldsymbol{\mathcal{G}} = \mathbf{T}^\star \boldsymbol{\mathcal{V}}$.

Functions such as the Lagrangian $L(x, v)$ or the Hamiltonian $H(x, p)$, respectively, are functions on the tangent or cotangent bundle, respectively, of a configuration space $\boldsymbol{\mathcal{V}}$. Because velocities v (or momenta p) are vectors (covectors) from different fibers for different position x ($\mathbf{T}_x \boldsymbol{\mathcal{V}} \neq \mathbf{T}_y \boldsymbol{\mathcal{V}}$ for $x \neq y$), we have to be a bit careful to use a partial derivative with respect of the position x. There is no problem with the definition

$$\frac{\partial L}{\partial v^{\mathbf{a}}}(x,v) \ : \qquad \delta v^{\mathbf{n}} \frac{\partial L}{\partial v^{\mathbf{n}}}(x,v) = \frac{d}{d\epsilon} L(x, v + \epsilon \delta v)|_{\epsilon=0} \tag{C.1}$$

— a *derivative with constant* x — but to define the *derivative with constant* v we need a connection ∇ on $\boldsymbol{\mathcal{V}}$

$$\frac{\nabla_{\mathbf{a}} L}{\partial x}(x,v) \ : \qquad \delta x^{\mathbf{n}} \frac{\nabla_{\mathbf{n}} L}{\partial x}(x,v) = \frac{d}{d\epsilon} L(x + \epsilon \delta x, v_\epsilon)|_{\epsilon=0} \quad , \tag{C.2}$$

where v_ϵ is the parallel transport of v in δx direction in the sense of the connection ∇ (i.e. $\frac{\nabla}{d\epsilon} v_\epsilon = 0$). Similarly, for a function on the cotangent bundle,

$$\begin{aligned} \frac{\partial H}{\partial p_{\mathbf{a}}}(x,p) \ &: \qquad \delta p_{\mathbf{n}} \frac{\partial H}{\partial p_{\mathbf{n}}}(x,p) = \frac{d}{d\epsilon} H(x, p + \epsilon \delta p)|_{\epsilon=0} \quad , \\ \frac{\nabla_{\mathbf{a}} H}{\partial x}(x,p) \ &: \qquad \delta x^{\mathbf{n}} \frac{\nabla_{\mathbf{n}} H}{\partial x}(x,p) = \frac{d}{d\epsilon} H(x + \epsilon \delta x, p_\epsilon)|_{\epsilon=0} \quad , \end{aligned} \tag{C.3}$$

where again $\frac{\nabla}{d\epsilon} p_\epsilon = 0$.

We will see that the cotangent bundle $\boldsymbol{\mathcal{G}} = \mathbf{T}^\star \boldsymbol{\mathcal{V}}$ has the structure of a phase space. Therefore it is useful to define a covariant generalization of "coordinate" vector fields and forms

$$\begin{aligned} &\frac{\partial^{\mathsf{A}}}{\partial p_{\mathbf{a}}} \qquad \text{a vector field on } \boldsymbol{\mathcal{G}} \text{ for which} \qquad \frac{\partial^{\mathsf{A}}}{\partial p_{\mathbf{a}}} \mathrm{d}_{\mathsf{A}} H = \frac{\partial H}{\partial p_{\mathbf{a}}} \quad , \\ &\frac{\nabla^{\mathsf{A}}_{\mathbf{a}}}{\partial x} \qquad \text{a vector field on } \boldsymbol{\mathcal{G}} \text{ for which} \qquad \frac{\nabla^{\mathsf{A}}_{\mathbf{a}}}{\partial x} \mathrm{d}_{\mathsf{A}} H = \frac{\nabla_{\mathbf{a}} H}{\partial x} \quad . \end{aligned} \tag{C.4}$$

$\frac{\partial}{\partial p}$ is actually the natural identification of the vector space $\mathbf{T}^\star_x \boldsymbol{\mathcal{V}}$ with its tangent space $\mathbf{T}(\mathbf{T}^\star_x \boldsymbol{\mathcal{V}})$ and $\frac{\nabla}{\partial x}$ is the horizontal shift of the connection ∇. Dual forms to these vector fields

$$\begin{aligned} &\mathrm{D}^{\mathbf{a}}_{\mathsf{A}} x \qquad \text{differential of the bundle projection} \qquad x \,:\, \mathbf{T} \boldsymbol{\mathcal{V}} \to \boldsymbol{\mathcal{V}},\ p|_x \to x \quad , \\ &\nabla_{\mathsf{A}} p_{\mathbf{a}} \qquad , \end{aligned} \tag{C.5}$$

are defined by

$$\frac{\nabla^{\mathsf{N}}_{\mathbf{a}}}{\partial x} \mathrm{D}^{\mathbf{b}}_{\mathsf{N}} x = \delta^{\mathbf{b}}_{\mathbf{a}} \quad , \quad \frac{\partial^{\mathsf{N}}}{\partial p_{\mathbf{b}}} \nabla_{\mathsf{N}} p_{\mathbf{a}} = \delta^{\mathbf{b}}_{\mathbf{a}} \quad , \quad \frac{\nabla^{\mathsf{N}}_{\mathbf{a}}}{\partial x} \nabla_{\mathsf{N}} p_{\mathbf{b}} = 0 \quad , \quad \frac{\partial^{\mathsf{N}}}{\partial p_{\mathbf{a}}} \mathrm{D}^{\mathbf{b}}_{\mathsf{N}} x = 0 \quad ,$$
$$\frac{\nabla^{\mathsf{A}}_{\mathbf{n}}}{\partial x} \mathrm{D}^{\mathbf{n}}_{\mathsf{B}} x + \frac{\partial^{\mathsf{A}}}{\partial p_{\mathbf{n}}} \nabla_{\mathsf{B}} p_{\mathbf{n}} = \delta^{\mathsf{A}}_{\mathsf{B}} \quad . \tag{C.6}$$

Now we can write down the canonical cotangent bundle symplectic form

$$\overset{\leftrightsquigarrow}{\omega}_{\mathsf{AB}} = \nabla_{\mathsf{A}} p_{\mathbf{a}} \wedge \mathrm{D}^{\mathbf{a}}_{\mathsf{B}} x = \nabla_{\mathsf{A}} p_{\mathbf{a}} \mathrm{D}^{\mathbf{a}}_{\mathsf{B}} x - \mathrm{D}^{\mathbf{a}}_{\mathsf{A}} x \nabla_{\mathsf{B}} p_{\mathbf{a}} \quad , \tag{C.7}$$

$$\overset{\leftrightsquigarrow}{\omega}^{-1\,\mathsf{AB}} = \frac{\partial^{\mathsf{A}}}{\partial p_{\mathbf{n}}} \frac{\nabla^{\mathsf{B}}_{\mathbf{n}}}{\partial x} - \frac{\nabla^{\mathsf{A}}_{\mathbf{n}}}{\partial x} \frac{\partial^{\mathsf{B}}}{\partial p_{\mathbf{n}}} \tag{C.8}$$

and we can even explicitly write the symplectic potential

$$\overset{\leftrightsquigarrow}{\omega}_{\mathsf{AB}} = \mathrm{d}_{\mathsf{A}} \theta_{\mathsf{B}} \quad , \quad \theta_{\mathsf{A}} = p_{\mathbf{n}} \mathrm{D}^{\mathbf{n}}_{\mathsf{A}} x \quad . \tag{C.9}$$

Canonical vector fields and Poisson brackets are

$$X_F = \frac{\partial F}{\partial p_{\mathbf{n}}} \frac{\nabla_{\mathbf{n}}}{\partial x} - \frac{\nabla_{\mathbf{n}} F}{\partial x} \frac{\partial}{\partial p_{\mathbf{n}}} \quad , \tag{C.10}$$

$$\{A, B\} = \frac{\partial A}{\partial p_{\mathbf{n}}} \frac{\nabla_{\mathbf{n}} B}{\partial x} - \frac{\nabla_{\mathbf{n}} A}{\partial x} \frac{\partial B}{\partial p_{\mathbf{n}}} \quad . \tag{C.11}$$

If we change the connection to another one,

$$\tilde{\nabla} = \nabla \oplus \Gamma \quad ,$$
$$\tilde{\nabla}_{\mathbf{a}} a^{\mathbf{b}} = \nabla_{\mathbf{a}} a^{\mathbf{b}} + \Gamma^{\mathbf{b}}_{\mathbf{an}} a^{\mathbf{n}} \quad , \quad \tilde{\nabla}_{\mathbf{a}} p_{\mathbf{b}} = \nabla_{\mathbf{a}} p_{\mathbf{b}} - \Gamma^{\mathbf{n}}_{\mathbf{ab}} p_{\mathbf{n}} \quad , \tag{C.12}$$

we get

$$\frac{\tilde{\nabla}^{\mathsf{A}}_{\mathbf{a}}}{\partial x}(x,p) = \frac{\nabla^{\mathsf{A}}_{\mathbf{a}}}{\partial x}(x,p) + p_{\mathbf{r}} \Gamma^{\mathbf{r}}_{\mathbf{as}}(x,p) \frac{\partial^{\mathsf{A}}}{\partial p_{\mathbf{s}}}(x,p) \quad ,$$
$$\tilde{\nabla}_{\mathsf{A}} p_{\mathbf{a}}(x,p) = \nabla_{\mathsf{A}} p_{\mathbf{a}}(x,p) - p_{\mathbf{r}} \Gamma^{\mathbf{r}}_{\mathbf{as}}(x,p) \mathrm{D}^{\mathbf{s}}_{\mathsf{A}} x(x,p) \quad . \tag{C.13}$$

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

Finally, coordinates x^{a} on $\boldsymbol{\mathcal{V}}$ generate coordinates $(x^{\mathrm{a}}, p_{\mathrm{a}})$ on $\boldsymbol{\mathcal{G}}$ by

$$p_{\mathrm{a}} = p_{\mathbf{a}} \frac{\partial^{\mathbf{a}}}{\partial x^{\mathrm{a}}} \tag{C.14}$$

and they define the coordinate connection ∂ on $\boldsymbol{\mathcal{V}}$ by

$$\partial \mathrm{d}x^{\mathrm{a}} = 0 \quad , \quad \partial \frac{\partial}{\partial x^{\mathrm{a}}} = 0 \qquad \text{for a} = 1, 2, \ldots, n \quad . \tag{C.15}$$

Using this connection, and expressing everything in coordinates, we get the standard relations

$$\overset{\leftrightsquigarrow}{\omega}_{\mathsf{AB}} = \mathrm{d}_{\mathsf{A}} p_{\mathrm{n}} \wedge \mathrm{d}_{\mathsf{B}} x^{\mathrm{n}} \quad , \quad \theta_{\mathsf{A}} = p_n \mathrm{d}_{\mathsf{A}} x^n \quad , \tag{C.16}$$

$$X_F{}^{\mathsf{A}} = \frac{\partial F}{\partial p_{\mathrm{n}}} \frac{\partial^{\mathsf{A}}}{\partial x^{\mathrm{n}}} - \frac{\partial F}{\partial x^{\mathrm{n}}} \frac{\partial^{\mathsf{A}}}{\partial p_{\mathrm{n}}} \quad , \tag{C.17}$$

$$\{A, B\} = \frac{\partial A}{\partial p_{\mathrm{n}}} \frac{\partial B}{\partial x^{\mathrm{n}}} - \frac{\partial A}{\partial x^{\mathrm{n}}} \frac{\partial B}{\partial p_{\mathrm{n}}} \quad , \tag{C.18}$$

$$\{x^{\mathrm{a}}, p_{\mathrm{b}}\} = -\delta^{\mathrm{a}}_{\mathrm{b}} \quad . \tag{C.19}$$

D Euclidian and physical versions of the theory

Euclidian theory

A very powerful tool in quantum field theory in flat spacetime is Wick rotation to the Euclidian sector of the theory. The Euclidian version of the theory is used to define objects which are not mathematically well-defined in the physical version. The desired results are computed in the Euclidian version and afterwards it "rotated" to the physical sector of the theory. The "rotation" means usually analytical continuation in the time coordinate from the real to the imaginary axis.

There exist different attempts to generalize this method to non-flat spacetime. The most straightforward generalization is analytical continuation in some special coordinates, but it lacks a good covariant foundation. There are two main approaches to more geometrical generalization of Wick rotation. The first is to change the spacetime to a complex manifold with complex coordinates and identify real submanifolds of the physical and Euclidian theory in this complex manifold. The another approach keeps the spacetime manifold fixed and uses complex fields living in the complexified bundles over the real spacetime manifold. Specifically, it uses the complexified metric g.

Both approaches have problems. The Wick rotation is not uniquely defined, if defined at all. But despite the problems, the Euclidian formulation is a useful tool at least in some special cases.

We adopt the latter approach to the Euclidian formulation of the theory in a curved spacetime. Our motivation will be following. We can encounter technical problems connected with the Lorentzian signature of the spacetime metric in definitions of some physical quantities, as e.g. transition amplitudes, propagator, etc.. For example, some integrals have an ugly oscillatory character. It is usually easier to define similar quantities for a positive definite metric. And if the dependence of the investigated quantity on the spacetime metric is sufficiently nice (in the best case analytical), we can hope that the definition of the quantity for Lorentzian metric can be obtained by an extension of the definition for the Euclidian metrics in the space of complex metrics to the "imaginary axis" with Lorentzian metrics.

This method is common in definitions of some distribution as the continuation of an analytical function to the border of analyticity. We give a trivial example. We want to define distributions $\frac{1}{1+g}$ or $\ln g$ for g on the negative real axis $\mathbb{R}^-$ ("Lorentzian values" of g). These functions are well defined for "Euclidian values" $g \in \mathbb{R}^+$, and we can use these Euclidian versions together with a specification of analytical continuation to define the Lorentzian versions of these distributions. There exist many analytical continuations from $\mathbb{R}^+$ to $\mathbb{R}^-$, and using different continuations we obtain different results. In our example, continuation through the upper or lower complex half-plane give for $g \in \mathbb{R}^-$

$$\frac{1}{1+g+i0} = \mathcal{P}\frac{1}{1+g} - i\pi\delta(1+g) \quad , \qquad \frac{1}{1+g-i0} = \mathcal{P}\frac{1}{1+g} + i\pi\delta(1+g) \quad , \tag{D.1}$$

$$\ln(g+i0) = \ln|g| + i\pi \quad , \qquad \ln(g-i0) = \ln|g| - i\pi \quad . \tag{D.2}$$

Here $\mathcal{P}$ denotes the distribution defined using the principal value.

We interpret the Euclidian version of the physical theory in a similar way. We use the Euclidian version to define mathematically well-defined objects which have a sufficiently nice dependence on the metric, and by specification of *generalized Wick rotation* — analytical continuation from Euclidian metrics to Lorentzian metrics — we define Lorentzian (physical) versions of the investigated objects.

Special Wick rotation in curved space

We have suggested that the generalization of Wick rotation is essentially some way how to analytically continue some functional of the spacetime metric from Euclidian metrics to Lorentzian. We will not study this concept in its generality — but it would be worthwhile to find how many different analytical continuation we have and how we may classify them. We will study a special case of continuation from Euclidian metrics to Lorentzian ones which is a straightforward generalization of the rotation of the time coordinate in flat spacetime.

Let us investigate a neighborhood U in a d-dimensional (spacetime) manifold which has topology $\mathbb{R} \times \Sigma$. In such a part of the manifold we can define the d-dimensional generalization of the $3+1$ splitting from chapter 2. I.e., we choose "time" coordinate t and time flow vector field $\vec{t}$ for which $\vec{t} \cdot \mathrm{d}t = 1$. This defines for us the foliation of the neighborhood U into hypersurfaces Σ_t defined by the condition $t = \text{const}$. Now we will investigate a complex metric g (symmetric non-degenerate quadratic form) on U in the following form

$$g = n^2\ {}^L\mathrm{n}{}^L\mathrm{n} + q \quad , \tag{D.3}$$

where n is a constant complex factor (usually just phase factor), ${}^L\mathrm{n}$ is the real form normal to the hypersurfaces Σ_t and q is a positive definite real metric on hypersurfaces[20] Σ_t. If the metric g is positive definite (for n real) we call it Euclidian, if it has signature $(-++\ldots)$ (for n imaginary) we call it Lorentzian. Choosing a contour in complex plane joining the Euclidian and Lorentzian values of n defines a specific continuation from Euclidian metric to Lorentzian metric — generalized Wick rotation. We will investigate only this type of Wick rotation, even if we can imagine more complicated transitions from the Euclidian sector to the Lorentzian.

Next we will define some useful quantities in the case of general signature. There are two useful conventions which we can adopt. One of them — which we call *Euclidian convention* — pretends that the metric is Euclidian and defines all quantities in the most natural way for a Euclidian metric. As a result some quantities can have a complex value for non-Euclidian metric. This convention suggests, that the Euclidian metrics are the "simplest" ones and that most relations should have a simple form using the Euclidian convention. And if we would express equations in the main text in this convention, we would see that they really simplify by the elimination of some numeric factor.

Another convention — which we call *Lorentzian convention* — tries explicitly to trace out the signature factor n and defines most quantities in the way that they are real even for complex metric g. Because the physical metric is in some sense a "complex metric" (the metric is Lorentzian for imaginary value of n), it will be more natural to adopt this convention to obtain the usual definitions of the quantities, and we will do so in the main text.

But it does not matter which convention we use — the choice is only a question of convenience in a specific problem. We can use both conventions, independently in which version of the theory we work — Euclidian or Lorentzian — or even if we work with a general complex metric.

Metric dependent quantities

Below we list some definitions of quantities connected with $(d-1)+1$ splitting in both conventions and translation between both conventions. We define lapse N and shift $\vec{N}$, normal vector $\vec{n}$, projector $\mathfrak{d}$ on hypersurface Σ_t, volume elements $\mathfrak{g}^{\frac{1}{2}}$ and $\mathfrak{q}^{\frac{1}{2}}$, and external curvature K. In the Euclidian (or Lorentzian respectively) convention we add the index ^{E} (or ^{L} respectively) in front of the a quantity. In the main text we drop the index ^{L}.

Euclidian	**translation**	**Lorentzian**	(D.4)
$g = {}^E\mathrm{n}{}^E\mathrm{n} + q$	${}^E\mathrm{n} = n\ {}^L\mathrm{n}$	$g = n^2\ {}^L\mathrm{n}{}^L\mathrm{n} + q \quad ,$	
${}^E\mathrm{n} = {}^E N \mathrm{d}t$	${}^E N = n\ {}^L N$	${}^L\mathrm{n} = {}^L N \mathrm{d}t \quad ,$	

$$
\begin{array}{lll}
{}^{E}\vec{n}\cdot{}^{E}n = 1 \qquad {}^{E}\vec{n}\cdot q = 0 & {}^{E}\vec{n} = \frac{1}{n}\,{}^{L}\vec{n} & {}^{L}\vec{n}\cdot{}^{L}n = 1 \qquad {}^{L}\vec{n}\cdot q = 0 \quad , \\
\mathfrak{d} = \delta - {}^{E}\vec{n}\,{}^{E}n & & \mathfrak{d} = \delta - {}^{L}\vec{n}\,{}^{L}n \quad , \\
g^{-1} = {}^{E}\vec{n}\,{}^{E}\vec{n} + q^{-1} & & g^{-1} = \frac{1}{n^2}\,{}^{L}\vec{n}\,{}^{L}\vec{n} + q^{-1} \quad , \\
{}^{E}\vec{n}\cdot g\cdot{}^{E}\vec{n} = 1 \quad {}^{E}n\cdot g^{-1}\cdot{}^{E}n = 1 & & {}^{L}\vec{n}\cdot g\cdot{}^{L}\vec{n} = n^2 \quad {}^{L}n\cdot g^{-1}\cdot{}^{L}n = \frac{1}{n^2} \quad , \\
{}^{E}n = g\cdot{}^{E}\vec{n} \quad {}^{E}\vec{n} = g^{-1}\cdot{}^{E}n & & {}^{L}n = \frac{1}{n^2}\,g\cdot{}^{L}\vec{n} \quad {}^{L}\vec{n} = n^2\,g^{-1}\cdot{}^{L}n \quad , \\
\vec{t} = {}^{E}N\,{}^{E}\vec{n} + \vec{N} & & \vec{t} = {}^{L}N\,{}^{L}\vec{n} + \vec{N} \quad , \\
{}^{E}\mathfrak{g} = \operatorname{Det} g & {}^{E}\mathfrak{g} = n^2\,{}^{L}\mathfrak{g} & {}^{L}\mathfrak{g} = \frac{1}{n^2}\operatorname{Det} g \quad , \\
\mathfrak{q}^{\frac{1}{2}} = \big(\operatorname{Det} q\big)^{\frac{1}{2}} & & \mathfrak{q}^{\frac{1}{2}} = \big(\operatorname{Det} q\big)^{\frac{1}{2}} \quad , \\
{}^{E}\mathfrak{g}^{\frac{1}{2}} = {}^{E}N dt\ \mathfrak{q}^{\frac{1}{2}} & {}^{E}\mathfrak{g}^{\frac{1}{2}} = n\,{}^{L}\mathfrak{g}^{\frac{1}{2}} & {}^{L}\mathfrak{g}^{\frac{1}{2}} = {}^{L}N dt\ \mathfrak{q}^{\frac{1}{2}} \quad , \\
{}^{E}\mathrm{K} = \mathfrak{d}\cdot\nabla\,{}^{E}n & {}^{E}\mathrm{K} = n\,{}^{L}\mathrm{K} & {}^{L}\mathrm{K} = \mathfrak{d}\cdot\nabla\,{}^{L}n \quad .
\end{array}
$$

Let's note that for these metric dependent quantities the relations between quantities in the Euclidian convention are the same as between quantities in Lorentzian convention with $n = 1$. But beware that this will not be always so — specifically for quantities connected with the action introduced in the next section.

Action dependent quantities

Now we turn to investigate the action and related quantities in Euclidian context. We will look first at a general theory in Lagrangian form. It can be formulated as a theory based on a one-dimensional inner manifold N (manifold of physical time parameter) with inner metric h which determines the choice of the physical time coordinate. History can be viewed as a map from the inner manifold N to some target manifold. Most physical theories can be reformulated in this form. A particle theory is already in this form, scalar field theory can be brought to this form using $(d-1)+1$ splitting discussed above.

In this case we speak about Euclidian or physical version of the theory if the inner space metric h is Euclidian (positive definite) or Lorentzian (i.e. in this case negative definite). The physical time t is coordinate on the inner space related to the metric h by

$$h = \nu^2 \mathrm{d}t\mathrm{d}t \quad , \quad \big(\operatorname{Det} h\big)^{\frac{1}{2}} = \nu dt \quad . \tag{D.5}$$

Here ν is equivalent of the signature factor n from the previous section for the inner metric h — i.e. it is a constant complex number which determines the version of the theory.

The action S is a functional on the space of histories. In the case of Euclidian theory it turns out to be more convenient to define the *Euclidian action* I. We will view the Euclidian action as the action in the Euclidian convention ($I = {}^{E}S$). Again, we can use both Euclidian and Lorentzian actions in both theories, depending which form is more convenient. The relation between both actions is

$$-I = \nu S \quad . \tag{D.6}$$

We assume that the action has a Lagrangian form, i.e. that it is expressed as the integral of a *Lagrangian* over inner manifold. We define Lagrangian L and related quantities — canonical momentum p, canonical velocity v and Hamiltonian H — in both Euclidian and Lorentzian convention.

These quantities are derivable from Euclidian or Lorentzian action in the same fashion.

$$
\begin{array}{lll}
\textbf{Euclidian} & \textbf{translation} & \textbf{Lorentzian} \\
I = \int {}^{E}\!L(x,\dot{x})dt & -\,{}^{E}\!L(x,v) = \nu\,{}^{L}\!L(x,v) & S = \int {}^{L}\!L(x,\dot{x})dt \quad , \\
{}^{E}\!p(x,v) = \dfrac{\partial\,{}^{E}\!L}{\partial v}(x,v) & -\,{}^{E}\!p(x,v) = \nu\,{}^{L}\!p(x,v) & {}^{L}\!p(x,v) = \dfrac{\partial\,{}^{L}\!L}{\partial v}(x,v) \quad , \\
{}^{E}\!v(x,{}^{E}\!p(x,v)) = v & {}^{E}\!v(x,p) = {}^{L}\!v(x,-\dfrac{p}{\nu}) & {}^{L}\!v(x,{}^{L}\!p(x,v)) = v \quad , \\
{}^{E}\!H(x,p) = & & {}^{L}\!H(x,p) = \\
\quad = p\cdot{}^{E}\!v(x,p) - {}^{E}\!L(x,{}^{E}\!v(x,p)) & {}^{E}\!H(x,p) = -\nu\,{}^{L}\!H(x,-\dfrac{p}{\nu}) & \quad = p\cdot{}^{L}\!v(x,p) - {}^{L}\!L(x,{}^{E}\!v(x,p)) \quad .
\end{array}
\tag{D.7}
$$

Specifically for the Lagrangian given by a sum of a quadratic kinetic term and a potential term we have

$$
\begin{array}{ll}
{}^{E}\!L(x,v) = \dfrac{1}{2}\dfrac{1}{\nu}\, v\cdot g(x)\cdot v + \nu V(x) & {}^{L}\!L(x,v) = -\dfrac{1}{2}\dfrac{1}{\nu^2}\, v\cdot g(x)\cdot v - V(x) \quad , \\
{}^{E}\!p(x,v) = \dfrac{1}{\nu}\, g(x)\cdot v & {}^{L}\!p(x,v) = -\dfrac{1}{\nu^2}\, g(x)\cdot v \quad , \\
{}^{E}\!H(x,p) = \nu\Big(\dfrac{1}{2}p\cdot g^{-1}(x)\cdot p - V(x)\Big) & {}^{L}\!H(x,p) = -\dfrac{1}{2}\nu^2\, p\cdot g^{-1}(x)\cdot p + V(x) \quad .
\end{array}
\tag{D.8}
$$

Here g is a metric on the target manifold. Let us note that now we have studied Wick rotation in inner manifold metric h, not in the target manifold metric g. It can be desirable to combine both methods as will be done in the last part of the work. But it only introduces a possibility for g to be a complex metric and does not change the definitions above.

Scalar field theory

Next we return to study a theory formulated on a d-dimensional spacetime manifold. It can be reduced to the previous case using $(d-1)+1$ splitting technique. But in chapter 1 we have formulated a general formalism without such splitting and we have applied it to the case of the scalar field theory in chapter 2. Now we present definitions from those chapters using both Euclidian and Lorentzian convention.

First we add the Laplace-like quadratic form and source term to our list of metric-dependent quantities

$$
\begin{array}{lll}
\textbf{Euclidian} & \textbf{translation} & \textbf{Lorentzian} \\
{}^{E}\!\mathcal{F}_d[\Omega] = (\chi[\Omega]\, V\ {}^{E}\mathcal{G}) + & & {}^{L}\!\mathcal{F}_d[\Omega] = (\chi[\Omega]\, V\ {}^{L}\mathcal{G}) + \\
\quad + \overleftarrow{\mathrm{d}}_{\boldsymbol{\alpha}} \bullet (\chi[\Omega] g^{-1\,\boldsymbol{\alpha\beta}}\ {}^{E}\mathcal{G}) \bullet \overrightarrow{\mathrm{d}}_{\boldsymbol{\beta}} & {}^{E}\!\mathcal{F}_d[\Omega] = n\ {}^{L}\!\mathcal{F}_d[\Omega] & \quad + \overleftarrow{\mathrm{d}}_{\boldsymbol{\alpha}} \bullet (\chi[\Omega] g^{-1\,\boldsymbol{\alpha\beta}}\ {}^{L}\mathcal{G}) \bullet \overrightarrow{\mathrm{d}}_{\boldsymbol{\beta}} \quad , \\
{}^{E}\!\overrightarrow{\mathcal{F}}[\Omega] = \chi[\Omega]\ V\ {}^{E}\mathcal{G} + & & {}^{L}\!\overrightarrow{\mathcal{F}}[\Omega] = \chi[\Omega]\ V\ {}^{L}\mathcal{G} + \\
\quad + \chi[\Omega]\ \overleftrightarrow{\mathrm{d}}_{\boldsymbol{\alpha}} \bullet \big(g^{-1\,\boldsymbol{\alpha\beta}}\ {}^{E}\mathcal{G}\overrightarrow{\mathrm{d}}_{\boldsymbol{\beta}}\big) & {}^{E}\!\overrightarrow{\mathcal{F}}[\Omega] = n\ {}^{L}\!\overrightarrow{\mathcal{F}}[\Omega] & \quad + \chi[\Omega]\ \overleftrightarrow{\mathrm{d}}_{\boldsymbol{\alpha}} \bullet \big(g^{-1\,\boldsymbol{\alpha\beta}}\ {}^{L}\mathcal{G}\overrightarrow{\mathrm{d}}_{\boldsymbol{\beta}}\big) \quad , \\
{}^{E}\partial\mathcal{F}[\partial\Omega] = {}^{E}\!\overrightarrow{\mathcal{F}}[\Omega] - {}^{E}\!\overleftarrow{\mathcal{F}}[\Omega] & {}^{E}\partial\mathcal{F}[\partial\Omega] = n\ {}^{L}\partial\mathcal{F}[\partial\Omega] & {}^{L}\partial\mathcal{F}[\partial\Omega] = {}^{L}\!\overrightarrow{\mathcal{F}}[\Omega] - {}^{L}\!\overleftarrow{\mathcal{F}}[\Omega] \quad , \\
{}^{E}\!\overrightarrow{d\mathcal{F}}_d[\partial\Omega] = {}^{E}\!\mathcal{F}_d[\Omega] - {}^{E}\!\overrightarrow{\mathcal{F}}[\Omega] & {}^{E}\!\overrightarrow{d\mathcal{F}}_d[\partial\Omega] = n\ {}^{L}\!\overrightarrow{d\mathcal{F}}_d[\partial\Omega] & {}^{L}\!\overrightarrow{d\mathcal{F}}_d[\partial\Omega] = {}^{L}\!\mathcal{F}_d[\Omega] - {}^{L}\!\overrightarrow{\mathcal{F}}[\Omega] \quad , \\
{}^{E}\mathcal{G} = {}^{E}\mathfrak{g}^{\frac{1}{2}}\,\delta & {}^{E}\mathcal{G} = n\ {}^{L}\mathcal{G} & {}^{L}\mathcal{G} = {}^{L}\mathfrak{g}^{\frac{1}{2}}\,\delta \quad , \\
{}^{E}J = {}^{E}\mathfrak{g}^{\frac{1}{2}}\,\tilde{J} & {}^{E}J = n\ {}^{L}J & {}^{L}J = {}^{L}\mathfrak{g}^{\frac{1}{2}}\,\tilde{J} \quad .
\end{array}
\tag{D.9}
$$

Next we list action-dependent quantities

$$
\begin{array}{lll}
\textbf{Euclidian} & \textbf{translation} & \textbf{Lorentzian} \\
I[\Omega] = \frac{1}{2}\phi \bullet {}^{E}\mathcal{F}_{d}[\Omega] \bullet \phi - {}^{E}J \bullet \phi & -I = nS & S[\Omega] = -\frac{1}{2}\phi \bullet {}^{L}\mathcal{F}_{d}[\Omega] \bullet \phi + {}^{E}J \bullet \phi \\
\mathrm{d}I[\Omega] = \chi[\Omega]\delta I - {}^{E}\mathfrak{P}[\partial\Omega] & -{}^{E}\mathfrak{P}[\partial\Omega] = n\,{}^{L}\mathfrak{P}[\partial\Omega] & \mathrm{d}S[\Omega] = \chi[\Omega]\delta S - {}^{L}\mathfrak{P}[\partial\Omega] \quad , \\
\delta I = {}^{E}\overset{\rightsquigarrow}{\mathcal{F}} \bullet \phi - {}^{E}J & -\delta I = n\delta S & n = -{}^{L}\overset{\rightsquigarrow}{\mathcal{F}} + {}^{L}J \quad , \\
\mathrm{d}^{E}\mathfrak{P} = -{}^{E}\partial\mathcal{F} = {}^{E}\underline{\pi} \cdot \underline{\varphi} - \underline{\varphi} \cdot {}^{E}\underline{\pi} & -\mathrm{d}^{E}\mathfrak{P} = n\,\mathrm{d}^{L}\mathfrak{P} & \mathrm{d}^{L}\mathfrak{P} = {}^{L}\partial\mathcal{F} = {}^{L}\underline{\pi} \cdot \underline{\varphi} - \underline{\varphi} \cdot {}^{L}\underline{\pi} \quad , \\
{}^{E}\overset{\leftrightsquigarrow}{d}\mathcal{F}_{d} = -{}^{E}\underline{\pi} \cdot \underline{\varphi} & -{}^{E}\underline{\pi} = n\,{}^{L}\underline{\pi} & {}^{L}\overset{\leftrightsquigarrow}{d}\mathcal{F}_{d} = {}^{L}\underline{\pi} \cdot \underline{\varphi} \quad , \\
{}^{E}\{A, B\}_{\boldsymbol{\mathcal{B}}} = \mathrm{d}A \diamond (\mathrm{d}^{E}\mathfrak{P})^{-1} \diamond \mathrm{d}B & -n\,{}^{E}\{\,,\,\}_{\boldsymbol{\mathcal{B}}} = {}^{L}\{\,,\,\}_{\boldsymbol{\mathcal{B}}} & {}^{L}\{A, B\}_{\boldsymbol{\mathcal{B}}} = \mathrm{d}A \diamond (\mathrm{d}^{L}\mathfrak{P})^{-1} \diamond \mathrm{d}B \quad , \\
\mathrm{d}^{E}\mathfrak{P} \diamond (\mathrm{d}^{E}\mathfrak{P})^{-1} = -\delta_{\boldsymbol{\mathcal{B}}} & -(\mathrm{d}^{E}\mathfrak{P})^{-1} = \frac{1}{n}(\mathrm{d}^{L}\mathfrak{P})^{-1} & \mathrm{d}^{L}\mathfrak{P} \diamond (\mathrm{d}^{L}\mathfrak{P})^{-1} = -\delta_{\boldsymbol{\mathcal{B}}} \quad .
\end{array}
\tag{D.10}
$$

Note that the relations between the metric-dependent and the action-dependent quantities are not always the same in Euclidian and Lorentzian conventions due to the extra minus sign in the definition of the Euclidian action.

E S-matrix

We want to prove the explicit form (8.112) of the S-matrix associated with a transition operator s. The following proof is generalization of the derivation for two-dimensional phase space presented in [31].

Let define for $\xi, \zeta \in \mathbb{R}$ a transition operator $s_{\xi,\zeta}$ in the form (8.113)

$$s_{\xi,\zeta} = \exp(\xi\mathcal{X}) \circ u_{i\,\zeta} = \exp(\xi\mathcal{X}) \circ \exp\bigl(\zeta \mathsf{J}_i \circ \psi\bigr) \quad , \tag{E.1}$$

where $\mathcal{X}$ and ψ are those from equation (8.113). Clearly we are interested in the case $\xi = \zeta = 1$.

For $\xi = 0$ the normal ordered form of the S-matrix (8.109) has the form

$$\hat{\mathrm{S}}_{0,\zeta} = \mathbf{:}\exp\Bigl(\langle\exp\bigl(\zeta\mathsf{J}_i \circ \psi\bigr) \circ \hat{\Phi}, \hat{\Phi}\rangle_i - \langle\hat{\Phi}, \hat{\Phi}\rangle_i\Bigr)\mathbf{:}_i \quad . \tag{E.2}$$

The derivative with respect of ζ is

$$\begin{aligned} \frac{d}{d\zeta}\hat{\mathrm{S}}_{0,\zeta} &= \mathbf{:}\,\langle\mathsf{J}_i \circ \psi \circ \exp\bigl(\zeta\mathsf{J}_i \circ \psi\bigr) \circ \hat{\Phi}, \hat{\Phi}\rangle_i \ \exp\Bigl(\langle\exp\bigl(\zeta\mathsf{J}_i \circ \psi\bigr) \circ \hat{\Phi}, \hat{\Phi}\rangle_i - \langle\hat{\Phi}, \hat{\Phi}\rangle_i\Bigr)\ \mathbf{:}_i = \\ &= -i\langle u_{i\,\zeta} \circ \psi \circ \hat{\Phi}, \hat{\mathrm{S}}_{0,\zeta}\hat{\Phi}\rangle_i = -i\langle u_{i\,\zeta} \circ \psi \circ \hat{\Phi}, u_{i\,\zeta} \circ \hat{\Phi}\rangle_i\ \hat{\mathrm{S}}_{0,\zeta} = \\ &= -i\langle\hat{\Phi}, \psi \circ \hat{\Phi}\rangle_i\ \hat{\mathrm{S}}_{0,\zeta} \quad , \end{aligned} \tag{E.3}$$

where we have used

$$\mathbf{:}\,\langle\hat{\Phi}, F(\hat{\Phi})\hat{\Phi}\rangle_i\,\mathbf{:}_i = \langle\hat{\Phi},\ \mathbf{:}F(\hat{\Phi})\mathbf{:}_i\,\hat{\Phi}\rangle_i \quad , \tag{E.4}$$

equation (8.62) and i-unitarity of $u_{i\,\zeta}$ operator. The solution of this differential equation together with initial conditions $\hat{\mathrm{S}}_{0,0} = \hat{\mathbb{1}}$ is

$$\hat{\mathrm{S}}_{0,\zeta} = \exp\Bigl(-i\zeta\langle\hat{\Phi}, \psi \circ \hat{\Phi}\rangle_i\Bigr) \quad . \tag{E.5}$$

For general ξ and $\zeta = 1$ the normal ordered form of the S-matrix has the form

$$\begin{aligned} \hat{\mathrm{S}}_{\xi,1} = \Bigl(\det\nolimits_{\boldsymbol{\mathcal{S}}} \mathrm{ch}(\xi\mathcal{X})\Bigr)^{-\frac{1}{4}} \mathbf{:}\exp\biggl(&\frac{1}{2}\bigl\langle\mathrm{th}(\xi\mathcal{X}) \circ \hat{\Phi}, \hat{\Phi}\bigr\rangle_i - \\ &- \frac{1}{2}\bigl\langle u_i \circ \hat{\Phi}, \mathrm{th}(\xi\mathcal{X}) \circ u_i \circ \hat{\Phi}\bigr\rangle_i + \bigl\langle\hat{\Phi}, \bigl(u_i^{-1} \circ \mathrm{ch}^{-1}(\xi\mathcal{X}) - \delta_{\boldsymbol{\mathcal{S}}}\bigr) \circ \hat{\Phi}\bigr\rangle_i\biggr)\mathbf{:}_i \quad . \end{aligned} \tag{E.6}$$

The derivative with respect of ξ is

$$\begin{aligned} \frac{d}{d\xi}\hat{\mathrm{S}}_{\xi,\zeta} = \mathbf{:}\biggl(&-\frac{1}{4}\,\mathrm{tr}_{\boldsymbol{\mathcal{S}}}\bigl(\mathcal{X} \circ \mathrm{th}(\xi\mathcal{X})\bigr) + \frac{1}{2}\Bigl\langle\frac{\mathcal{X}}{\mathrm{ch}^2(\xi\mathcal{X})} \circ \hat{\Phi},\ \hat{\Phi}\Bigr\rangle_i - \\ &- \frac{1}{2}\Bigl\langle u_i \circ \hat{\Phi},\ \frac{\mathcal{X}}{\mathrm{ch}^2(\xi\mathcal{X})} \circ u_i \circ \hat{\Phi}\Bigr\rangle_i - \Bigl\langle u_i \circ \hat{\Phi},\ \frac{\mathcal{X} \circ \mathrm{sh}(\xi\mathcal{X})}{\mathrm{ch}^2(\xi\mathcal{X})} \circ \hat{\Phi}\Bigr\rangle_i\biggr) \times \\ \times \Bigl(\det\nolimits_{\boldsymbol{\mathcal{S}}} \mathrm{ch}(\xi\mathcal{X})\Bigr)^{-\frac{1}{4}}\ \exp\biggl(&\frac{1}{2}\bigl\langle\mathrm{th}(\xi\mathcal{X}) \circ \hat{\Phi}, \hat{\Phi}\bigr\rangle_i - \\ &- \frac{1}{2}\bigl\langle u_i \circ \hat{\Phi}, \mathrm{th}(\xi\mathcal{X}) \circ u_i \circ \hat{\Phi}\bigr\rangle_i + \bigl\langle\hat{\Phi}, \bigl(u_i^{-1} \circ \mathrm{ch}^{-1}(\xi\mathcal{X}) - \delta_{\boldsymbol{\mathcal{S}}}\bigr) \circ \hat{\Phi}\bigr\rangle_i\biggr)\mathbf{:}_i = \end{aligned}$$

$$
\begin{aligned}
&= -\frac{1}{4}\,\mathrm{tr}_{\boldsymbol{\mathcal{S}}}\big(\mathcal{X}\circ\mathrm{th}(\xi\mathcal{X})\big)\;\hat{\mathrm{S}}_{\xi,1} + \hat{\mathrm{S}}_{\xi,1}\;\frac{1}{2}\Big\langle \frac{\mathcal{X}}{\mathrm{ch}^2(\xi\mathcal{X})}\circ\hat{\Phi},\,\hat{\Phi}\Big\rangle_i - \\
&\qquad -\frac{1}{2}\Big\langle u_i\circ\hat{\Phi},\,\frac{\mathcal{X}}{\mathrm{ch}^2(\xi\mathcal{X})}\circ u_i\circ\hat{\Phi}\Big\rangle_i\,\hat{\mathrm{S}}_{\xi,1} - \Big\langle u_i\circ\hat{\Phi},\,\hat{\mathrm{S}}_{\xi,1}\frac{\mathcal{X}\circ\mathrm{sh}(\xi\mathcal{X})}{\mathrm{ch}^2(\xi\mathcal{X})}\circ\hat{\Phi}\Big\rangle_i = \\
&= \hat{\mathrm{S}}_{\xi,1}\bigg(-\frac{1}{2}\,\mathrm{tr}_{\boldsymbol{\mathcal{S}}}\big(\mathcal{X}\circ\mathrm{th}(\xi\mathcal{X})\big) + \frac{1}{2}\Big\langle\frac{\mathcal{X}}{\mathrm{ch}^2(\xi\mathcal{X})}\circ\hat{\Phi},\,\hat{\Phi}\Big\rangle_i - \\
&\qquad -\frac{1}{2}\Big\langle\exp(-\xi\mathcal{X})\circ\hat{\Phi},\,\frac{\mathcal{X}\circ\exp(-\xi\mathcal{X})}{\mathrm{ch}^2(\xi\mathcal{X})}\circ\hat{\Phi}\Big\rangle_i - \Big\langle\exp(-\xi\mathcal{X})\circ\hat{\Phi},\,\frac{\mathcal{X}\circ\mathrm{sh}(\xi\mathcal{X})}{\mathrm{ch}^2(\xi\mathcal{X})}\circ\hat{\Phi}\Big\rangle_i\bigg) \quad .
\end{aligned}
\tag{E.7}
$$

Here we have used (E.4) and

$$
\begin{aligned}
&{:}\langle\hat{\Phi},\,F(\hat{\Phi})\,A\circ\hat{\Phi}\rangle_i{:}_i = \langle\hat{\Phi},A\circ\hat{\Phi}\rangle_i\;{:}F(\hat{\Phi}){:}_i \quad , \\
&{:}\langle A\circ\hat{\Phi},\,F(\hat{\Phi})\,\hat{\Phi}\rangle_i{:}_i = {:}F(\hat{\Phi}){:}_i\;\langle A\circ\hat{\Phi},\hat{\Phi}\rangle_i
\end{aligned}
\tag{E.8}
$$

for an i-antilinear operator A, the fact that $\mathcal{X}$ is i-antilinear, and again relation (8.62). Using trigonometric identities we can rearrange expression (E.7) to

$$
\begin{aligned}
&\hat{\mathrm{S}}_{\xi,1}\bigg(\frac{1}{2}\big\langle\mathcal{X}\circ\hat{\Phi},\hat{\Phi}\big\rangle_i - \frac{1}{2}\big\langle\hat{\Phi},\mathcal{X}\circ\hat{\Phi}\big\rangle_i - \frac{1}{4}\,\mathrm{tr}_{\boldsymbol{\mathcal{S}}}\big(\mathcal{X}\circ\mathrm{th}(\xi\mathcal{X})\big) + \\
&\qquad + \frac{1}{2}\big\langle\mathrm{th}(\xi\mathcal{X})\circ\hat{\Phi},\mathcal{X}\circ\hat{\Phi}\big\rangle_i - \frac{1}{2}\big\langle\hat{\Phi},\mathrm{th}(\xi\mathcal{X})\circ\mathcal{X}\circ\hat{\Phi}\big\rangle_i\bigg) = \\
&= \hat{\mathrm{S}}_{\xi,1}\frac{1}{2}\Big(\big\langle\mathcal{X}\circ\hat{\Phi},\hat{\Phi}\big\rangle_i - \big\langle\hat{\Phi},\mathcal{X}\circ\hat{\Phi}\big\rangle_i\Big) \quad ,
\end{aligned}
\tag{E.9}
$$

where we have used i-antilinearity of the operator $\mathcal{X}$ and equation (6.45). Integration with respect of ξ, using equation (E.5) as initial conditions, gives the desired result

$$
\hat{\mathrm{S}} = \hat{\mathrm{S}}_{1,1} = \exp\Big(-i\langle\hat{\Phi},\psi\circ\hat{\Phi}\rangle_i\Big)\;\exp\Big(\big\langle\mathcal{X}\circ\hat{\Phi},\hat{\Phi}\big\rangle_i - \big\langle\hat{\Phi},\mathcal{X}\circ\hat{\Phi}\big\rangle_i\Big) \quad . \tag{E.10}
$$

F Asymptotic expansion of the leading term in the heat kernel

Vector space

In a vector space V equipped with a positive nondegenerate quadratic form g a simple Gaussian integration gives

$$\begin{aligned}
&\frac{1}{(2\pi\nu\tau)^{\frac{d}{2}}}\int\limits_{X,Z\in V}\mathfrak{g}^{\frac{1}{2}}(X)\mathfrak{g}^{\frac{1}{2}}(Z)\varphi(X)\psi(Z)\exp\Big(-\frac{1}{2\nu\tau}(X-Z)\cdot g\cdot(X-Z)\Big)=\\
&\quad=\frac{1}{(2\pi\nu)^{\frac{d}{2}}}\int\limits_{X\in V}\mathfrak{g}^{\frac{1}{2}}(X)\varphi(X)\int\limits_{Y\in V}\mathfrak{g}^{\frac{1}{2}}(Y)\psi(X+\sqrt{\tau}Y)\exp\Big(-\frac{1}{2\nu}Y\cdot g\cdot Y\Big)=\\
&\quad=\frac{1}{(2\pi\nu)^{\frac{d}{2}}}\int\limits_{X\in V}\mathfrak{g}^{\frac{1}{2}}(X)\varphi(X)\sum_{k\in\mathbb{N}_0}\tau^{\frac{k}{2}}\big[\partial_{\boldsymbol{\alpha}_1}\dots\partial_{\boldsymbol{\alpha}_k}\psi\big](X)\times\\
&\qquad\qquad\times\frac{1}{k!}\int\limits_{Y\in V}\mathfrak{g}^{\frac{1}{2}}(Y)\,Y^{\boldsymbol{\alpha}_1}\dots Y^{\boldsymbol{\alpha}_k}\exp\Big(-\frac{1}{2\nu}Y\cdot g\cdot Y\Big)=\\
&\quad=\int\limits_{X\in V}\mathfrak{g}^{\frac{1}{2}}(X)\varphi(X)\sum_{m\in\mathbb{N}_0}\frac{(2m-1)!}{(2m)!}(\tau\nu)^m\ \big[(g^{-1\,\boldsymbol{\alpha}\boldsymbol{\beta}}\partial_{\boldsymbol{\alpha}}\partial_{\boldsymbol{\beta}})^m\psi\big](X)=\\
&\quad=\sum_{m\in\mathbb{N}_0}\frac{1}{m!}\Big(-\frac{\nu\tau}{2}\Big)^m\varphi\bullet\mathcal{L}^m\bullet\psi\quad.
\end{aligned}\tag{F.1}$$

Here φ, ψ are test functions, $\mathfrak{g}^{\frac{1}{2}}$ is the constant volume element of the metric g, ν is a number ($\mathrm{Re}\,\frac{1}{\nu}\geqslant 0$) and $\mathcal{L}^m$ represents a bi-distribution

$$\varphi\bullet\mathcal{L}^m\bullet\psi=\int\limits_V\mathfrak{g}^{\frac{1}{2}}\varphi\big[(g^{-1\,\boldsymbol{\alpha}\boldsymbol{\beta}}\partial_{\boldsymbol{\alpha}}\partial_{\boldsymbol{\beta}})^m\psi\big]=\int\limits_V\mathfrak{g}^{\frac{1}{2}}\psi\big[(g^{-1\,\boldsymbol{\alpha}\boldsymbol{\beta}}\partial_{\boldsymbol{\alpha}}\partial_{\boldsymbol{\beta}})^m\varphi\big]\quad.\tag{F.2}$$

It can be viewed as an "m-th" power of the Laplace quadratic form $\mathcal{L}$ associated with the metric g on the vector space V.

So we can write the asymptotic expansion for small τ as

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\mathfrak{g}^{\frac{1}{2}}(X)\mathfrak{g}^{\frac{1}{2}}(Z)\exp\Big(-\frac{1}{2\nu\tau}(X-Z)\cdot g\cdot(X-Z)\Big)=\sum_{m\in\mathbb{N}_0}\frac{1}{m!}\Big(-\frac{\tau\nu}{2}\Big)^m\mathcal{L}^m\quad.\tag{F.3}$$

Here we allowed the metric g to be Lorentzian — this case can be obtained by analytical continuation in g. The nature of g is given by a value of the phase factor n as discussed in appendix D and the extra factor n in (F.3) came from the Lorentzian convention for the volume element $\mathfrak{g}^{\frac{1}{2}}$.

In the case of the vector space the expression on the left side of eq. (F.3) is the heat kernel of the operator $\mathcal{L}$. Because the right side is formally the exponential we see that the expansion is exact. To say more about convergence it is necessary to specify functional spaces on which all the operators act and we will not do this here. But see e.g. [28] for some details.

Manifold without a boundary

Now we would like to find the expansion of the similar expression in a general manifold M without boundary. More precisely, we want to expand

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\Delta(x|z)\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\exp\Big(-\frac{1}{\nu\tau}\sigma(x|z)\Big) \tag{F.4}$$

for small τ.

We smooth both arguments with test functions φ, ψ and note that for a small τ the integration over x and z is dominated by a diagonal $x\approx z$ thanks to $\sigma(x|z)\approx 0$ for $x\approx z$. Therefore for a fixed x we can restrict integration over z to a normal neighborhood of x. In this neighborhood we can change variables $z\to Z$ with

$$z=\boldsymbol{u}_x(\sqrt{\tau}Z)\approx x+\sqrt{\tau}Z \quad , \tag{F.5}$$

where $\boldsymbol{u}_x(\epsilon Z)$ is a geodesic with an origin x and initial tangent vector Z (see (G.1)). This is the exact meaning of "adding" of a vector to a point as mentioned after equation (13.25).

The Jacobian associated with this change of variables is given by Van-Vleck Morette determinant (see (G.43))

$$(\boldsymbol{u}_x^{-1\star}\mathfrak{g}^{\frac{1}{2}})(\sqrt{\tau}Z)=\tau^{\frac{d}{2}}\mathfrak{g}^{\frac{1}{2}}(x)[Z]\,\Delta^{-1}(x|z) \quad , \tag{F.6}$$

where $\mathfrak{g}^{\frac{1}{2}}(x)[Z]$ is understood as a constant measure on the target vector space $\mathbf{T}_xM$ at vector Z. After a change of variables, using (G.16), expanding ψ and performing a Gaussian integration, we get

$$\begin{aligned}
&\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\int\limits_{x,z\in M}\Delta(x|z)\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\varphi(x)\psi(z)\exp\Big(-\frac{1}{\nu\tau}\sigma(x|z)\Big)=\\
&\quad=\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\int\limits_{x\in M}\mathfrak{g}^{\frac{1}{2}}(x)\varphi(x)\int\limits_{Z\in\mathbf{T}_xM}\mathfrak{g}^{\frac{1}{2}}(x)[Z]\times\\
&\qquad\qquad\times\Big(\sum_{k\in\mathbb{N}_0}\frac{1}{k!}\tau^{\frac{k}{2}}\psi_{k\,\boldsymbol{\alpha_1}\dots\boldsymbol{\alpha_k}}(x)\,Z^{\boldsymbol{\alpha_1}}\dots Z^{\boldsymbol{\alpha_k}}\Big)\,\exp\Big(-\frac{1}{\nu\tau}Z\cdot g(x)\cdot Z\Big)=\\
&\quad=\int\limits_M\mathfrak{g}^{\frac{1}{2}}\varphi\,\Big(\psi+\frac{\nu\tau}{2}\,g^{-1\,\boldsymbol{\alpha\beta}}\psi_{2\,\boldsymbol{\alpha\beta}}+\mathcal{O}(\tau^2)\Big)\quad .
\end{aligned} \tag{F.7}$$

Using (G.27) we have $\psi_2=\nabla\mathrm{d}\psi$, so we get

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\Delta(x|z)\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\exp\Big(-\frac{1}{\nu\tau}\sigma(x|z)\Big)=\mathcal{G}-\frac{\nu\tau}{2}\mathcal{L}+\mathcal{O}(\tau^2) \quad . \tag{F.8}$$

Half line

Next we will investigate the simplest case of the manifold with the boundary — half line $\mathbb{R}^+$. We assume it is equipped with a special coordinate η which selects a measure and derivative

$$\mu=d\eta \quad , \quad \mathcal{M}=\mu\delta \quad , \quad \partial=\frac{\partial}{\partial\eta} \quad . \tag{F.9}$$

We define bi-distributions of the m-th derivative

$$\omega \bullet \overrightarrow{\partial}^{\langle m\rangle} \bullet \varphi = \omega \bullet (\partial^m \varphi) = \int_{\mathbb{R}^+} \omega(\partial^m \varphi) \quad , \quad \overleftarrow{\partial}^{\langle m\rangle} = \overrightarrow{\partial}^{\langle m\rangle\top} \quad , \tag{F.10}$$

and

$$\overrightarrow{\partial} = \overrightarrow{\partial}^{\langle 1\rangle} \quad , \quad \overleftarrow{\partial} = \overleftarrow{\partial}^{\langle 1\rangle} \quad . \tag{F.11}$$

We can define also a boundary delta bi-distribution $\mathcal{D}$ as

$$\varphi \bullet \mathcal{D} \bullet \psi = (\varphi\psi)|_{\text{boundary}} \quad . \tag{F.12}$$

Integration by parts can be expressed by the relation

$$\begin{gathered} \overleftarrow{\partial} \bullet \mathcal{M} + \mathcal{M} \bullet \overrightarrow{\partial} = -\mathcal{D} \quad , \\ \overleftarrow{\partial}^{\langle m+1\rangle} \bullet \mathcal{M} + (-1)^m \mathcal{M} \bullet \overrightarrow{\partial}^{\langle m+1\rangle} = -\sum_{k=0,\ldots,m} \overleftarrow{\partial}^{\langle m-k\rangle} \bullet \mathcal{D} \bullet \overrightarrow{\partial}^{\langle k\rangle} \quad . \end{gathered} \tag{F.13}$$

Next we define quadratic forms of powers of the Laplace operator

$$\begin{gathered} \overrightarrow{\mathcal{L}} = -\mathcal{M} \bullet \overrightarrow{\partial}^{\langle 2\rangle} \quad , \quad \overrightarrow{\mathcal{L}}^{\langle m\rangle} = (-1)^m \mathcal{M} \bullet \overrightarrow{\partial}^{\langle 2m\rangle} \quad , \\ \overleftarrow{\mathcal{L}} = -\overleftarrow{\partial}\langle 2\rangle \bullet \mathcal{M} \quad , \quad \overleftarrow{\mathcal{L}}^{\langle m\rangle} = (-1)^m \overleftarrow{\partial}^{\langle 2m\rangle} \bullet \mathcal{M} \quad , \\ \overleftrightarrow{\mathcal{L}} = \frac{1}{2}\big(\overleftarrow{\mathcal{L}} + \overrightarrow{\mathcal{L}}\big) \quad , \quad \overleftrightarrow{\mathcal{L}}^{\langle m\rangle} = \frac{1}{2}\big(\overleftarrow{\mathcal{L}}^{\langle m\rangle} + \overrightarrow{\mathcal{L}}^{\langle m\rangle}\big) \quad , \\ \mathcal{L} = \overleftarrow{\partial} \bullet \mathcal{M} \bullet \overrightarrow{\partial} \quad . \end{gathered} \tag{F.14}$$

The symplectic form on the boundary is

$$\partial\mathcal{L} = \overrightarrow{\mathcal{L}} - \overleftarrow{\mathcal{L}} = -\overleftarrow{\partial} \bullet \mathcal{D} + \mathcal{D} \bullet \overrightarrow{\partial} \quad . \tag{F.15}$$

It is straightforward to check that

$$\overrightarrow{\mathcal{L}}^{\langle m\rangle} - \overleftarrow{\mathcal{L}}^{\langle m\rangle} = (-1)^m \sum_{\substack{k,l\in\mathbb{N}_0 \\ k+l+1=2m}} \overleftarrow{\partial}^{\langle k\rangle} \bullet \mathcal{D} \bullet \overrightarrow{\partial}^{\langle l\rangle} \quad . \tag{F.16}$$

Now we prove the following expansion for small τ

$$\begin{aligned} &\frac{1}{\sqrt{2\pi\tau\nu}} \exp\Big(-\frac{1}{2\tau\nu}(\xi-\zeta)^2\Big)\, \mu(\xi)\mu(\zeta) = \\ &= \sum_{m\in\mathbb{N}_0} \frac{1}{\Gamma\big(\frac{m}{2}+1\big)} \Big(\frac{\tau\nu}{2}\Big)^{\frac{m}{2}} \frac{1}{2}\Big(\overleftarrow{\partial}^{\langle m\rangle} \bullet \mathcal{M} + \mathcal{M} \bullet \overrightarrow{\partial}^{\langle m\rangle}\Big) = \\ &= \sum_{m\in\mathbb{N}_0} \frac{(-1)^m}{m!} \Big(\frac{\tau\nu}{2}\Big)^m \overleftrightarrow{\mathcal{L}}^{\langle m\rangle} + \\ &\quad + \sum_{m\in\mathbb{N}_0} \frac{(-1)^{m+1}}{\Gamma\big(m+\frac{3}{2}\big)} \Big(\frac{\tau\nu}{2}\Big)^{m+\frac{1}{2}} \frac{1}{2} \sum_{\substack{k,l\in\mathbb{N}_0 \\ k+l=2m}} (-1)^{\frac{k-l}{2}} \overleftarrow{\partial}^{\langle k\rangle} \bullet \mathcal{D} \bullet \overrightarrow{\partial}^{\langle l\rangle} \quad . \end{aligned} \tag{F.17}$$

Here ν is a complex number such that $\frac{1}{\nu}$ has non-negative real part. Strictly speaking, the following derivation needs a positive real part; but for an imaginary value of ν the relation can be obtained by limiting procedure. Because only a combination the $\tau\nu$ appears in the equation, we drop ν in the following derivation — it can be easily restored by inspection of the τ-dependence.

Clearly, the second equality follows from integration by parts (F.13). To prove the first one we smooth it with test functions φ and ψ and get

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi\tau}}\int\limits_{\xi,\zeta\in\mathbb{R}^+}\exp\Big(-\frac{1}{2\tau}(\xi-\zeta)^2\Big)\;\varphi(\xi)\psi(\zeta)\;\mu(\xi)\mu(\zeta)=\\
&\quad=\frac{1}{\sqrt{2\pi\tau}}\int\limits_{\xi\in\langle 0,\epsilon\rangle}d\xi\int\limits_{\zeta\in\mathbb{R}^+}d\zeta\,\varphi(\xi)\psi(\zeta)\exp\Big(-\frac{1}{2\tau}(\xi-\zeta)^2\Big)+\\
&\quad+\frac{1}{\sqrt{2\pi\tau}}\int\limits_{\xi\in\langle\epsilon,\infty\rangle}d\xi\int\limits_{\zeta\in\mathbb{R}^+}d\zeta\,\varphi(\xi)\psi(\zeta)\exp\Big(-\frac{1}{2\tau}(\xi-\zeta)^2\Big)
\end{aligned}\tag{F.18}$$

for some $\epsilon\in\mathbb{R}^+$.

For a small τ the exponential suppresses any contribution except from $\xi\approx\zeta$. Therefore for small ϵ only small values of ξ and ζ contribute to the first term of the last equation. We can rescale variables by factor $\sqrt{\tau}$ and expand φ and ψ at zero and obtain

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi\tau}}\int\limits_{\xi\in\langle 0,\epsilon\rangle}d\xi\int\limits_{\zeta\in\mathbb{R}^+}d\zeta\,\varphi(\xi)\psi(\zeta)\exp\Big(-\frac{1}{2\tau}(\xi-\zeta)^2\Big)=\\
&\quad=\frac{\tau}{\sqrt{2\pi\tau}}\int\limits_{\xi\in\langle 0,\frac{\epsilon}{\sqrt{\tau}}\rangle}d\xi\,\varphi(\sqrt{\tau}\xi)\sum_{l\in\mathbb{N}_0}\tau^{\frac{l}{2}}\psi^{\langle l\rangle}(0)\,\frac{1}{l!}\int\limits_{l\in\mathbb{R}^+}d\zeta\,\zeta^l\exp\Big(-\frac{1}{2}(\xi-\zeta)^2\Big)=\\
&\quad=\frac{1}{\sqrt{2\pi}}\sum_{k,l\in\mathbb{N}_0}\tau^{\frac{k+l+1}{2}}\;\varphi^{\langle k\rangle}(0)\;\psi^{\langle l\rangle}(0)\;\frac{1}{k!}\int\limits_{\xi\in\langle 0,\frac{\epsilon}{\sqrt{\tau}}\rangle}d\xi\,\xi^k\mathrm{R}_{l+1}(\xi)\quad,
\end{aligned}\tag{F.19}$$

where we have used the definition of special functions R_l (H.1). Properties of these special functions are summarized in appendix H. Using equation (H.17) the last expression gives

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi}}\sum_{k,l\in\mathbb{N}_0}\tau^{\frac{k+l+1}{2}}\;\varphi^{\langle k\rangle}(0)\;\psi^{\langle l\rangle}(0)\times\\
&\quad\times\Bigg(\;(-1)^{l+1}\mathrm{R}_{k+l+2}(0)+\\
&\qquad+\frac{\sqrt{2\pi}}{l!k!}\sum_{\substack{m\in\mathbb{N}_0\\2m\leqslant l}}\frac{(2m-1)!!}{k+l-2m+1}\binom{l}{2m}\Big(\frac{\epsilon}{\sqrt{\tau}}\Big)^{k+l-2m+1}+\\
&\qquad+(-1)^l\sum_{m=0,\dots,k}\frac{1}{m!}\Big(\frac{\epsilon}{\sqrt{\tau}}\Big)^m\;\mathrm{R}_{k+l-m+2}\big(-\tfrac{\epsilon}{\sqrt{\tau}}\big)\Bigg)=\\
&=\sum_{m\in\mathbb{N}_0}\tau^{\frac{m+1}{2}}\Big(2^{\frac{m+1}{2}}\Gamma\big(\frac{m+1}{2}+1\big)\Big)^{-1}\frac{1}{2}\sum_{l=0,\dots,m}(-1)^{l+1}\,\varphi^{\langle m-l\rangle}(0)\;\psi^{\langle l\rangle}(0)+\\
&\quad+\sum_{m\in\mathbb{N}_0}\frac{\tau^m}{(2m)!!}\sum_{k,l\in\mathbb{N}_0}\frac{\epsilon^{k+l+1}}{k!\,l!\,(k+l+1)}\,\varphi^{\langle k\rangle}(0)\;\psi^{\langle l+2m\rangle}(0)+\\
&\quad+\exp\Big(-\frac{1}{2}\frac{\epsilon^2}{\tau}\Big)\;\mathcal{O}(\tau)=
\end{aligned}$$

$$
\begin{aligned}
&= -\sum_{m\in\mathbb{N}} \frac{\tau^m}{(2m)!!}\frac{1}{2} \sum_{l=0,\dots,2m-1} (-1)^l\, \varphi^{\langle 2m-l-1\rangle}(0)\, \psi^{\langle l\rangle}(0) + \\
&\quad + \sum_{m\in\mathbb{N}_0} \frac{\tau^{m+\frac{1}{2}}}{(2m+1)!!}\frac{-1}{\sqrt{2\pi}} \sum_{l=0,\dots,2m} (-1)^l\, \varphi^{\langle 2m-l\rangle}(0)\, \psi^{\langle l\rangle}(0) + \\
&\quad + \sum_{m\in\mathbb{N}_0} \frac{\tau^m}{(2m)!!} \sum_{k,l\in\mathbb{N}_0} \frac{\epsilon^{k+l+1}}{k!\,l!\,(k+l+1)}\, \varphi^{\langle k\rangle}(0)\, \psi^{\langle l+2m\rangle}(0) + \\
&\quad + \exp\Big(-\frac{1}{2}\frac{\epsilon^2}{\tau}\Big)\, \mathcal{O}(\tau) \quad .
\end{aligned}
\tag{F.20}
$$

Here we have used relations (H.10) and (H.14).

In the second term of the expression (F.18) we change variables $\zeta \to \eta = \frac{1}{\sqrt{\tau}}(\xi - \zeta)$ using again the fact that only the contribution from $\zeta \approx \xi$ is not suppressed by the exponential. Next we expand ψ around $\eta = 0$ and obtain

$$
\begin{aligned}
&\frac{1}{\sqrt{2\pi\tau}} \int\limits_{\xi\in\langle\epsilon,\infty\rangle} d\xi \int\limits_{\zeta\in\mathbb{R}+} d\zeta\, \varphi(\xi)\psi(\zeta) \exp\Big(-\frac{1}{2\tau}(\xi-\zeta)^2\Big) = \\
&= \frac{1}{\sqrt{2\pi\tau}} \int\limits_{\xi\in\langle\epsilon,\infty\rangle} d\xi\, \varphi(\xi) \sum_{k\in\mathbb{N}_0} \psi^{\langle k\rangle}(\xi)\, \tau^{\frac{k}{2}} \times \\
&\quad \times \Bigg(\frac{1}{k!} \int\limits_{\eta\in\mathbb{R}} d\eta\, \eta^k \exp\Big(-\frac{1}{2}\eta^2\Big) - \frac{1}{k!} \int\limits_{\eta\in\langle-\infty,\frac{\xi}{\sqrt{\tau}}\rangle} d\eta\, \eta^k \exp\Big(-\frac{1}{2}\eta^2\Big)\Bigg) = \\
&= \sum_{m=\mathbb{N}_0} \frac{\tau^m}{(2m)!!} \int\limits_{\xi\in\langle\epsilon,\infty\rangle} d\xi\, \varphi(\xi)\psi^{\langle 2m\rangle}(\xi) - \\
&\quad - \frac{1}{\sqrt{2\pi\tau}} \sum_{k\in\mathbb{N}_0} \tau^{\frac{k}{2}} \sum_{l=0,\dots,k} \frac{(-1)^k}{l!} \int\limits_{\langle\epsilon,\infty\rangle} d\xi \Big(\frac{\xi}{\sqrt{\tau}}\Big)^l\, \mathrm{R}_{k-l+1}\big(-\tfrac{\xi}{\sqrt{\tau}}\big)\, \varphi(\xi)\, \psi^{\langle k\rangle}(\xi) = \\
&= \sum_{m=\mathbb{N}_0} \frac{\tau^m}{(2m)!!} \int\limits_{\xi\in\mathbb{R}+} d\xi\, \varphi(\xi)\psi^{\langle 2m\rangle}(\xi) - \sum_{m=\mathbb{N}_0} \frac{\tau^m}{(2m)!!} \int\limits_{\xi\in\langle 0,\epsilon\rangle} d\xi\, \varphi(\xi)\psi^{\langle 2m\rangle}(\xi) + \\
&\quad + \exp\Big(-\frac{1}{2}\frac{\epsilon^2}{\tau}\Big)\, \mathcal{O}(\tau) \quad .
\end{aligned}
\tag{F.21}
$$

Here we used (H.15), (H.11), (H.16) and (H.14). For small ϵ we can expand φ and $\psi^{\langle 2m\rangle}$ about zero in the second term of the last expression. Performing also an integration by parts in the first term transforms the last expression to

$$
\begin{aligned}
&\sum_{m\in\mathbb{N}_0} \frac{\tau^m}{(2m)!!}\frac{1}{2} \int\limits_{\xi\in\mathbb{R}+} d\xi \Big(\varphi^{\langle 2m\rangle}(\xi)\psi(\xi) + \varphi(\xi)\psi^{\langle 2m\rangle}(\xi)\Big) + \\
&\quad + \sum_{m\in\mathbb{N}} \frac{\tau^m}{(2m)!!}\frac{1}{2} \sum_{l=0,\dots,2m-1} (-1)^l\, \varphi^{\langle 2m-l-1\rangle}(0)\, \psi^{\langle l\rangle}(0) - \\
&\quad - \sum_{m\in\mathbb{N}_0} \frac{\tau^m}{(2m)!!} \sum_{k,l\in\mathbb{N}_0} \frac{\epsilon^{k+l+1}}{k!\,l!\,(k+l+1)}\, \varphi^{\langle k\rangle}(0)\, \psi^{\langle l+2m\rangle}(0) + \\
&\quad + \exp\Big(-\frac{1}{2}\frac{\epsilon^2}{\tau}\Big)\mathcal{O}(\tau) \quad .
\end{aligned}
\tag{F.22}
$$

Substituting equations (F.20) and (F.22) to equation (F.18) and ignoring exponentially suppressed terms $\exp\bigl(-\frac{1}{2}\frac{\epsilon^2}{\tau}\bigr)\mathcal{O}(\tau)$ we obtain the desired relation (F.17).

Next we will prove another expansion for small τ

$$\begin{aligned}\frac{1}{\sqrt{2\pi\nu\tau}}\,\omega\Bigl(\frac{\xi\zeta}{\xi+\zeta}\Bigr)\,\exp\Bigl(-\frac{1}{2\nu\tau}(\xi+\zeta)^2\Bigr)\,\mu(\xi)\mu(\zeta) =\\ =\sum_{n\in\mathbb{N}_0}\Bigl(\frac{\tau\nu}{2}\Bigr)^{\frac{n+1}{2}}\frac{1}{\Gamma\bigl(\frac{n+1}{2}\bigr)}\sum_{\substack{m,k,l\in\mathbb{N}_0\\ k+l+m=n}}\frac{\omega^{\langle m\rangle}(0)}{n+m+1}\frac{\binom{m+k}{k}\binom{m+l}{l}}{\binom{n+m}{m}}\,\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}\quad,\end{aligned}\tag{F.23}$$

where ω is some smooth function. As a corollary for $\omega=1$ we get

$$\begin{aligned}\frac{1}{\sqrt{2\pi\nu\tau}}\,\exp\Bigl(-\frac{1}{2\nu\tau}(\xi+\zeta)^2\Bigr)\,\mu(\xi)\mu(\zeta) =\\ =\sum_{k,l\in\mathbb{N}_0}\frac{1}{\Gamma\bigl(\frac{k+l+1}{2}+1\bigr)}\Bigl(\frac{\tau\nu}{2}\Bigr)^{\frac{k+l+1}{2}}\frac{1}{2}\,\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle} =\\ =\sum_{m\in\mathbb{N}}\frac{1}{m!}\Bigl(\frac{\tau\nu}{2}\Bigr)^{m}\frac{1}{2}\sum_{\substack{k,l\in\mathbb{N}_0\\ k+l+1=2m}}\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}+\\ +\sum_{m\in\mathbb{N}_0}\frac{1}{\Gamma\bigl(m+\frac{3}{2}\bigr)}\Bigl(\frac{\tau\nu}{2}\Bigr)^{m+\frac{1}{2}}\frac{1}{2}\sum_{\substack{k,l\in\mathbb{N}_0\\ k+l=2m}}\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}\quad.\end{aligned}\tag{F.24}$$

As before, we drop the factor ν in the proof because it can easily be restored from the τ dependence. Again, we smooth the relation with test functions φ and ψ. Thanks to the exponential suppression, only small values of ξ and ζ contributes to the integrals. Therefore we can rescale ξ and ζ by $\sqrt{\tau}$, expand φ, ψ, and ω about zero, and get

$$\begin{aligned}\frac{1}{2\pi\tau}\int\limits_{\xi,\zeta\in\mathbb{R}^+}\varphi(\xi)\psi(\zeta)\,\omega\Bigl(\frac{\xi\zeta}{\xi+\zeta}\Bigr)\,\exp\Bigl(-\frac{1}{2\tau}(\xi+\zeta)^2\Bigr)\,d\xi\,d\zeta =\\ =\frac{1}{2\pi\tau}\sum_{n\in\mathbb{N}_0}\tau^{\frac{n}{2}+1}\sum_{\substack{k,l,m\in\mathbb{N}_0\\ k+l+m=n}}\frac{n!}{k!\,l!\,m!}\,\varphi^{\langle k\rangle}(0)\,\psi^{\langle l\rangle}(0)\,\omega^{\langle m\rangle}(0)\times\\ \times\frac{1}{n!}\int\limits_{\xi,\zeta\mathbb{R}^+}d\xi\,d\zeta\,\frac{\xi^{m+k}\zeta^{m+l}}{(\xi+\zeta)^m}\,\exp\Bigl(-\frac{1}{2}(\xi+\zeta)^2\Bigr) =\\ =\sum_{n\in\mathbb{N}_0}\Bigl(\frac{\tau}{2}\Bigr)^{\frac{n+1}{2}}\frac{1}{\Gamma\bigl(\frac{n+1}{2}\bigr)}\sum_{\substack{k,l,m\in\mathbb{N}_0\\ k+l+m=n}}\frac{\omega^{\langle m\rangle}(0)}{n+m+1}\frac{\binom{m+k}{k}\binom{m+l}{l}}{\binom{n+m}{m}}\,\varphi^{\langle k\rangle}(0)\,\psi^{\langle l\rangle}(0)\quad,\end{aligned}\tag{F.25}$$

what proves the relation (F.23). Here we have used the integral (H.18).

Manifold with boundary — no reflection contribution

Now we find an expansion of the contribution to the short time amplitude from the trajectories near the geodesic without reflection in the domain Ω with boundary $\partial\Omega$. We will prove for small τ

$$\begin{aligned}\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\,\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z)\exp\Bigl(-\frac{1}{\nu\tau}\sigma(x|z)\Bigr) =\\ =\mathcal{G}+\sqrt{\tau}\Bigl(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\Bigr)\mathcal{Q}-\tau\frac{\nu}{2}\overleftrightarrow{\mathcal{L}}+\mathcal{O}(\tau^{\frac{3}{2}})\quad.\end{aligned}\tag{F.26}$$

As usual, we will be proving a smoothed version of this relation — we multiply the expression by test functions $\varphi(x)$ and $\psi(z)$, and integrate over x and z. Thanks to the exponential suppression the only non-trivial contribution is from $x \approx z$. Therefore it is sufficient to prove the relation locally. Clearly, for φ and ψ with support inside of interior of the domain Ω the boundary does not have any influence and the relation reduces to the case without boundary. Therefore we will investigate only the case when φ and ψ are localized near the boundary. Thanks to locality we can also, without losing generality, assume that the test functions are localized on the neighborhood $U \subset \Omega$ of the boundary with topology $\mathbb{R} \times \partial\Omega$ on which the geodesics normal to the boundary do not cross. In such a neighborhood we can use the method described in appendix G and change the integration over a neighborhood to integration over the boundary $\partial\Omega$ and geodesic distance from the boundary (see (G.60))

$$\begin{aligned} x \to \hat{x}, \xi \quad &, \quad x = \hat{\boldsymbol{w}}(\hat{x}, \xi) \quad , \\ y \to \hat{y}, \zeta \quad &, \quad y = \hat{\boldsymbol{w}}(\hat{y}, \zeta) \quad . \end{aligned} \tag{F.27}$$

The Jacobian associated with this change of variables is

$$\mathfrak{g}^{\frac{1}{2}}(\hat{x}) = d\xi\, \hat{\mathfrak{q}}^{\frac{1}{2}}(\hat{x}, \xi) = d\xi\, \hat{\jmath}(\hat{x}, \xi)\, \mathfrak{q}^{\frac{1}{2}} \quad . \tag{F.28}$$

Here we use the convention (G.62) — we denote the spacetime dependent object $A(x)$ in variables $\hat{x}$, ξ and tensor indices moved to the boundary as $\widehat{A}(\hat{x}, \xi)$. Changing variables we get

$$\begin{aligned} &\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{x,z\in\Omega} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z) \exp\Big(-\frac{1}{\nu\tau}\sigma(x|z)\Big)\varphi(x)\psi(z) = \\ &= \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{\substack{\hat{x},\hat{z}\in\partial\Omega \\ \xi,\zeta\in\mathbb{R}^+}} d\xi\, d\zeta\;\, \hat{\jmath}(\hat{x},\xi)\mathfrak{q}^{\frac{1}{2}}(\hat{x})\, \hat{\jmath}(\hat{z},\zeta)\mathfrak{q}^{\frac{1}{2}}(z)\, \widehat{\Delta}(\hat{x},\xi|\hat{z},\zeta)\times \\ &\qquad\qquad\qquad \times \exp\Big(-\frac{1}{\nu\tau}\hat{\sigma}(\hat{x},\xi|\hat{z},\zeta)\Big)\; \hat{\varphi}(\hat{x},\xi)\hat{\psi}(\hat{z},\zeta) = \\ &= \int\limits_{\hat{x}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\hat{x})\, \frac{n}{(2\pi\nu\tau)^{\frac{1}{2}}} \int\limits_{\xi,\zeta\in\mathbb{R}^+} d\xi\, d\zeta\;\, \hat{\varphi}(\hat{x},\xi)\times \\ &\quad \times \frac{1}{(2\pi\nu\tau)^{\frac{d}{2}}} \int\limits_{\hat{z}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\hat{z})\; \Delta(\hat{x}|\hat{z})\, \hat{\psi}(\hat{z},\zeta)\;\, \exp\Big(-\frac{1}{\nu\tau}\hat{\sigma}(\hat{x},\xi|\hat{z},\zeta) + \hat{l}(\hat{x},\xi|\hat{z},\zeta)\Big) \quad . \end{aligned} \tag{F.29}$$

Here we have defined

$$\hat{l}(\hat{x},\xi|\hat{z},\zeta) = \ln\bigg(\hat{\jmath}(\hat{x},\xi)\frac{\widehat{\Delta}(\hat{x},\xi|\hat{z},\zeta)}{\Delta(\hat{x}|\hat{z})}\hat{\jmath}(\hat{z},\zeta)\bigg) \quad , \tag{F.30}$$

where $\Delta(\hat{x}|\hat{z})$ is the Van-Vleck Morette determinant of the metric q in the boundary manifold.

Exponential suppression ensures again that the only contributions comes from $\hat{x} \approx \hat{z}$. So we can change variables

$$\begin{aligned} \hat{x} \to \hat{y} = \hat{x} \quad &, \\ \hat{z} \to Y \in \mathbf{T}_{\hat{y}}\partial\Omega \quad , \quad &\hat{z} = \boldsymbol{v}_{\hat{y}}(\sqrt{\tau}Y) \quad , \end{aligned} \tag{F.31}$$

with the exponential map $\boldsymbol{v}_{\hat{y}}(Y)$ defined as in (G.1) but on the boundary manifold. The Jacobian for this change of variables is given by an equation similar to (G.43), only with the Van-Vleck Morette determinant $\Delta(\hat{x}, \hat{y})$ defined using the metric q on the boundary manifold. We use covariant expansions

$$\widehat{\sigma}(\widehat{y},\xi|\widehat{y},\sqrt{\tau}Y,\zeta) = \tau n^2 \frac{1}{2}(\xi-\zeta)^2 + \sum_{k=2,3,\dots} \tau^{\frac{k}{2}} \frac{1}{k!}\, \widehat{\sigma}_{0,k\,\boldsymbol{\mu}_1\dots\boldsymbol{\mu}_k}(\widehat{y};\xi,\zeta)\, Y^{\boldsymbol{\mu}_1}\dots Y^{\boldsymbol{\mu}_k} \quad , \tag{F.32}$$

$$\widehat{l}\,(\widehat{y},\xi|\widehat{y},\sqrt{\tau}Y,\zeta) = \sum_{k=\mathbb{N}_0} \tau^{\frac{k}{2}} \frac{1}{k!}\, \widehat{l}_{0,k\,\boldsymbol{\mu}_1\dots\boldsymbol{\mu}_k}(\widehat{y};\xi,\zeta)\, Y^{\boldsymbol{\mu}_1}\dots Y^{\boldsymbol{\mu}_k} \quad , \tag{F.33}$$

$$\widehat{\psi}(\widehat{y},\sqrt{\tau}Y,\zeta) = \sum_{k=\mathbb{N}_0} \tau^{\frac{k}{2}} \frac{1}{k!}\, \widehat{\psi}_{k\,\boldsymbol{\mu}_1\dots\boldsymbol{\mu}_k}(\widehat{y};\zeta)\, Y^{\boldsymbol{\mu}_1}\dots Y^{\boldsymbol{\mu}_k} \quad , \tag{F.34}$$

with coefficients given by expressions (G.99–G.103), (G.104–G.106), and (G.27). Expanding the exponential, gathering all terms up to order $\mathcal{O}(\tau)$, and performing a Gaussian integration over Y lead to

$$\int\limits_{\widehat{y}\in\partial\Omega} \frac{n}{(2\pi\nu\tau)^{\frac{1}{2}}} \int\limits_{\xi,\zeta\in\mathbb{R}^+} d\xi\, d\zeta\ \exp\Big(-\frac{n^2}{2\nu\tau}(\zeta-\xi)^2\Big)\, \tilde{j}(\widehat{y};\xi,\zeta)\, \Big(\omega_0(\widehat{y};\xi,\zeta)+\tau\omega_1(\widehat{y};\xi,\zeta)+\mathcal{O}(\tau^2)\Big) \tag{F.35}$$

with

$$\begin{aligned} \tilde{j}(\widehat{y};\xi\zeta) &= \widehat{j}\,(\widehat{y},\xi)\, \widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\, \widehat{j}\,(\widehat{y},\zeta)\, \mathfrak{q}^{\frac{1}{2}}(\widehat{y})\, \Big(\mathrm{Det}_{\shortparallel}\, \widehat{\sigma}_{0,2}(\widehat{y};\xi,\zeta)\Big)^{-\frac{1}{2}} = \\ &= \Big(\widehat{j}\,(\widehat{y},\xi)\, \widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\, \widehat{j}\,(\widehat{y},\zeta)\Big)^{\frac{1}{2}} \quad , \end{aligned} \tag{F.36}$$

$$\omega_0(\widehat{y};\xi,\zeta) = \widehat{\varphi}(\widehat{y},\xi)\, \widehat{\psi}(\widehat{y},\zeta) \quad , \tag{F.37}$$

$$\begin{aligned} \omega_1(\widehat{y};\xi,\zeta) = \nu\, \widehat{\varphi}(\widehat{y},\xi)\, \widehat{\psi}(\widehat{y},\zeta)\, \Big(&-\frac{1}{8}\widehat{\sigma}_{0,4\,\boldsymbol{\mu\nu\kappa\lambda}}\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2} \widehat{\sigma}^{-1\,\boldsymbol{\kappa\lambda}}_{0,2} + \frac{1}{2}\widehat{l}_{0,2\,\boldsymbol{\mu\nu}}\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2} + \\ &+ \frac{1}{8}\widehat{\sigma}_{0,3\,\boldsymbol{\mu\nu\alpha}}\, \widehat{\sigma}_{0,3\,\boldsymbol{\kappa\lambda\beta}}\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2} \widehat{\sigma}^{-1\,\boldsymbol{\alpha\beta}}_{0,2} \widehat{\sigma}^{-1\,\boldsymbol{\kappa\lambda}}_{0,2} - \frac{1}{2}\widehat{l}_{0,1\,\boldsymbol{\mu}}\, \widehat{\sigma}_{0,3\,\boldsymbol{\kappa\lambda\nu}}\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2} \widehat{\sigma}^{-1\,\boldsymbol{\kappa\lambda}}_{0,2} + \\ &+ \frac{1}{12}\widehat{\sigma}_{0,3\,\boldsymbol{\mu\kappa\alpha}}\, \widehat{\sigma}_{0,3\,\boldsymbol{\nu\lambda\beta}}\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2} \widehat{\sigma}^{-1\,\boldsymbol{\alpha\beta}}_{0,2} \widehat{\sigma}^{-1\,\boldsymbol{\kappa\lambda}}_{0,2} + \frac{1}{2}\widehat{l}_{0,1\,\boldsymbol{\mu}}\, \widehat{l}_{0,1\,\boldsymbol{\nu}}\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2}\Big)(\widehat{y};\xi,\zeta) + \\ &+ \nu\, \widehat{\varphi}(\widehat{y};\xi)\, \widehat{\psi}_{1\,\boldsymbol{\mu}}(\widehat{y};\zeta)\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2}\, \Big(\widehat{l}_{0,1\,\boldsymbol{\nu}} - \frac{1}{2}\widehat{\sigma}_{0,3\,\boldsymbol{\kappa\lambda\nu}}\, \widehat{\sigma}^{-1\,\boldsymbol{\kappa\lambda}}_{0,2}\Big)(\widehat{y};\xi,\zeta) + \\ &+ \nu\, \widehat{\varphi}(\widehat{y};\xi)\, \widehat{\psi}_{2\,\boldsymbol{\mu\nu}}(\widehat{y};\zeta)\, \widehat{\sigma}^{-1\,\boldsymbol{\mu\nu}}_{0,2}(\widehat{y};\xi,\zeta) \quad . \end{aligned} \tag{F.38}$$

The equality in (F.36) is proved in (G.76). Applying the expansion in (F.17) in (F.35) and using (F.6) we get

$$\begin{aligned} &\int\limits_{y\in\Omega} \mathfrak{g}^{\frac{1}{2}}(y)\, \varphi(y)\, \psi(y) + \\ &\quad + \sqrt{\tau}\Big(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\Big) \int\limits_{\widehat{y}\in\Omega} \mathfrak{q}^{\frac{1}{2}}(\widehat{y})\, \varphi(\widehat{y})\, \psi(\widehat{y}) + \\ &\quad + \tau \int\limits_{\substack{\widehat{y}\in\partial\Omega \\ \eta\in\mathbb{R}^+}} d\eta\, \mathfrak{q}^{\frac{1}{2}}(\widehat{y})\, \widehat{j}\,(\widehat{y};\eta)\, \Big(\frac{\nu}{4n^2}\, \tilde{j}^{-1}\big(\tilde{j}\omega_0\big)^{\mathbf{l}'\,\mathbf{l}'} + \frac{\nu}{4n^2}\, \tilde{j}^{-1}\big(\tilde{j}\omega_0\big)^{\mathbf{r}'\,\mathbf{r}'} + \omega_1\Big)(\widehat{y};\eta,\eta) + \\ &\quad + \mathcal{O}(\tau^{\frac{3}{2}}) \quad , \end{aligned} \tag{F.39}$$

where $f^{\mathbf{l}'}(\xi,\zeta)$ (or $f^{\mathbf{r}'}(\xi,\zeta)$) means derivative of a function f with respect of the left (or right) argument.

We see that we have proved already the desired expansion up to order $\sqrt{\tau}$. Now we proceed to prove it in the order τ. We split the integrand of the last term to pieces and compute each of them. First we note that (see (G.101))

$$[\hat{\sigma}_{0,2}] = \hat{q} \quad , \tag{F.40}$$

where by a coincidence limit of a function $f(\xi,\zeta)$ depending on two real parameters we mean $[f](\eta) = f(\eta,\eta)$. Using (G.107) and (G.108) we get

$$\begin{aligned} &\frac{1}{n}\big[(\ln\tilde{j})^{\mathrm{r}\prime}\big] = \frac{1}{2}n\,\hat{k} \quad , \\ &\frac{1}{n^2}\big[(\ln\tilde{j})^{\mathrm{r}\prime\mathrm{r}\prime}\big] = \frac{1}{2n^2}\,(\ln\hat{j})^{\mathrm{r}\prime\mathrm{r}\prime} + \frac{1}{2n^2}\big[(\ln\hat{\Delta})^{\mathrm{r}\prime\mathrm{r}\prime}\big] = -\frac{n^2}{6}\hat{\mathrm{K}}^2 + \frac{1}{3}\hat{k}' \quad , \end{aligned} \tag{F.41}$$

and therefore

$$\frac{1}{n^2}\big[\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathrm{r}\prime\,\mathrm{r}\prime}\big] = \frac{1}{n^2}\,\hat{\varphi}\hat{\psi}'' + \hat{k}\,\varphi\hat{\psi}' + \Big(\frac{1}{3}\hat{k}' - \frac{1}{6}n^2\hat{\mathrm{K}}^2 + \frac{1}{4}\hat{k}^2\Big)\,\hat{\varphi}\hat{\psi} \quad . \tag{F.42}$$

Here $\hat{k}$ is a trace of extrinsic curvature and $\hat{\mathrm{K}}^2$ is a square of the extrinsic curvature (eq. (G.51)). Next, using (G.27), (G.105), and (G.102), transforming the connection ∇ to $\hat{\nabla}$ (eq. (G.64)) and performing an integration by parts gives

$$\begin{aligned} &\frac{\nu}{2}\int\limits_{\partial\Omega} \mathfrak{q}^{\frac{1}{2}}\hat{j}\,\hat{\varphi}\,\Big(\hat{q}^{-1\,\mu\nu}\,\hat{\psi}_{2\,\mu\nu} + \hat{\psi}_{1\,\mu}\,\hat{q}^{-1\,\mu\nu}\,\Big(\big[\hat{l}_{0,1\,\nu}\big] - \frac{1}{2}\big[\hat{\sigma}_{0,3\,\kappa\lambda\nu}\big]\,\hat{q}^{-1\,\kappa\lambda}\Big)\Big) = \\ &\quad = -\frac{\nu}{2}\int\limits_{\partial\Omega} \hat{\mathfrak{q}}^{\frac{1}{2}}\,\mathrm{D}_{\mu}\hat{\varphi}\,\hat{q}^{-1\,\mu\nu}\,\mathrm{D}_{\nu}\hat{\psi} \quad . \end{aligned} \tag{F.43}$$

Substituting for $[\hat{\sigma}_{0,k}]$ and $[\hat{l}_{0,k}]$ in remaining terms of $[\omega_1]$, a straightforward long calculation gives

$$\begin{aligned} &-\frac{1}{8}\big[\hat{\sigma}_{0,4\,\mu\nu\kappa\lambda}\big]\,\hat{q}^{-1\,\mu\nu}\hat{q}^{-1\,\kappa\lambda} + \frac{1}{2}\big[\hat{l}_{0,2\,\mu\nu}\big]\,\hat{q}^{-1\,\mu\nu} + \\ &\quad + \frac{1}{8}\big[\hat{\sigma}_{0,3\,\mu\nu\alpha}\big]\,\big[\hat{\sigma}_{0,3\,\kappa\lambda\beta}\big]\,\hat{q}^{-1\,\mu\nu}\hat{q}^{-1\,\alpha\beta}\hat{q}^{-1\,\kappa\lambda} + \frac{1}{2}\big[\hat{l}_{0,1\,\mu}\big]\,\big[\hat{l}_{0,1\,\nu}\big]\,\hat{q}^{-1\,\mu\nu} + \\ &\quad + \frac{1}{12}\big[\hat{\sigma}_{0,3\,\mu\kappa\alpha}\big]\,\big[\hat{\sigma}_{0,3\,\nu\lambda\beta}\big]\,\hat{q}^{-1\,\mu\nu}\hat{q}^{-1\,\alpha\beta}\hat{q}^{-1\,\kappa\lambda} - \frac{1}{2}\big[\hat{l}_{0,1\,\mu}\big]\,\big[\hat{\sigma}_{0,3\,\kappa\lambda\nu}\big]\,\hat{q}^{-1\,\mu\nu}\hat{q}^{-1\,\kappa\lambda} = \\ &\quad = \nu\Big(-\frac{1}{6}\hat{k}' + \frac{n^2}{12}\hat{\mathrm{K}}^2 - \frac{n^2}{8}\hat{k}^2\Big) \quad . \end{aligned} \tag{F.44}$$

Putting together (F.42–F.44), and integrating by parts we find

$$\begin{aligned} &\int\limits_{\substack{\hat{y}\in\partial\Omega\\ \eta\in\mathbb{R}^+}} d\eta\,\mathfrak{q}^{\frac{1}{2}}(\hat{y})\,\hat{j}(\hat{y};\eta)\,\Big(\frac{\nu}{4n^2}\,\tilde{j}^{-1}(\tilde{j}\omega_0)^{1\prime\,1\prime} + \frac{\nu}{4n^2}\,\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathrm{r}\prime\,\mathrm{r}\prime} + \omega_1\Big)(\hat{y};\eta,\eta) = \\ &\quad = \nu\int\limits_{\mathbb{R}^+} d\eta\int\limits_{\partial\Omega}\hat{\mathfrak{q}}^{\frac{1}{2}}\Big(\frac{1}{4n^2}\Big(\hat{\varphi}''\hat{\psi} + \hat{\varphi}\hat{\psi}'' + n^2\hat{k}\,\big(\hat{\varphi}'\hat{\psi} + \hat{\varphi}\hat{\psi}'\big)\Big) - \frac{1}{2}\mathrm{D}_{\mu}\hat{\varphi}\,\hat{q}^{-1\,\mu\nu}\,\mathrm{D}_{\nu}\hat{\psi}\Big) = \\ &\quad = -\frac{\nu}{2}\int\limits_{\mathbb{R}^+} d\eta\int\limits_{\partial\Omega} n\hat{\mathfrak{q}}^{\frac{1}{2}}\Big(\frac{1}{n^2}\,\hat{\varphi}'\hat{\psi}' + \mathrm{D}_{\mu}\hat{\varphi}\,\hat{q}^{-1\,\mu\nu}\,\mathrm{D}_{\nu}\hat{\psi}\Big) - \frac{\nu}{4n^2}\int\limits_{\partial\Omega}\mathfrak{q}^{\frac{1}{2}}\,\big(\hat{\varphi}'\hat{\psi} + \hat{\varphi}\hat{\psi}'\big) = \\ &\quad = -\frac{\nu}{2}\int\limits_{\Omega}\mathfrak{g}^{\frac{1}{2}}\,\mathrm{d}_{\mu}\varphi\,g^{-1\,\mu\nu}\,\mathrm{d}_{\nu}\psi - \frac{\nu}{4n^2}\int\limits_{\partial\Omega}\mathfrak{q}^{\frac{1}{2}}\,\big(\psi\,\vec{n}^{\mu}\mathrm{d}_{\mu}\varphi + \varphi\,\vec{n}^{\mu}\mathrm{d}_{\mu}\psi\big) = \\ &\quad = -\frac{\nu}{2}\,\varphi\bullet\Big(\mathcal{L}_d - \frac{1}{2}\big(\overleftarrow{d}\mathcal{L}_d + \overrightarrow{d}\mathcal{L}_d\big)\Big)\bullet\psi = -\frac{\nu}{2}\,\varphi\bullet\overleftrightarrow{\mathcal{L}}\bullet\psi \quad . \end{aligned} \tag{F.45}$$

This concludes the proof of the expansion in (F.26).

Manifold with boundary — reflection contribution

Finally we will prove the last expansion we have needed in the main text:

$$\begin{aligned}&\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\,\Delta_{\mathrm{b}}^{1\text{-}p}(x|z)\,\beta(\tau,x|z)\,\exp\Big(-\frac{1}{\nu\tau}\sigma_{\mathrm{b}}(x|z)\Big)=\\&\quad=\sqrt{\tau}\,\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\,\mathcal{Q}-\tau\frac{\nu}{2}\,\frac{1}{2}(\overleftrightarrow{d\mathcal{F}}_d+\overrightarrow{d\mathcal{F}}_d)-\tau\frac{\nu}{2}\,\Big(\frac{1+p}{3}k+\beta\text{-terms}\Big)+\mathcal{O}(\tau^{\frac{3}{2}})\quad.\end{aligned}\tag{F.46}$$

Similarly to the previous section, we smooth this expression with test functions, perform a change of variables (F.27) and consequently (F.31), and use the covariant expansions (F.34),

$$\begin{aligned}\widehat{\beta}(\tau,\widehat{x},\xi|\widehat{z},\zeta)&=\widehat{\beta}_0(\widehat{x},\xi|\widehat{z},\zeta)+\sqrt{\tau}\widehat{\beta}_{\frac{1}{2}}(\widehat{x},\xi|\widehat{z},\zeta)+\mathcal{O}(\tau)\quad,\\ \widehat{\beta}_0(\widehat{y},\xi|\widehat{y},\sqrt{\tau}Y,\zeta)&=\sum_{k=\mathbb{N}_0}\tau^{\frac{k}{2}}\frac{1}{k!}\,\widehat{\beta}_{0;0,k\,\boldsymbol{\mu}_1\dots\boldsymbol{\mu}_k}(\widehat{y};\xi,\zeta)\,Y^{\boldsymbol{\mu}_1}\dots Y^{\boldsymbol{\mu}_k}\quad;\end{aligned}\tag{F.47}$$

similarly for $\beta_{\frac{1}{2}}(x|z)$; and

$$\widehat{\sigma}_{\mathrm{b}}(\widehat{y},\xi|\widehat{y},\sqrt{\tau}Y,\zeta)=\tau n^2\frac{1}{2}(\xi+\zeta)^2+\sum_{k=2,3,\dots}\tau^{\frac{k}{2}}\frac{1}{k!}\,\widehat{\sigma}_{\mathrm{b}\,0,k\,\boldsymbol{\mu}_1\dots\boldsymbol{\mu}_k}(\widehat{y};\xi,\zeta)\,Y^{\boldsymbol{\mu}_1}\dots Y^{\boldsymbol{\mu}_k}\quad,\tag{F.48}$$

$$\widehat{l}_{\mathrm{b}}(\widehat{y},\xi|\widehat{y},\sqrt{\tau}Y,\zeta)=\sum_{k=\mathbb{N}_0}\tau^{\frac{k}{2}}\frac{1}{k!}\,\widehat{l}_{\mathrm{b}\,0,k\,\boldsymbol{\mu}_1\dots\boldsymbol{\mu}_k}(\widehat{y};\xi,\zeta)\,Y^{\boldsymbol{\mu}_1}\dots Y^{\boldsymbol{\mu}_k}\quad,\tag{F.49}$$

where

$$\widehat{l}_{\mathrm{b}}(\widehat{x},\xi|\widehat{z},\zeta)=\ln\Big(\widehat{j}(\widehat{x},\xi)\frac{\widehat{\Delta}_{\mathrm{b}}^{1\text{-}p}(\widehat{x},\xi|\widehat{z},\zeta)}{\Delta(\widehat{x}|\widehat{z})}\widehat{j}(\widehat{z},\zeta)\Big)\quad.\tag{F.50}$$

This leads to a Gaussian integration in the variable $Y\in\mathbf{T}_{\widehat{y}}\partial\Omega$ in which only leading terms in expansions survive and we get

$$\begin{aligned}&\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\int\limits_{x,z\in\Omega}\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\,\varphi(x)\psi(z)\,\Delta_{\mathrm{b}}^{1\text{-}p}(x|z)\,\beta(\tau,x|z)\,\exp\Big(-\frac{1}{\nu\tau}\sigma_{\mathrm{b}}(x|z)\Big)=\\&\quad=\int\limits_{\widehat{y}\in\partial\Omega}\frac{n}{(2\pi\nu\tau)^{\frac{1}{2}}}\,\mathfrak{q}^{\frac{1}{2}}(\widehat{y})\int\limits_{\xi,\zeta\in\mathbb{R}^+}d\xi\,d\zeta\,\exp\Big(-\frac{n^2}{2\nu\tau}(\xi+\zeta)^2\Big)\,\widehat{\varphi}(\widehat{y},\xi)\,\widehat{\psi}(\widehat{y},\zeta)\times\\&\qquad\times\tilde{j}_{\mathrm{b}}(\widehat{y};\xi,\tfrac{\xi\zeta}{\xi+\zeta},\zeta)\,\Big(\tilde{\beta}_0(\widehat{y};\xi,\tfrac{\xi\zeta}{\xi+\zeta},\zeta)+\sqrt{\tau}\,\tilde{\beta}_{\frac{1}{2}}(\widehat{y};\xi,\tfrac{\xi\zeta}{\xi+\zeta},\zeta)+\mathcal{O}(\tau)\Big)\quad,\end{aligned}\tag{F.51}$$

where

$$\begin{aligned}\tilde{j}_{\mathrm{b}}(\widehat{y};\xi,\tfrac{\xi\zeta}{\xi+\zeta},\zeta)&=\widehat{j}(\widehat{y},\xi)\,\widehat{\Delta}_{\mathrm{b}}^{1\text{-}p}(\widehat{y};\xi|\widehat{y},\zeta)\,\widehat{j}(\widehat{y},\zeta)\,\mathfrak{q}^{\frac{1}{2}}(\widehat{y})\,\Big(\mathrm{Det}_{\shortparallel}\,\widehat{\sigma}_{\mathrm{b}\,0,2}(\widehat{y};\xi,\zeta)\Big)^{-\frac{1}{2}}=\\&=\Big(\widehat{j}(\widehat{y},\xi)\,\widehat{\Delta}_{\mathrm{b}}^{1\text{-}2p}(\widehat{y};\xi|\widehat{y},\zeta)\,\widehat{j}(\widehat{y},\zeta)\Big)^{\frac{1}{2}}\quad,\end{aligned}\tag{F.52}$$

$$\tilde{\beta}_0(\widehat{y};\xi,\tfrac{\xi\zeta}{\xi+\zeta},\zeta)=\widehat{\beta}_0(\widehat{y},\xi|\widehat{y},\zeta)\quad,\tag{F.53}$$

with analytical dependence of $\tilde{j}_{\mathrm{b}}$ and $\tilde{\beta}_0$ on their three real arguments. $\tilde{\beta}_{\frac{1}{2}}$ is defined in similar way as $\tilde{\beta}_0$. Here we anticipate that $\widehat{\Delta}_{\mathrm{b}}$ and $\widehat{\beta}$ can have more complicated analytical dependence on ξ

and ζ. The equality in (F.52) follows from (G.98). Using the expansion (F.23) we obtain

$$\begin{aligned}\int\limits_{\widehat{y}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\widehat{y})\Big(&\sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\,\tilde{\beta}_0(\widehat{y};0,0,0)\,\varphi(\widehat{y})\psi(\widehat{y})+\\ &+\tau\frac{\nu}{4n^2}\,\tilde{\beta}_0(\widehat{y};0,0,0)\,\Big(\widehat{\varphi}'(\widehat{y},0)\widehat{\psi}(\widehat{y},0)+\widehat{\varphi}(\widehat{y},0)\widehat{\psi}'(\widehat{y},0)\Big)+\\ &+\tau\,\Big(\frac{\nu}{4n^2}\big(\tilde{j}_{\mathrm{b}}\tilde{\beta}_0\big)^{\mathtt{l}'}+\frac{\nu}{4n^2}\big(\tilde{j}_{\mathrm{b}}\tilde{\beta}_0\big)^{\mathtt{r}'}+\\ &\qquad+\frac{\nu}{12n^2}\big(\tilde{j}_{\mathrm{b}}\tilde{\beta}_0\big)^{\mathtt{m}'}+\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\,\tilde{\beta}_{\frac{1}{2}}\Big)(\widehat{y};0,0,0)\,\varphi(\widehat{y})\psi(\widehat{y})+\\ &+\mathcal{O}(\tau^{\frac{3}{2}})\Big)\quad.\end{aligned}\tag{F.54}$$

Using the expansion (G.116) of $\tilde{j}_{\mathrm{b}}$ and obvious relations for $\tilde{\beta}_0(\widehat{y};0,0,0)$ and $\tilde{\beta}_{\frac{1}{2}}(\widehat{y};0,0,0)$, this expression is equal to

$$\begin{aligned}\int\limits_{\widehat{y}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\widehat{y})\Big(&\sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\,\beta(0,\widehat{y}|\widehat{y})\,\varphi(\widehat{y})\psi(\widehat{y})+\\ &+\tau\frac{\nu}{4n^2}\,\beta(0,\widehat{y}|\widehat{y})\,\Big(\widehat{\varphi}'(\widehat{y},0)\widehat{\psi}(\widehat{y},0)+\widehat{\varphi}(\widehat{y},0)\widehat{\psi}'(\widehat{y},0)\Big)+\\ &+\frac{\tau\nu}{2}\,\Big(-\frac{1+6}{3}\beta(0,\widehat{y}|\widehat{y})k(\widehat{y})+\frac{2}{n}\sqrt{\frac{1}{2\pi\nu}}\,\dot{\beta}(0,\widehat{y}|\widehat{y})+\\ &\qquad+\Big(\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{l}'}+\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{r}'}+\frac{1}{6n^2}\tilde{\beta}_0{}^{\mathtt{m}'}\Big)(\widehat{y};0,0,0)\Big)\,\varphi(\widehat{y})\psi(\widehat{y})+\\ &+\mathcal{O}(\tau^{\frac{3}{2}})\Big)\quad.\end{aligned}\tag{F.55}$$

Using the normalization condition (14.17) concludes the proof of the expansion (F.46). By inspection we see that the β-terms have form

$$\beta\text{-terms}=-\frac{2}{n}\sqrt{\frac{1}{2\pi\nu}}\,\dot{\beta}(0,\widehat{y}|\widehat{y})-\Big(\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{l}'}+\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{r}'}+\frac{1}{6n^2}\tilde{\beta}_0{}^{\mathtt{m}'}\Big)(\widehat{y};0,0,0)\quad.\tag{F.56}$$

G Geodesic theory

Basic definitions

In this appendix we review some facts from geodesic theory and list a number of useful expansion, some of which we have used in this work. The material related to a manifold without boundary is well known — see for example the classical works [1, 32] and [33]. The theory of expansion near a boundary is less known. Some material can be found in [26, 34, 35]. The calculations are usually straightforward but cumbersome. We will present mostly only results. But all expressions presented were computed and checked by the author (see [36]).

We start with introducing the *covariant expansion* in a curved manifold. We would like to expand a sufficiently smooth tensor field $A^{\boldsymbol{\alpha}\cdots}_{\boldsymbol{\beta}\cdots}$ on a manifold around a point x. First we change the dependence on a point z in the manifold M to the dependence on a vector Z from $\mathbf{T}_x\, M$, then we transform vector indices from different tangent spaces to one common tensor space, and finally we do the usual Taylor expansion of a linear-space-valued function on a vector space.

To transform the tensor field on the manifold to a linear-space-valued function we need to know how to move tensors from one tangent point to another. We assume that we have given a metric g which define a parallel transport. It allows us to transform tensors from the tangent space at point z in a normal neighborhood of the point x to the space $\mathbf{T}_x\, M$ along the geodetic joining these two points. In the normal neighborhood of x we can parametrize a geodesic by its tangent vector at x, i.e. we can define an *exponential map* $\boldsymbol{u}_x$

$$\boldsymbol{u}_x : \mathbf{T}_x\, M \to M \quad , \tag{G.1}$$

$$\frac{\nabla}{d\tau}\frac{\mathrm{D}}{d\tau}\boldsymbol{u}_x(\tau X) = 0 \quad , \quad \frac{\mathrm{D}}{d\tau}\boldsymbol{u}_x(\tau X)|_{\tau=0} = X \quad . \tag{G.2}$$

If $f(z)$ is some manifold dependent function, we use notation $f(x;Z) = f(\boldsymbol{u}_x(Z))$. This transformation concludes our first step. Next we parallel transform vector indices of the tensor field to the space $\mathbf{T}_x\, M$ along the geodesics starting from x. We define the *tensor of geodesic transport* $\iota(x|z)$ from z to x

$$\iota^{\boldsymbol{\mu}}{}_{\boldsymbol{\nu}}(x|z) \in \mathbf{T}_x\, M \otimes \mathbf{T}^\star_z\, M \quad , \quad \frac{\nabla}{d\tau}\iota(x, \boldsymbol{u}_x(\tau X)) = 0 \quad , \tag{G.3}$$

and its version with indices up and down

$$\bar{\iota} = \iota \cdot g^{-1} \quad , \quad \underline{\iota} = g \cdot \iota \quad . \tag{G.4}$$

Using this tensor we can write down the tensor field A with transported indices explicitly. We obtain the linear-space-valued function on a linear space

$$A^{\boldsymbol{\mu}\cdots}_{\boldsymbol{\nu}\cdots}(x;.)\; \iota^{\boldsymbol{\alpha}}{}_{\boldsymbol{\mu}}(x|x;.)\ldots\; \iota^{-1\,\boldsymbol{\nu}}{}_{\boldsymbol{\beta}}(x|x;.)\ldots \quad : \mathbf{T}_x\, M \to \mathbf{T}_x{}^k_l\, M \quad . \tag{G.5}$$

Finally we can write the *covariant expansion*

$$A^{\boldsymbol{\mu}\cdots}_{\boldsymbol{\nu}\cdots}(x;Z)\; \iota^{\boldsymbol{\alpha}}{}_{\boldsymbol{\mu}}(x|x;Z)\ldots\; \iota^{-1\,\boldsymbol{\nu}}{}_{\boldsymbol{\beta}}(x|x;Z)\ldots = \sum_{k\in\mathbb{N}_0} \frac{1}{k!} A_k{}^{\boldsymbol{\alpha}\cdots}_{\boldsymbol{\beta}\cdots\,\boldsymbol{\mu}_1\ldots\boldsymbol{\mu}_k}(x)\; Z^{\boldsymbol{\mu}_1}\ldots Z^{\boldsymbol{\mu}_k} \quad . \tag{G.6}$$

We call $A_k(x)$ the coefficients of the covariant expansion of the field A at x. They are tensors at x symmetric in indices $\mu_1, \ldots, \mu_k$.

To compute these coefficients we need to develop geodesic theory to greater detail. First we define the *world function* $\sigma(x|z)$ of the metric g. It is given by half of the squared geodesic distance between points x and z — see (13.27). For time-like separated points it is negative. The *geodesic distance* is then given by

$$s(x|z) = |2\sigma(x|z)|^{\frac{1}{2}} \quad . \tag{G.7}$$

We define *geodesic tangent vectors* $\overrightarrow{\sigma}$, $\overleftarrow{\sigma}$

$$\overrightarrow{\sigma}(x|z) = g^{-1}(x) \cdot \mathrm{d}_{\mathbf{l}}\sigma(x|z) \quad , \quad \overleftarrow{\sigma}(x|z) = \mathrm{d}_{\mathbf{r}}\sigma(x|z) \cdot g^{-1}(z) \quad . \tag{G.8}$$

Here, as before, $\mathrm{d}_{\mathbf{l}} f$ or $\mathrm{d}_{\mathbf{r}} f$ denote the gradient in the left or right argument of a bi-function $f(x|z)$.

The basic properties of the world function (see e.g. [1]) are that its gradient vector $\overrightarrow{\sigma}(x|z)$ is really tangent to the geodesic between x and z and it is normalized to the length of the geodesic. I.e.

$$-Z = \overrightarrow{\sigma}(x|x;Z) \quad . \tag{G.9}$$

We also introduce a special notation for the second derivatives of the world function

$$\overrightarrow{\overrightarrow{\sigma}} = \nabla_{\mathbf{l}}\mathrm{d}_{\mathbf{l}}\sigma \quad , \quad \overleftrightarrow{\sigma} = \mathrm{d}_{\mathbf{l}}\mathrm{d}_{\mathbf{r}}\sigma \quad , \quad \overleftarrow{\overleftarrow{\sigma}} = \nabla_{\mathbf{r}}\mathrm{d}_{\mathbf{r}}\sigma \quad . \tag{G.10}$$

To conclude our definition we introduce also determinants of ι, $\underline{\iota}$, $\overleftrightarrow{\sigma}$. They are well-defined objects — bi-densities on M

$$\mathfrak{i}(x|z) = \frac{1}{n^2}\,\mathrm{Det}\,\iota(x|z) = \mathfrak{g}^{-\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z) \quad , \quad \underline{\mathfrak{i}}(x|z) = \frac{1}{n^2}\,\mathrm{Det}\,\underline{\iota}(x|z) = \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z) \quad , \tag{G.11}$$

$$\mathfrak{s}(x|z) = \frac{1}{n^2}\,\mathrm{Det}\big(-\mathfrak{s}(x|z)\big) \quad \in \tilde{\mathbb{R}}_x\, M \otimes \tilde{\mathbb{R}}_z\, M \quad . \tag{G.12}$$

Finally we define *Van-Vleck Morette determinant*

$$\Delta(x|z) = \mathfrak{s}(x|z)\,\underline{\mathfrak{i}}^{-1}(x|z) = \mathfrak{s}(x|z)\,\mathfrak{g}^{-\frac{1}{2}}(x)\mathfrak{g}^{-\frac{1}{2}}(z) \quad . \tag{G.13}$$

For a bi-tensor $F(x|z)$ on the manifold — a tensor object depending on two points in the manifold — we denote the *coincidence limit*

$$[F](x) = F(x|x) \quad . \tag{G.14}$$

The generalized Synge's theorem (see e.g. [37]) tells us that

$$\nabla[F] = [\nabla_{\mathbf{l}}F] + [\nabla_{\mathbf{r}}F] \quad . \tag{G.15}$$

Coincidence limits and covariant expansions

Equation (G.9) gives

$$\sigma = \frac{1}{2}\,\mathrm{d}_{\mathbf{r}}\sigma \cdot g^{-1} \cdot \mathrm{d}_{\mathbf{r}}\sigma = \frac{1}{2}\,\mathrm{d}_{\mathbf{l}}\sigma \cdot g^{-1} \cdot \mathrm{d}_{\mathbf{l}}\sigma = \frac{1}{2}\,\overrightarrow{\sigma} \cdot g \cdot \overrightarrow{\sigma} = \frac{1}{2}\,\overleftarrow{\sigma} \cdot g \cdot \overleftarrow{\sigma} \quad . \tag{G.16}$$

Taking repeatedly derivatives of this expression in both arguments we can derive

$$\overrightarrow{\sigma} \cdot g = \overrightarrow{\sigma} \cdot \overrightarrow{\overrightarrow{\sigma}} = \overleftrightarrow{\sigma} \cdot \overleftarrow{\sigma} \quad , \quad g \cdot \overleftarrow{\sigma} = \overleftarrow{\overleftarrow{\sigma}} \cdot \overleftarrow{\sigma} = \overrightarrow{\sigma} \cdot \overleftrightarrow{\sigma} \quad , \tag{G.17}$$

and following identities

$$\overrightarrow{\sigma}^{\mu} \mathrm{d}_{1\mu}\sigma = 2\sigma \quad , \tag{G.18}$$

$$\begin{aligned} \overrightarrow{\sigma}^{\mu} \nabla_{1\mu} \overrightarrow{\sigma}^{\alpha} &= \overrightarrow{\sigma}^{\alpha} \quad , \\ \overrightarrow{\sigma}^{\mu} \nabla_{1\mu} \overleftarrow{\sigma}^{\alpha} &= \overleftarrow{\sigma}^{\alpha} \quad , \end{aligned} \tag{G.19}$$

$$\begin{aligned} \overrightarrow{\sigma}^{\mu} \nabla_{1\mu} \overrightarrow{\overrightarrow{\sigma}}_{\alpha\beta} &= \overrightarrow{\overrightarrow{\sigma}}_{\alpha\beta} - \overrightarrow{\overrightarrow{\sigma}}_{\alpha\mu} \overrightarrow{\overrightarrow{\sigma}}_{\beta\nu} g^{-1\,\mu\nu} - \mathrm{R}_{\alpha\mu\beta\nu} \overrightarrow{\sigma}^{\mu} \overrightarrow{\sigma}^{\nu} \quad , \\ \overrightarrow{\sigma}^{\mu} \nabla_{1\mu} \overleftrightarrow{\sigma}_{\alpha\beta} &= \overleftrightarrow{\sigma}_{\alpha\beta} - \overrightarrow{\overrightarrow{\sigma}}_{\alpha\mu} g^{-1\,\mu\nu} \overleftrightarrow{\sigma}_{\nu\beta} \quad , \\ \overrightarrow{\sigma}^{\mu} \nabla_{1\mu} \overleftarrow{\overleftarrow{\sigma}}_{\alpha\beta} &= \overleftarrow{\overleftarrow{\sigma}}_{\alpha\beta} - g^{-1\,\mu\nu} \overleftrightarrow{\sigma}_{\mu\alpha} \overleftrightarrow{\sigma}_{\nu\beta} \quad , \\ \overrightarrow{\sigma}^{\mu} \nabla_{1\alpha} \nabla_{1\beta} \nabla_{1\mu}\sigma &= \overrightarrow{\overrightarrow{\sigma}}_{\alpha\beta} - \overrightarrow{\overrightarrow{\sigma}}_{\alpha\mu} \overrightarrow{\overrightarrow{\sigma}}_{\beta\nu} g^{-1\,\mu\nu} \quad . \end{aligned} \tag{G.20}$$

Similar, more complicated relations hold for higher derivatives. Using the fact that coincidence limits of the world function and tangent geodesic vector are zero, taking coincidence limits of relations above and similar relations for higher derivatives, and using the Synge's theorem, we get

$$[\sigma] = 0 \quad , \tag{G.21}$$

$$[\mathrm{d}_1\sigma] = [\mathrm{d}_\mathrm{r}\sigma] = 0 \quad , \tag{G.22}$$

$$[\nabla_1\nabla_1\sigma] = -[\nabla_1\nabla_\mathrm{r}\sigma] = [\nabla_\mathrm{r}\nabla_\mathrm{r}\sigma] = g \quad , \tag{G.23}$$

$$[\nabla_1\nabla_1\nabla_1\sigma] = [\nabla_1\nabla_1\nabla_\mathrm{r}\sigma] = [\nabla_1\nabla_\mathrm{r}\nabla_\mathrm{r}\sigma] = [\nabla_\mathrm{r}\nabla_\mathrm{r}\nabla_\mathrm{r}\sigma] = 0 \quad , \tag{G.24}$$

$$\begin{aligned} &[\nabla_{1\alpha}\nabla_{1\beta}\nabla_{1\mu}\nabla_{1\nu}\sigma] = -[\nabla_{1\beta}\nabla_{1\mu}\nabla_{1\nu}\nabla_{\mathrm{r}\alpha}\sigma] = [\nabla_{1\mu}\nabla_{1\nu}\nabla_{\mathrm{r}\beta}\nabla_{\mathrm{r}\alpha}\sigma] = \\ &= -[\nabla_{1\nu}\nabla_{\mathrm{r}\mu}\nabla_{\mathrm{r}\beta}\nabla_{\mathrm{r}\alpha}\sigma] = [\nabla_{\mathrm{r}\nu}\nabla_{\mathrm{r}\mu}\nabla_{\mathrm{r}\beta}\nabla_{\mathrm{r}\alpha}\sigma] = -\frac{1}{3}\big(\mathrm{R}_{\alpha\mu\beta\nu} + \mathrm{R}_{\alpha\nu\beta\mu}\big) \quad . \end{aligned} \tag{G.25}$$

Similar relation for the fifth and sixth derivative can be found in [36].

Now we are prepared to compute at least some coefficients of covariant expansion. We start with the simplest case of the covariant expansion of a function f on the manifold. In this case we do not have problems with tensor nature of f and we do not have to worry about parallel transport of tensor indices. The equation (G.6) can be rewritten using (G.9) as

$$f(z) = \sum_{k\in\mathbb{N}_0} \frac{(-1)^k}{k!} f_{k\,\mu_1\ldots\mu_k}(x)\; \overrightarrow{\sigma}^{\mu_1}(x,z)\ldots\overrightarrow{\sigma}^{\mu_k}(x,z) \quad . \tag{G.26}$$

Taking derivatives of this equation and coincidence limits we can find that the coefficients are given by

$$f_{k\,\mu_1\ldots\mu_k} = \nabla_{(\mu_1}\ldots\nabla_{\mu_k)} f \quad . \tag{G.27}$$

To do a similar calculation for a general tensor field A we need to know the coincidence limits of the geodesic transport tensor. They can be calculated from the equation

$$\overrightarrow{\sigma} = -\iota\cdot\overleftarrow{\sigma} \tag{G.28}$$

by taking derivatives and coincidence limits. We give only a list of some of them (see [33,37] or [36]).

$$[\underline{\iota}] = g \quad , \tag{G.29}$$

$$[\nabla_1\underline{\iota}] = [\nabla_\mathrm{r}\underline{\iota}] = 0 \quad , \tag{G.30}$$

$$-[\nabla_{1\beta}\nabla_{1\alpha}\underline{\iota}_{\mu\nu}] = [\nabla_{1\alpha}\nabla_{\mathrm{r}\beta}\underline{\iota}_{\mu\nu}] = -[\nabla_{\mathrm{r}\alpha}\nabla_{\mathrm{r}\beta}\underline{\iota}_{\mu\nu}] = \frac{1}{2}\mathrm{R}_{\alpha\beta\mu\nu} \quad , \tag{G.31}$$

$$[\nabla_{1\gamma}\nabla_{1\beta}\nabla_{1\alpha}\underline{\iota}_{\mu\nu}] = -\frac{1}{3}\nabla_\gamma\mathrm{R}_{\alpha\beta\mu\nu} - \frac{1}{3}\nabla_\beta\mathrm{R}_{\alpha\gamma\mu\nu} \quad , \tag{G.32}$$

$$
\begin{aligned}
&[\nabla_{1\delta}\nabla_{1\gamma}\nabla_{1\beta}\nabla_{1\alpha}\underline{\iota}_{\mu\nu}] = \\
&\quad -\frac{1}{4}\nabla_\delta\nabla_\gamma \mathrm{R}_{\mu\nu\alpha\beta} - \frac{1}{4}\nabla_\delta\nabla_\beta \mathrm{R}_{\mu\nu\alpha\gamma} - \frac{1}{4}\nabla_\gamma\nabla_\beta \mathrm{R}_{\mu\nu\alpha\delta} + \\
&\quad + \frac{1}{8}\,\mathrm{R}_{\mu\nu\delta\lambda}\,\mathrm{R}_{\kappa\alpha\beta\gamma}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\mu\nu\gamma\lambda}\,\mathrm{R}_{\kappa\alpha\beta\delta}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\mu\nu\beta\lambda}\,\mathrm{R}_{\kappa\alpha\gamma\delta}\,g^{\text{-}1\kappa\lambda} + \\
&\quad + \frac{1}{24}\,\mathrm{R}_{\mu\nu\delta\lambda}\,\mathrm{R}_{\kappa\beta\alpha\gamma}\,g^{\text{-}1\kappa\lambda} + \frac{1}{24}\,\mathrm{R}_{\mu\nu\gamma\lambda}\,\mathrm{R}_{\kappa\beta\alpha\delta}\,g^{\text{-}1\kappa\lambda} + \frac{1}{24}\,\mathrm{R}_{\mu\nu\delta\lambda}\,\mathrm{R}_{\kappa\gamma\alpha\beta}\,g^{\text{-}1\kappa\lambda} + \\
&\quad + \frac{1}{8}\,\mathrm{R}_{\nu\lambda\gamma\delta}\,\mathrm{R}_{\kappa\mu\alpha\beta}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\nu\lambda\beta\delta}\,\mathrm{R}_{\kappa\mu\alpha\gamma}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\nu\lambda\beta\gamma}\,\mathrm{R}_{\kappa\mu\alpha\delta}\,g^{\text{-}1\kappa\lambda} + \\
&\quad + \frac{1}{8}\,\mathrm{R}_{\nu\lambda\alpha\delta}\,\mathrm{R}_{\kappa\mu\beta\gamma}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\nu\lambda\alpha\gamma}\,\mathrm{R}_{\kappa\mu\beta\delta}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\nu\lambda\alpha\beta}\,\mathrm{R}_{\kappa\mu\gamma\delta}\,g^{\text{-}1\kappa\lambda} + \\
&\quad + \frac{1}{24}\,\mathrm{R}_{\mu\nu\kappa\gamma}\,\mathrm{R}_{\alpha\beta\delta\lambda}\,g^{\text{-}1\kappa\lambda} + \frac{1}{24}\,\mathrm{R}_{\mu\nu\kappa\beta}\,\mathrm{R}_{\alpha\gamma\delta\lambda}\,g^{\text{-}1\kappa\lambda} + \frac{1}{24}\,\mathrm{R}_{\mu\nu\kappa\beta}\,\mathrm{R}_{\alpha\delta\gamma\lambda}\,g^{\text{-}1\kappa\lambda} + \\
&\quad + \frac{1}{24}\,\mathrm{R}_{\mu\nu\kappa\alpha}\,\mathrm{R}_{\beta\gamma\delta\lambda}\,g^{\text{-}1\kappa\lambda} + \frac{1}{24}\,\mathrm{R}_{\mu\nu\kappa\alpha}\,\mathrm{R}_{\beta\delta\gamma\lambda}\,g^{\text{-}1\kappa\lambda} + \frac{1}{8}\,\mathrm{R}_{\nu\mu\kappa\alpha}\,\mathrm{R}_{\beta\lambda\gamma\delta}\,g^{\text{-}1\kappa\lambda}
\end{aligned}
\tag{G.33}
$$

Derivatives in other argument can be obtained using Synge's theorem and commuting covariant derivatives.

Now it is straightforward to compute the coefficients in a covariant expansion of a general field. It can be done by taking covariant derivatives and coincidence limits of the rewritten equation (G.6)

$$
A^{\mu\dots}_{\nu\dots}(z)\;\iota^{\alpha}_{\mu}(x|z)\dots\;\iota^{\text{-}1\nu}{}_{\beta}(x|z)\dots = \sum_{k\in\mathbb{N}_0}\frac{(-1)^k}{k!}A_k{}^{\alpha\dots}_{\beta\dots\,\mu_1\dots\mu_k}(x)\;\vec{\sigma}^{\mu_1}(x|z)\dots\vec{\sigma}^{\mu_k}(x|z) \quad . \tag{G.34}
$$

We will not list explicit results.

We can also expand a bi-tensor $A(x|z)$ in both its arguments around some point y. We denote coefficients of such expansion $A_{k,l}(y)$. I.e.

$$
\iota^\star(y|y;X)\iota^\star(y|y;Z)A(y;X|y;Z) = \sum_{k,l\in\mathbb{N}} A_{k,l\,\mu_1\dots\mu_k\nu_1\dots\nu_l}(y)\;X^{\mu_1}\dots X^{\mu_k}\;Z^{\nu_1}\dots Z^{\nu_k} \quad , \tag{G.35}
$$

where by $\iota^\star(y|z)A(z)$ we mean a parallel transport of all indices from z to y. In the case of a bi-scalar $f(x|z)$, similarly to (G.27) we can derive that

$$
f_{k,l\,\mu_1\dots\mu_k\nu_1\dots\nu_l} = [\nabla_{(1\mu_1}\dots\nabla_{1\mu_k)}\nabla_{(\mathrm{r}\nu_1}\dots\nabla_{\mathrm{r}\nu_l)}f] \quad . \tag{G.36}
$$

For calculations in appendix F we need the covariant expansion of the world function $\sigma(x|z)$. When we expand both its arguments at point y using the method described above we obtain

$$
\sigma(y;X|y;Z) = \frac{1}{2}\big(X-Z\big)^\mu\,g_{\mu\nu}(y)\,\big(X-Z\big)^\nu - \frac{1}{6}X^\mu X^\nu Z^\kappa Z^\lambda\;\mathrm{R}_{\mu\kappa\nu\lambda}(y) + \dots \quad . \tag{G.37}
$$

Clearly, the expansion of the world function at one of its arguments is given by equation (G.16).

Similarly, it is possible to derive (see [36, 37]) that coincidence limits of derivatives of the Van-Vleck Morette determinant are

$$
[\Delta] = 1 \quad , \tag{G.38}
$$

$$
[\mathrm{d_l}\Delta] = [\mathrm{d_r}\Delta] = 0 \quad , \tag{G.39}
$$

$$
[\nabla_{1\mu}\nabla_{1\nu}\Delta] = -[\nabla_{1\mu}\nabla_{\mathrm{r}\nu}\Delta] = [\nabla_{\mathrm{r}\mu}\nabla_{\mathrm{r}\nu}\Delta] = \frac{1}{3}\mathrm{Ric}_{\mu\nu} \quad . \tag{G.40}
$$

and the covariant expansion

$$
\Delta(y;X|y;Z) = 1 + \frac{1}{6}\,(X-Z)\cdot\mathrm{Ric}\cdot(X-Z) + \dots \quad . \tag{G.41}
$$

Finally let us note that the Jacobian associated with a map

$$\boldsymbol{u}_x^{-1} : z \to Z = -\vec{\sigma}(x|z) \tag{G.42}$$

is given by

$$\left|\mathrm{Det}\,\mathrm{D}\boldsymbol{u}_x^{-1}(z)\right| = \left|\mathrm{Det}\big(g^{-1}(x)\cdot \overset{\leftrightarrow}{\sigma}(x|z)\big)\right| = \mathfrak{g}^{-1}(x)\,\mathfrak{s}(x|z) = \mathfrak{i}(x|z)\,\Delta(x|z) \quad . \tag{G.43}$$

$(d-1)+1$ splitting near a boundary

Now we turn to investigate the domain Ω with a boundary. We will study this situation locally — i.e. we will work on a neighborhood of the boundary with topology $\mathbb{R}\times\Sigma$ where Σ is part of boundary manifold. In such neighborhood we can perform a $(d-1)+1$ splitting which we discussed already in appendix D (see also e.g. [2]). It is given by a *time function* t and *time flow vector* $\vec{t}$ such that $\vec{t}\cdot\mathrm{d}t = 1$. We use notation of usual $3+1$ splitting of spacetime even if we do not necessarily assume that t plays the role of a time coordinate. We assume that the condition $t=0$ defines the boundary and that $t>0$ inside of the domain Ω. We denote Σ_t hypersurfaces defined by conditions $t=\text{const}$. We denote n and $\vec{n}$ inside oriented normalized normal form and vector, q orthogonal projection of the metric g on the hypersurfaces Σ_t, and $\mathfrak{d}$ orthogonal projector to hypersurfaces Σ_t. I.e.

$$g = n^2\,nn + q \quad , \quad g^{-1} = n^{-2}\,\vec{n}\vec{n} + q^{-1} \quad , \quad \delta = \vec{n}n + \mathfrak{d} \quad , \tag{G.44}$$

where q^{-1} is inverse of g in the tangent space to the hypersurfaces. The phase factor n governs the signature of the metric g and the character of the hypersurfaces (see appendix D). We will use shorthands

$$A^{\cdots\shortparallel\alpha\cdots\perp\cdots}_{\cdots\perp\cdots} = A^{\cdots\beta\cdots\mu\cdots}_{\cdots\nu\cdots}\,\mathfrak{d}^{\alpha}_{\beta}\,\vec{n}^{\nu}\,n_{\mu} \quad . \tag{G.45}$$

We also use

$$\overset{\twoheadrightarrow}{\sigma}_{\shortparallel} \overset{\text{def}}{=} \overset{\twoheadrightarrow}{\sigma}_{\shortparallel\shortparallel} \quad , \quad \overset{\leftrightarrow}{\sigma}_{\shortparallel} \overset{\text{def}}{=} \overset{\leftrightarrow}{\sigma}_{\shortparallel\shortparallel} \quad , \quad \overset{\twoheadleftarrow}{\sigma}_{\shortparallel} \overset{\text{def}}{=} \overset{\leftrightarrow}{\sigma}_{\shortparallel\shortparallel} \quad . \tag{G.46}$$

Decomposition of the time flow vector $\vec{t}$ defines *lapse* N and *shift* $\vec{N}$

$$\vec{t} = N\vec{n} + \vec{N} \quad , \quad \mathrm{d}t = Nn \quad . \tag{G.47}$$

We denote D the *hypersurface gradient* — an orthogonal projection of a spacetime gradient to the hypersurfaces Σ_t

$$\mathrm{D}f = \mathfrak{d}\cdot\mathrm{d}f \quad , \tag{G.48}$$

and $\triangledown$ the *hypersurface connection* of the metric q. It is related to the spacetime connection as

$$\triangledown A = \mathfrak{d}^{\star}\nabla A \qquad \text{for } A \text{ such that} \qquad A = \mathfrak{d}^{\star}A \quad . \tag{G.49}$$

where by $\mathfrak{d}^{\star}A$ we mean projection of all tensor indices to the spaces tangent to the boundary. We denote by R, RIC, $\mathcal{R}$, and $\triangledown^2$ the Riemann curvature tensor, Ricci tensor, scalar curvature and Laplace operator of the metric q.

The *extrinsic curvature* K is given by covariant derivative of the normal form

$$\mathrm{K} = \mathfrak{d}\cdot\nabla n \quad , \tag{G.50}$$

and we use shorthands

$$\begin{aligned} k &= \mathrm{K}_{\mu\nu}g^{-1\,\mu\nu} \quad , \\ \mathrm{K}^2 &= \mathrm{K}_{\kappa\mu}\mathrm{K}_{\lambda\nu}g^{-1\,\kappa\lambda}g^{-1\,\mu\nu} \quad . \end{aligned} \tag{G.51}$$

We define the *time derivative* of a tensor field A tangent to the hypersurfaces:

$$A' = \mathfrak{d}^{\star}\mathcal{L}_{\vec{t}}A \qquad \text{for } A \text{ such that} \qquad A = \mathfrak{d}^{\star}A \quad . \tag{G.52}$$

Now we list a number of useful relations between spacetime quantities and "space" quantities, derivations of which are straightforward and for the case $n^2 = -1$ can be mostly found, for example, in [2].

$$\begin{aligned} \vec{n} \cdot \nabla n &= -\mathrm{D} \ln N \quad , \\ \nabla \cdot \vec{n} &= n^2 k \quad , \end{aligned} \tag{G.53}$$

$$\begin{aligned} \vec{n} \cdot \nabla q &= n\Big(n\,(\mathrm{D}\ln N) + (\mathrm{D}\ln N)\,n\Big) \quad , \\ \mathfrak{d}^{\mu}_{\gamma}\,\nabla_{\mu} q_{\alpha\beta} &= -n_{\alpha}\mathrm{K}_{\beta\gamma} - n_{\beta}\mathrm{K}_{\alpha\gamma} \quad , \end{aligned} \tag{G.54}$$

$$\begin{aligned} \nabla \cdot \mathfrak{d} &= -n^2 n k + \mathrm{D}\ln N \quad , \\ \mathfrak{d} \cdot (\nabla \mathfrak{d}) \cdot \mathfrak{d} &= -\mathrm{K}\,\vec{n} \end{aligned} \tag{G.55}$$

$$\begin{aligned} q' &= 2n^2 N\mathrm{K} + \mathcal{L}_{\vec{N}} q \quad , \\ \mathrm{K}' &= N\,\big(\vec{n} \cdot \nabla \mathrm{K}\big)_{\shortparallel\shortparallel} + 2n^2 N\,\mathrm{K} \cdot q^{-1} \cdot \mathrm{K} + \mathcal{L}_{\vec{N}}\mathrm{K} \quad , \\ k' &= N\,\vec{n} \cdot \mathrm{d}k + \vec{N}k \quad . \end{aligned} \tag{G.56}$$

The curvature tensors of the spacetime metric g and of the space metric q are related by

$$\begin{aligned} \mathrm{R}_{\shortparallel\alpha\,\shortparallel\beta\,\shortparallel\gamma\,\shortparallel\delta} &= \mathrm{R}_{\alpha\beta\gamma\delta} + n^2\big(\mathrm{K}_{\alpha\delta}\mathrm{K}_{\beta\gamma} - \mathrm{K}_{\alpha\gamma}\mathrm{K}_{\beta\delta}\big) \quad , \\ \mathrm{R}_{\shortparallel\alpha\shortparallel\beta\gamma\perp} &= n^2\big(\nabla_{\alpha}\mathrm{K}_{\beta\gamma} - \nabla_{\beta}\mathrm{K}_{\alpha\gamma}\big) \quad , \\ \mathrm{R}_{\shortparallel\perp\shortparallel\perp} &= n^4\big(\mathrm{K}k - \mathrm{K}\cdot q^{-1}\cdot\mathrm{K}\big) - n^2\Big(\nabla\nabla\ln N + (\mathrm{D}\ln N)\,(\mathrm{D}\ln N) + \big(\nabla\cdot(\vec{n}\mathrm{K})\big)_{\shortparallel\shortparallel}\Big) = \\ &= n^4\mathrm{K}\cdot q^{-1}\cdot\mathrm{K} - n^2\Big(\nabla\nabla\ln N + (\mathrm{D}\ln N)\,(\mathrm{D}\ln N) + \frac{1}{N}\mathrm{K}' - \frac{1}{N}\mathcal{L}_{\vec{N}}\mathrm{K}\Big) \quad , \end{aligned} \tag{G.57}$$

$$\begin{aligned} \mathrm{Ric}_{\shortparallel\shortparallel} &= \mathrm{RIC} - \nabla\nabla\ln N - (\mathrm{D}\ln N)\,(\mathrm{D}\ln N) - \big(\nabla\cdot(\vec{n}\mathrm{K})\big)_{\shortparallel\shortparallel} \quad , \\ \mathrm{Ric}_{\shortparallel\perp} &= n^2\big(\nabla\cdot q^{-1}\cdot\mathrm{K} - \mathrm{D}k\big) \quad , \\ \mathrm{Ric}_{\perp\perp} &= n^4(k^2 - \mathrm{K}^2) - n^2\nabla\cdot\big(\vec{n}\,k + q^{-1}\cdot(\mathrm{D}\ln N)\big) = \\ &= -n^4\mathrm{K}^2 - n^2\Big(\nabla^2\ln N + (\mathrm{D}\ln N)\cdot q^{-1}\cdot(\mathrm{D}\ln N) + \vec{n}\cdot\mathrm{d}k\Big) \end{aligned} \tag{G.58}$$

$$\begin{aligned} R &= \mathcal{R} + n^2(k^2 - \mathrm{K}^2) - 2\nabla\cdot\big(\vec{n}\,k + q^{-1}\cdot(\mathrm{D}\ln N)\big) = \\ &= \mathcal{R} - n^2(k^2 + \mathrm{K}^2) - 2\Big(\vec{n}\cdot\mathrm{d}k + \nabla^2\ln N + (\mathrm{D}\ln N)\cdot q^{-1}\cdot(\mathrm{D}\ln N)\Big) \end{aligned} \tag{G.59}$$

Geodesic theory near a boundary

We can develop geodesic theory on a hypersurface Σ similarly to what we did for the spacetime M. On the boundary we denote the exponential map $\boldsymbol{v}_x$, the tensor of geodesic transform and its determinant ς and $\jmath$, the world function, its derivatives and its determinant ρ, $\overrightarrow{\rho}$, $\overleftarrow{\rho}$, $\overset{\twoheadrightarrow}{\rho}$, $\overleftrightarrow{\rho}$, $\overset{\twoheadleftarrow}{\rho}$ and $\mathfrak{r}$, and Van-Vleck Morette determinant $\vartriangle$. Finally, we denote $\{.\}$ the coincidence limit on the boundary.

In the neighborhood of a part of the boundary Σ of the domain Ω in which geodesics orthogonal to the boundary do not cross we can also define the map $\hat{\boldsymbol{w}}$

$$\begin{gathered} \hat{\boldsymbol{w}} : \Sigma \times \mathbb{R} \to M \quad , \\ \hat{\boldsymbol{w}}(x,\eta) \quad \text{is geodesic} \quad , \quad \hat{\boldsymbol{w}}(x,0) = x \quad , \quad \hat{\boldsymbol{w}}'(x,0) = \vec{n} \quad . \end{gathered} \tag{G.60}$$

It maps point x on the boundary "orthogonally" to the domain Ω by the distance η. We denote Σ_η the hypersurface which we obtain by shifting $\Sigma = \Sigma_0$ by the distance η. We also use the notation

$$\begin{aligned} \hat{\boldsymbol{w}}_\eta : \Sigma \to \Sigma_\eta \quad &, \quad \hat{\boldsymbol{w}}_\eta(x) = \hat{\boldsymbol{w}}(x,\eta) \quad , \\ \hat{\boldsymbol{w}}_{\xi,\zeta} : \Sigma_\xi \to \Sigma_\zeta \quad &, \quad \hat{\boldsymbol{w}}_{\xi,\zeta} = \hat{\boldsymbol{w}}_\xi(\hat{\boldsymbol{w}}_\zeta^{-1}) \quad . \end{aligned} \tag{G.61}$$

This foliation is special case of the foliation discussed above. We obtain it for the choice of lapse and shift $N = 1$ and $\vec{N} = 0$.

For a tensor field $A(x)$ on spacetime we denote by $A(\hat{x}, \xi)$ its dependence on $\hat{x}$ and ξ, and $\widehat{A}(\hat{x}, \xi)$ the tensor field on the boundary manifold given by

$$A(\hat{x}, \xi) = A\big(\hat{\boldsymbol{w}}(\hat{x}, \xi)\big)\,\widehat{A}(\hat{x}, \xi) = \hat{\boldsymbol{w}}_{\xi}^{\star} A\big(\hat{\boldsymbol{w}}_{\xi}(\hat{x})\big) \quad , \tag{G.62}$$

where $\hat{\boldsymbol{w}}_{\xi}^{\star}$ is the induced transformation on tangent bundles. For a bi-tensor $A(x|z)$ we mean by the *boundary coincidence limit*

$$\{A\}(\hat{y}; \xi, \zeta) = A(\hat{y}, \xi|\hat{y}, \zeta) \quad . \tag{G.63}$$

Specially, we have a metric $\hat{q}(\hat{y}, \eta)$ (generally different from $q(\hat{y})$) on the boundary manifold, volume element $\hat{\mathrm{q}}^{\frac{1}{2}}(\hat{y}, \eta)$, and associated connection $\hat{\nabla}$. It is related to the connection ∇ by

$$\hat{\nabla} = \nabla \oplus \hat{\gamma} \quad . \tag{G.64}$$

The relation of corresponding curvature tensors is (see e.g. [2])

$$\begin{aligned} \hat{\mathrm{R}}_{\gamma\alpha}{}^{\delta}{}_{\beta} &= \mathrm{R}_{\gamma\alpha}{}^{\delta}{}_{\beta} + \hat{\nabla}_{\gamma}\hat{\gamma}^{\delta}_{\alpha\beta} - \hat{\nabla}_{\alpha}\hat{\gamma}^{\delta}_{\gamma\beta} + \hat{\gamma}^{\delta}_{\alpha\mu}\hat{\gamma}^{\mu}_{\gamma\beta} - \hat{\gamma}^{\delta}_{\gamma\mu}\hat{\gamma}^{\mu}_{\alpha\beta} \quad , \\ \mathrm{R\hat{I}C}_{\alpha\beta} &= \mathrm{RIC}_{\alpha\beta} + \hat{\nabla}_{\mu}\hat{\gamma}^{\mu}_{\alpha\beta} - \hat{\nabla}_{\alpha}\hat{\gamma}^{\mu}_{\beta\mu} + \hat{\gamma}^{\nu}_{\alpha\mu}\hat{\gamma}^{\mu}_{\beta\nu} - \hat{\gamma}^{\nu}_{\mu\nu}\hat{\gamma}^{\mu}_{\alpha\beta} \quad . \end{aligned} \tag{G.65}$$

From the definition of the map $\hat{\boldsymbol{w}}$ we have

$$\{\vec{\sigma}\}(\hat{y}; \xi, \zeta) = (\xi - \zeta)\,\vec{n}(\hat{y}, \xi) \quad , \tag{G.66}$$

$$\{\mathrm{D}_1\sigma\} = 0 \quad . \tag{G.67}$$

Differentiating this equation we obtain the differential map $\mathrm{D}\hat{\boldsymbol{w}}$

$$\begin{aligned} &\mathrm{D}\hat{\boldsymbol{w}}_{\xi,\zeta}(x) : \mathbf{T}_x\,\Sigma_{\xi} \to \mathbf{T}_z\,\Sigma_{\zeta} \quad , \quad z = \hat{\boldsymbol{w}}_{\xi,\zeta}(x) \quad , \\ &\mathrm{D}^{\nu}_{\mu}\hat{\boldsymbol{w}}_{\xi,\zeta}(x) = -\big(\nabla_{1\mu}\nabla_{1\kappa}\sigma\big)(x|z)\;\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1\,\kappa\nu}(x|z) \quad . \end{aligned} \tag{G.68}$$

In the special case $\xi = 0$ we get

$$\mathrm{D}^{\nu}_{\mu}\hat{\boldsymbol{w}}_{\eta}(\hat{y}) = -\big(\eta n^2 \mathrm{K}_{\mu\kappa}(\hat{y}) + \vec{\vec{\sigma}}_{\shortparallel\,\mu\kappa}(\hat{y}|\hat{y}, \eta)\big)\;\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1\,\kappa\nu}(\hat{y}|\hat{y}, \eta) \quad . \tag{G.69}$$

Here $\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1}$ is the inverse of $\overset{\leftrightarrow}{\sigma}_{\shortparallel}$ in spaces tangent to hypersurfaces Σ_{η}. Because $\mathrm{D}\hat{\boldsymbol{w}}_{\xi,\zeta} = \mathrm{D}\hat{\boldsymbol{w}}^{-1}_{\zeta,\xi}$ we have

$$\{\overset{\leftrightarrow}{\sigma}_{\shortparallel\,\mu\nu}\} = \big\{\big(\nabla_{1\mu}\nabla_{1\kappa}\sigma\big)\big(\nabla_{\mathrm{r}\nu}\nabla_{\mathrm{r}\lambda}\sigma\big)\,\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1\,\kappa\lambda}\big\} \quad . \tag{G.70}$$

Using this relation, the definition of the Van-Vleck Morette determinant and

$$\vec{n}(x)\cdot\overset{\leftrightarrow}{\sigma}(x|z) = -\vec{n}(z)\cdot g(z) \qquad \text{for} \qquad z = \hat{\boldsymbol{w}}_{\xi,\zeta}(x) \quad , \tag{G.71}$$

we get an expression for the Jacobian associated with the map $\hat{\boldsymbol{w}}_{\xi,\zeta}$,

$$\begin{aligned} \hat{\jmath}(\hat{y}; \xi, \zeta) &= \big|\mathrm{Det}_{\shortparallel}\,\mathrm{D}\hat{\boldsymbol{w}}_{\xi,\zeta}\big|\,(\hat{y}, \xi) = \\ &= \big\{\Delta^{-1}\,\mathrm{q}^{-1}\big(\mathrm{Det}_{\shortparallel}\,\nabla_1\nabla_1\sigma\big\}\big)(\hat{y}; \xi, \zeta) = \big\{\Delta\,\mathrm{q}\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathrm{r}}\nabla_{\mathrm{r}}\sigma\big\}^{-1}\big)(\hat{y}; \xi, \zeta) \quad . \end{aligned} \tag{G.72}$$

As special cases we have

$$\hat{\jmath}(\hat{y}, \eta) = \hat{\jmath}(\hat{y}; 0, \eta) \quad , \quad \hat{\jmath}(\hat{y}; \xi, \zeta) = \hat{\jmath}^{-1}(\hat{y}, \xi)\,\hat{\jmath}(\hat{y}, \zeta) \quad . \tag{G.73}$$

This also gives the expression for the Van-Vleck Morette determinant,

$$\Delta(\hat{y},\xi|\hat{y},\zeta) = \mathfrak{q}^{-\frac{1}{2}}(\hat{y},\xi)\,\mathfrak{q}^{-\frac{1}{2}}(\hat{y},\zeta)\,\Big(\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{l}}\nabla_{\mathbf{l}}\sigma\big)\,\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma\big)\Big)^{\frac{1}{2}}(\hat{y},\xi|\hat{y},\zeta) \quad . \tag{G.74}$$

Finally we can prove that

$$\hat{\jmath}(\hat{y},\xi)\,\hat{\Delta}(\hat{y},\xi|\hat{y},\zeta)\,\hat{\jmath}(\hat{y},\zeta) = \mathfrak{q}^{-1}(\hat{y})\,\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{l}}\nabla_{\mathbf{l}}\hat{\sigma}\big)(\hat{y},\xi|\hat{y},\zeta) = \mathfrak{q}^{-1}(\hat{y})\,\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\hat{\sigma}\big)(\hat{y},\xi|\hat{y},\zeta) \quad . \tag{G.75}$$

Thanks to (G.67), (G.72), and (G.73), the function $\tilde{\jmath}$ defined in (F.36) is

$$\begin{aligned}
\tilde{\jmath}(\hat{y};\xi,\zeta) &= \hat{\jmath}(\hat{y},\xi)\,\hat{\Delta}(\hat{y},\xi|\hat{y},\zeta)\;\hat{\jmath}(\hat{y},\zeta)\;\mathfrak{q}^{\frac{1}{2}}(\hat{y})\,\Big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\hat{\sigma}\Big)^{-\frac{1}{2}}(\hat{y},\xi|\hat{y},\zeta) = \\
&= \hat{\jmath}(\hat{y},\xi)\,\hat{\Delta}(\hat{y},\xi|\hat{y},\zeta)\;\hat{\mathfrak{q}}^{\frac{1}{2}}(\hat{y},\zeta)\,\Big(\mathrm{Det}_{\shortparallel}\,\hat{\nabla}_{\mathbf{r}}\hat{\nabla}_{\mathbf{r}}\hat{\sigma}\Big)^{-\frac{1}{2}}(\hat{y},\xi|\hat{y},\zeta) = \\
&= j(x)\Delta(x|z)\;\mathfrak{q}^{\frac{1}{2}}(z)\,\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma\big)^{-\frac{1}{2}}(x|z) = j(x)\;\Delta^{\frac{1}{2}}(x|z)\;\hat{\jmath}(\hat{y};\xi,\zeta)^{\frac{1}{2}} = \\
&= \Big(\hat{\jmath}(\hat{y},\xi)\,\hat{\Delta}(\hat{y},\xi|\hat{y},\zeta)\,\hat{\jmath}(\hat{y},\zeta)\Big)^{\frac{1}{2}} \quad .
\end{aligned} \tag{G.76}$$

The equation previous to this one is a straightforward consequence.

Reflection on the boundary

In chapter 14 we have worked with the *geodesic reflected on the boundary*. We recall its definition here and list some useful properties which allows us to prove the relation (F.52).

We will study the geodesic $\bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)$ between points x and z which is reflecting on the boundary at point $b(x|z)$ — an extreme trajectory of the functional given by the half of squared length, with the condition that it has to touch the boundary. We use the convention, that for any quantity depending on two spacetime points $f(x|z)$ we denote

$$f_{\mathrm{l}}(x|z) = f(x|b(x|z)) \quad , \quad f_{\mathrm{r}}(x|z) = f(b(x|z)|z) \quad . \tag{G.77}$$

If we denote the parameter at which the geodesic reflects on the boundary $\lambda_{\mathrm{r}}(x|z)$ and its complement $\lambda_{\mathrm{l}}(x|z)$

$$\begin{gathered}
b(x|z) = \bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)|_{\lambda_{\mathrm{r}}(x|z)} \in \partial\Omega \quad , \\
1 = \lambda_{\mathrm{l}}(x|z) + \lambda_{\mathrm{r}}(x|z) \quad .
\end{gathered} \tag{G.78}$$

we can write the reflected geodesic as joining of two geodesics

$$[\tau, \bar{\boldsymbol{x}}_{\mathrm{b}}] = [\lambda_{\mathrm{l}}\tau, \bar{\boldsymbol{x}}_{\mathrm{l}}] \odot [\lambda_{\mathrm{r}}\tau, \bar{\boldsymbol{x}}_{\mathrm{r}}] \quad . \tag{G.79}$$

The extremum conditions on position of the reflection point and reflection parameter are

$$\frac{(\mathrm{D}\sigma)_{\mathrm{l}}}{\lambda_{\mathrm{l}}} + \frac{(\mathrm{D}\sigma)_{\mathrm{r}}}{\lambda_{\mathrm{r}}} = 0 \quad , \quad \frac{\sigma_{\mathrm{l}}}{\lambda_{\mathrm{l}}^2} = \frac{\sigma_{\mathrm{r}}}{\lambda_{\mathrm{r}}^2} \quad . \tag{G.80}$$

We define *reflection world function* σ_{b} as

$$\sigma_{\mathrm{b}} = \frac{\sigma_{\mathrm{l}}}{\lambda_{\mathrm{l}}} + \frac{\sigma_{\mathrm{r}}}{\lambda_{\mathrm{r}}} = \frac{\sigma_{\mathrm{l}}}{\lambda_{\mathrm{l}}^2} = \frac{\sigma_{\mathrm{r}}}{\lambda_{\mathrm{r}}^2} \quad . \tag{G.81}$$

Clearly

$$\begin{gathered}
\lambda_{\mathrm{l}} = \sqrt{\frac{\sigma_{\mathrm{l}}}{\sigma_{\mathrm{b}}}} \quad , \quad \lambda_{\mathrm{r}} = \sqrt{\frac{\sigma_{\mathrm{r}}}{\sigma_{\mathrm{b}}}} \quad , \\
\sqrt{\sigma_{\mathrm{b}}} = \sqrt{\sigma_{\mathrm{l}}} + \sqrt{\sigma_{\mathrm{r}}} \quad , \quad 0 = (\mathrm{D}\sqrt{\sigma})_{\mathrm{l}} + (\mathrm{D}\sqrt{\sigma})_{\mathrm{r}} \quad ,
\end{gathered} \tag{G.82}$$

Using the last equation we can get

$$\mathrm{d}_{\mathbf{1}}\sqrt{\sigma_{\mathrm{b}}} = (\mathrm{d}_{\mathbf{1}}\sqrt{\sigma})_{\mathrm{l}} \quad , \quad \mathrm{d}_{\mathbf{r}}\sqrt{\sigma_{\mathrm{b}}} = (\mathrm{d}_{\mathbf{r}}\sqrt{\sigma})_{\mathrm{r}} \quad . \tag{G.83}$$

Similarly to the case without boundary we define

$$s_{\mathrm{b}} = \left|\sqrt{2\sigma_{\mathrm{b}}}\right| = s_{\mathrm{l}} + s_{\mathrm{r}} \tag{G.84}$$

$$\overrightarrow{\sigma}_{\mathrm{b}} = g^{-1} \cdot \mathrm{d}_{\mathbf{1}}\sigma_{\mathrm{b}} = \frac{\overrightarrow{\sigma}_{\mathrm{l}}}{\lambda_{\mathrm{l}}} \quad , \quad \overleftarrow{\sigma}_{\mathrm{b}} = \mathrm{d}_{\mathbf{r}}\sigma_{\mathrm{b}} \cdot g^{-1} = \frac{\overleftarrow{\sigma}_{\mathrm{r}}}{\lambda_{\mathrm{r}}} \quad , \tag{G.85}$$

$$\overset{\twoheadrightarrow}{\sigma}_{\mathrm{b}} = \nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sigma_{\mathrm{b}} \quad , \quad \overleftrightarrow{\sigma}_{\mathrm{b}} = \mathrm{d}_{\mathbf{1}}\mathrm{d}_{\mathbf{r}}\sigma_{\mathrm{b}} \quad , \quad \overset{\twoheadleftarrow}{\sigma}_{\mathrm{b}} = \nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}} \quad . \tag{G.86}$$

Additionally we define

$$s_{\perp} = -\frac{1}{\lambda_{\mathrm{l}}}\, \vec{n}(b) \cdot (\mathrm{d}_{\mathbf{r}}\sigma)_{\mathrm{l}} = -\frac{1}{\lambda_{\mathrm{r}}}\, \vec{n}(b) \cdot (\mathrm{d}_{\mathbf{1}}\sigma)_{\mathrm{r}} = \vec{n} \cdot (\mathrm{d}_{\mathbf{1}}\sigma_{\mathrm{b}}) = \vec{n} \cdot (\mathrm{d}_{\mathbf{r}}\sigma_{\mathrm{b}}) \quad , \tag{G.87}$$

and we denote differentials of maps $x \to b(x|z)$ and $z \to b(x|z)$ as

$$\overrightarrow{b} = \mathrm{D}_{\mathbf{1}}b \quad , \quad \overleftarrow{b} = \mathrm{D}_{\mathbf{r}}b \quad , \tag{G.88}$$

i.e. if we displace points x and z in directions X and Z, the reflection point moves in direction $X \cdot \overrightarrow{b}(x|z) + \overleftarrow{b}(x|z) \cdot Z$.

Finally we define the *reflection Van-Vleck Morette determinant* Δ_{b}

$$\Delta_{\mathrm{b}} = |\mathrm{Det}\, \overleftrightarrow{\sigma}_{\mathrm{b}}|\ \underline{\mathfrak{i}}^{-1} \quad . \tag{G.89}$$

Some long algebra gives

$$\begin{aligned}
\overset{\twoheadrightarrow}{\sigma}_{\mathrm{b}} &= -\overrightarrow{b} \cdot B \cdot \overrightarrow{b} - \frac{1}{2\sigma_{\mathrm{b}}}\frac{\lambda_{\mathrm{r}}}{\lambda_{\mathrm{l}}}(\mathrm{d}_{\mathbf{1}}\sigma_{\mathrm{b}})(\mathrm{d}_{\mathbf{1}}\sigma_{\mathrm{b}}) + \frac{1}{\lambda_{\mathrm{l}}}\overset{\twoheadrightarrow}{\sigma}_{\mathrm{l}} \quad , \\
\overleftrightarrow{\sigma}_{\mathrm{b}} &= -\overrightarrow{b} \cdot B \cdot \overleftarrow{b} + \frac{1}{2\sigma_{\mathrm{b}}}(\mathrm{d}_{\mathbf{1}}\sigma_{\mathrm{b}})(\mathrm{d}_{\mathbf{r}}\sigma_{\mathrm{b}}) \quad , \\
\overset{\twoheadleftarrow}{\sigma}_{\mathrm{b}} &= -\overleftarrow{b} \cdot B \cdot \overleftarrow{b} - \frac{1}{2\sigma_{\mathrm{b}}}\frac{\lambda_{\mathrm{l}}}{\lambda_{\mathrm{r}}}(\mathrm{d}_{\mathbf{r}}\sigma_{\mathrm{b}})(\mathrm{d}_{\mathbf{r}}\sigma_{\mathrm{b}}) + \frac{1}{\lambda_{\mathrm{r}}}\overset{\twoheadleftarrow}{\sigma}_{\mathrm{l}} \quad ,
\end{aligned} \tag{G.90}$$

where

$$B = 2\sqrt{\sigma_{\mathrm{b}}}\left(\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sqrt{\sigma})_{\mathrm{l}} + \nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sqrt{\sigma})_{\mathrm{r}}\right) = \frac{\overset{\twoheadleftarrow}{\sigma}_{\shortparallel\mathrm{l}}}{\lambda_{\mathrm{l}}} + \frac{\overset{\twoheadrightarrow}{\sigma}_{\shortparallel\mathrm{r}}}{\lambda_{\mathrm{r}}} + \frac{1}{2}\frac{\sigma_{\mathrm{b}}}{\sigma_{\mathrm{l}}\sigma_{\mathrm{r}}}(\mathrm{D}_{\mathbf{1}}\sigma)_{\mathrm{r}}(\mathrm{D}_{\mathbf{r}}\sigma)_{\mathrm{l}} + 2s_{\perp}\mathrm{K}(b) \quad . \tag{G.91}$$

Using these relations, a more intricate calculation gives the space coincidence limits

$$\left\{\overleftrightarrow{\sigma}_{\mathrm{b}\shortparallel}\right\} = -\left\{\overrightarrow{b} \cdot B \cdot \overleftarrow{b}\right\} \quad , \tag{G.92}$$

$$\left\{\frac{\overleftrightarrow{\sigma}_{\shortparallel\mathrm{l}}}{\lambda_{\mathrm{l}}}\right\} = -\left\{\overrightarrow{b} \cdot B\right\} \quad , \quad \left\{\frac{\overleftrightarrow{\sigma}_{\shortparallel\mathrm{r}}}{\lambda_{\mathrm{r}}}\right\} = -\left\{B \cdot \overleftarrow{b}\right\} \quad , \tag{G.93}$$

$$\begin{aligned}
\left\{(\nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sigma_{\mathrm{b}})^{-1}\right\} &= \left\{\overleftrightarrow{\sigma}^{-1}_{\mathrm{b}\shortparallel} \cdot (\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}})^{-1} \cdot \overleftrightarrow{\sigma}^{-1}_{\mathrm{b}\shortparallel}\right\} = \\
&= \left\{\overleftrightarrow{\sigma}^{-1}_{\shortparallel\mathrm{l}} \cdot (\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma)_{\mathrm{l}} \cdot \Big(\lambda_{\mathrm{l}}(\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma)^{-1}_{\mathrm{l}} + \lambda_{\mathrm{r}}(\nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sigma)^{-1}_{\mathrm{r}}\Big) \cdot (\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma)_{\mathrm{l}} \cdot \overleftrightarrow{\sigma}^{-1}_{\shortparallel\mathrm{l}}\right\} \quad ,
\end{aligned} \tag{G.94}$$

$$\left\{(\nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sigma_{\mathrm{b}})^{-1} \cdot \overleftrightarrow{\sigma}_{\mathrm{b}\shortparallel}\right\} = \left\{\overleftrightarrow{\sigma}^{-1}_{\mathrm{b}\shortparallel} \cdot (\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}})\right\} \quad . \tag{G.95}$$

Here inverses are taken in the spaces tangent to the boundary. Taking the determinant of the last equation, we find

$$\begin{aligned}
\left\{(\mathrm{Det}_{\shortparallel}\overleftrightarrow{\sigma}_{\mathrm{b}\shortparallel})^2\right\} &= \left\{(\mathrm{Det}_{\shortparallel}\, \nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sigma_{\mathrm{b}})\,(\mathrm{Det}_{\shortparallel}\, \nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}})\right\} \quad , \\
\Delta_{\mathrm{b}}(\hat{y},\xi|\hat{y},\zeta) &= \Big(\mathfrak{q}^{-\frac{1}{2}}(\hat{y},\xi)\, \mathfrak{q}^{-\frac{1}{2}}(\hat{y},\zeta)\ (\mathrm{Det}_{\shortparallel}\, \nabla_{\mathbf{1}}\nabla_{\mathbf{1}}\sigma_{\mathrm{b}})\,(\mathrm{Det}_{\shortparallel}\, \nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}})\Big)^{\frac{1}{2}}(\hat{y},\xi|\hat{y},\zeta) \quad .
\end{aligned} \tag{G.96}$$

and

$$\frac{j^2(x)}{\mathfrak{q}(x)}\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{l}}\nabla_{\mathbf{l}}\sigma_{\mathrm{b}}\big)(x|z) = \frac{j^2(z)}{\mathfrak{q}(z)}\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}}\big)(x|z) = \\ = \frac{j^2(\hat{y})}{\mathfrak{q}(\hat{y})}\Big(\lambda_{\mathrm{l}}(\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma)_{\mathrm{l}}^{-1} + \lambda_{\mathrm{r}}(\nabla_{\mathbf{l}}\nabla_{\mathbf{l}}\sigma)_{\mathrm{r}}^{-1}\Big)(x|z) \tag{G.97}$$

for $x = \hat{\boldsymbol{w}}(\hat{y},\xi)$ and $z = \hat{\boldsymbol{w}}(\hat{y},\zeta)$. Putting these relation together we obtain

$$j(x)\,\Delta_{\mathrm{b}}(x|z) j(z) = \frac{j^2(x)}{\mathfrak{q}(x)}\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{l}}\nabla_{\mathbf{l}}\sigma_{\mathrm{b}}\big)(x|z) = \frac{j^2(z)}{\mathfrak{q}(z)}\big(\mathrm{Det}_{\shortparallel}\,\nabla_{\mathbf{r}}\nabla_{\mathbf{r}}\sigma_{\mathrm{b}}\big)(x|z) \tag{G.98}$$

for $x = \hat{\boldsymbol{w}}(\hat{y},\xi)$ and $z = \hat{\boldsymbol{w}}(\hat{y},\zeta)$. The equality in (F.52) is a straightforward consequence of this relation.

Covariant expansions near boundary

Finally we will write down coefficients in covariant expansions (F.32) and (F.33) of the world function σ and function l defined in (F.30). These are expansions *inside* of the boundary manifold of $\hat{\boldsymbol{w}}$-mapped functions $\hat{\sigma}(\hat{x},\xi|\hat{z},\zeta)$ and $\hat{l}(\hat{x},\xi|\hat{z},\zeta)$ around point $\hat{x}$. The derivation is long and technical. It uses the general method discussed above and a transformation of the connection ∇ to the connection $\hat{\nabla}$. Fortunately, we need only the spacetime coincidence limit of the coefficients (i.e. $\hat{\sigma}_{k,l}(\hat{y};\eta,\eta)$), which simplifies the calculations significantly. But even then the calculations is too long and uninteresting to be included it here. We list only the results. See also [26,34,35] for similar calculations.

The coefficients of the boundary covariant expansion of the spacetime world function $\hat{\sigma}$ at some general point $\hat{y}$ (slight generalization of eq. (F.32)) are

$$\hat{\sigma}_{0,0}(\hat{y};\xi,\zeta) = \frac{1}{2}n^2\,(\xi-\zeta)^2 \quad , \tag{G.99}$$

$$\hat{\sigma}_{0,1}(\hat{y};\xi,\zeta) = \hat{\sigma}_{1,0}(\hat{y};\xi,\zeta) = 0 \quad , \tag{G.100}$$

$$[\hat{\sigma}_{2,0}] = -[\hat{\sigma}_{1,1}] = [\hat{\sigma}_{0,2}] = \hat{q} \quad , \tag{G.101}$$

$$[\hat{\sigma}_{3,0\,\alpha\beta\gamma}] = [\hat{\sigma}_{0,3\,\alpha\beta\gamma}] = 3\hat{\gamma}^{\;\mu}_{(\alpha\beta}\hat{q}_{\gamma)\mu} \quad , \quad [\hat{\sigma}_{2,1\,\alpha\beta\,\kappa}] = [\hat{\sigma}_{1,2\,\kappa\,\alpha\beta}] = -\hat{\gamma}^{\;\mu}_{\alpha\beta}\hat{q}_{\kappa\mu} \quad , \tag{G.102}$$

$$[\hat{\sigma}_{4,0\,\alpha\beta\gamma\delta}] = [\hat{\sigma}_{0,4\,\alpha\beta\gamma\delta}] = \\ = -n^2\hat{\mathrm{K}}_{(\alpha\beta}\hat{\mathrm{K}}_{\gamma\delta)} + 4(\hat{\nabla}_{(\alpha}\hat{\gamma}^{\;\mu}_{\beta\gamma})\hat{q}_{\delta)\mu} + 8\hat{\gamma}^{\;\nu}_{\mu(\alpha}\hat{\gamma}^{\;\mu}_{\beta\gamma}\hat{q}_{\delta)\nu} + 3\hat{\gamma}^{\;\mu}_{(\alpha\beta}\hat{\gamma}^{\;\nu}_{\gamma\delta)}\hat{q}_{\mu\nu} \quad , \\ [\hat{\sigma}_{3,1\,\alpha\beta\gamma\,\kappa}] = [\hat{\sigma}_{1,3\,\kappa\,\alpha\beta\gamma}] = \\ = n^2\hat{\mathrm{K}}_{(\alpha\beta}\hat{\mathrm{K}}_{\gamma)\kappa} - (\hat{\nabla}_{(\alpha}\hat{\gamma}^{\;\mu}_{\beta\gamma)})\hat{q}_{\mu\kappa} - \hat{\gamma}^{\;\mu}_{(\alpha\beta}\hat{\gamma}^{\;\nu}_{\gamma)\mu}\hat{q}_{\nu\kappa} \quad , \\ [\hat{\sigma}_{2,2\,\alpha\beta\,\kappa\lambda}] = -\frac{1}{3}\big(\mathrm{R}_{\alpha\kappa\beta\lambda} + \mathrm{R}_{\alpha\lambda\beta\kappa}\big) - \\ -\frac{1}{3}n^2\hat{\mathrm{K}}_{\alpha\kappa}\hat{\mathrm{K}}_{\beta\lambda} - \frac{1}{3}n^2\hat{\mathrm{K}}_{\alpha\lambda}\hat{\mathrm{K}}_{\beta\kappa} - n^2\hat{\mathrm{K}}_{\alpha\beta}\hat{\mathrm{K}}_{\kappa\lambda} - \hat{\gamma}^{\;\mu}_{\alpha\beta}\hat{\gamma}^{\;\nu}_{\kappa\lambda}\hat{q}_{\mu\nu} \quad . \tag{G.103}$$

The coefficients of the boundary covariant expansion of the function l at some general point $\hat{y}$ (slight generalization of eq. (F.33)) are

$$[\hat{l}_{0,0}] = 2\ln\hat{j} \quad , \tag{G.104}$$

$$[\hat{l}_{1,0\,\alpha}] = [\hat{l}_{0,1\,\alpha}] = \hat{\gamma}^{\;\mu}_{\alpha\mu} \quad , \tag{G.105}$$

$$
\begin{aligned}
[\hat{l}_{2,0\,\alpha\beta}] = [\hat{l}_{0,2\,\alpha\beta}] &= \\
= \frac{1}{3}\Big(&-\hat{\mathrm{K}}'_{\alpha\beta} + 2n^2\hat{\mathrm{K}}_{\alpha\mu}\hat{\mathrm{K}}_{\beta\nu}\hat{q}^{-1\,\mu\nu} - n^2\hat{\mathrm{K}}_{\alpha\beta}\hat{k} + \\
&+ 3\hat{\nabla}_{(\mu}\hat{\gamma}^{\ \mu}_{\alpha\beta)} + \hat{\gamma}^{\ \mu}_{\alpha\nu}\hat{\gamma}^{\ \nu}_{\beta\mu} + 2\hat{\gamma}^{\ \mu}_{\alpha\beta}\hat{\gamma}^{\ \nu}_{\mu\nu}\Big) \quad , \\
[\hat{l}_{1,1\,\alpha\,\beta}] = \frac{1}{3}\Big(&\hat{\mathrm{K}}'_{\alpha\beta} - 2n^2\hat{\mathrm{K}}_{\alpha\mu}\hat{\mathrm{K}}_{\beta\nu}\hat{q}^{-1\,\mu\nu} + n^2\hat{\mathrm{K}}_{\alpha\beta}\hat{k}\Big)
\end{aligned}
\tag{G.106}
$$

Computing normal derivatives we also get

$$
\begin{aligned}
\frac{1}{n}(\ln\hat{\jmath})' &= n\hat{k} \quad , \\
\frac{1}{n^2}(\ln\hat{\jmath})'' &= \hat{k}' \quad ,
\end{aligned}
\tag{G.107}
$$

and

$$
\begin{aligned}
\frac{1}{n}[(\ln\hat{\jmath})^{\mathbf{r}'}] &= 0 \quad , \\
\frac{1}{n^2}[(\ln\hat{\jmath})^{\mathbf{r}'\mathbf{r}'}] &= -\frac{1}{3}\mathrm{l}(\hat{k}' + n^2\hat{\mathrm{K}}^2) \quad .
\end{aligned}
\tag{G.108}
$$

Finally, we have boundary coincidence limits

$$
\{\sigma_{\mathrm{b}}\}(\hat{y};\xi,\zeta) = \frac{1}{2}n^2(\xi+\zeta)^2 \quad , \quad \{s_\perp\}(\hat{y};\xi,\zeta) = n^2(\xi+\zeta) \quad , \tag{G.109}
$$

$$
\{\vec{\sigma}_{\mathrm{b}}\}(\hat{y};\xi,\zeta) = (\xi+\zeta)\vec{n}(\hat{y},\xi) \quad , \quad \{\overleftarrow{\sigma}_{\mathrm{b}}\}(\hat{y};\xi,\zeta) = (\xi+\zeta)\vec{n}(\hat{y},\zeta) \quad , \tag{G.110}
$$

$$
\{\lambda_{\mathrm{l}}\}(\hat{y};\xi,\zeta) = \frac{\xi}{\xi+\zeta} \quad , \quad \{\lambda_{\mathrm{r}}\}(\hat{y};\xi,\zeta) = \frac{\zeta}{\xi+\zeta} \quad . \tag{G.111}
$$

Using these relations, equations (G.92), (G.93), with help of (G.69) and

$$
\{\vec{\vec{\sigma}}_{\shortparallel\mathrm{r}}\}(\hat{y};\xi,\zeta) = q(\hat{y}) + \mathcal{O}(\zeta^2) \quad , \quad \{\overleftarrow{\overleftarrow{\sigma}}_{\shortparallel\mathrm{l}}\}(\hat{y};\xi,\zeta) = q(\hat{y}) + \mathcal{O}(\xi^2) \tag{G.112}
$$

we can derive

$$
-\{\overleftrightarrow{\sigma}_{\mathrm{b}\shortparallel}\}(\hat{y};\xi,\zeta) = q(\hat{y}) + \Big(\xi+\zeta-2\frac{\xi\zeta}{\xi+\zeta}\Big)n^2\mathrm{K}(\hat{y}) + \mathcal{O}((\xi+\zeta)^2) \quad . \tag{G.113}
$$

From this follows

$$
\{\hat{\Delta}_{\mathrm{b}}\}(\hat{y};\xi,\zeta) = 1 + \Big(\xi+\zeta-2\frac{\xi\zeta}{\xi+\zeta}\Big)n^2k(\hat{y}) + \mathcal{O}((\xi+\zeta)^2) \quad . \tag{G.114}
$$

Together with

$$
\hat{\jmath}(\hat{y},\eta) = 1 + n^2k(\hat{y})\eta + \mathcal{O}(\eta^2) \tag{G.115}
$$

and the definition (F.52), it finally gives the expansion for $\tilde{\jmath}_{\mathrm{b}}$,

$$
\tilde{\jmath}_{\mathrm{b}}(\hat{y};\xi,\lambda,\zeta) = 1 + \Big(\frac{\xi+\zeta}{2} - (1-2p)\lambda\Big)n^2k(\hat{y}) + \mathcal{O}((\xi+\zeta+\lambda)^2) \quad . \tag{G.116}
$$

H Special functions R_ν

In appendix F we have used various integrals of exponentials of quadratic exponent and integrals of such integrals. Here we summarize properties of such integrals. We will introduce a special function R_ν closely related to error functions $\mathrm{erfc}(x)$, the definition and properties of which can be found, for example, in [38]. The derivation of the properties below are not all simple, and we do not include them here.

We define the function $\mathrm{R}_\nu(x)$ for positive ν as

$$\mathrm{R}_\nu(z) = \frac{1}{\Gamma(\nu)} \int\limits_{\mathbb{R}^+} dx\, x^{\nu-1} \exp\Big(-\frac{1}{2}(x-z)^2\Big) \quad . \tag{H.1}$$

It is a solution of the differential equation

$$\mathrm{R}'_\nu(z) = \nu \mathrm{R}_{\nu+1}(z) - z\mathrm{R}_\nu(z) \quad , \quad \mathrm{R}_\nu \xrightarrow{z\to-\infty} 0 \quad . \tag{H.2}$$

In the limit $\nu \to 0$ and for $\nu = 1$ we have

$$\mathrm{R}_0(z) = \exp\Big(-\frac{1}{2}z^2\Big) \quad , \tag{H.3}$$

$$\mathrm{R}_1(z) = \sqrt{2\pi} - \sqrt{\frac{\pi}{2}}\,\mathrm{erfc}\Big(\frac{z}{\sqrt{2}}\Big) \quad . \tag{H.4}$$

We also have the recurrence relation

$$\mathrm{R}_{\nu+2}(z) = \frac{1}{\nu+1}\big(z\,\mathrm{R}_{\nu+1}(z) + \mathrm{R}_\nu(z)\big) \quad . \tag{H.5}$$

For $\nu \in \mathbb{N}$ these functions are combinations of R_0 and R_1 with polynomial coefficients

$$\mathrm{R}_{n+1} = \mathrm{p}_n \mathrm{R}_1 + \mathrm{q}_{n-1}\mathrm{R}_0 \qquad \text{for} \qquad n \in \mathbb{N} \quad , \tag{H.6}$$

where

$$\begin{aligned} \mathrm{p}_{n+1}(z) &= \frac{1}{n+1}\big(z\,\mathrm{p}_n(z) + \mathrm{p}_{n-1}(z)\big) \quad , \quad \mathrm{p}_0 = 1 \quad , \quad \mathrm{p}_1 = z \quad , \\ \mathrm{q}_{n+1}(z) &= \frac{1}{n+2}\big(z\,\mathrm{q}_n(z) + \mathrm{q}_{n-1}(z)\big) \quad , \quad \mathrm{q}_0 = 1 \quad , \quad \mathrm{q}_1 = \frac{1}{2}z \quad . \end{aligned} \tag{H.7}$$

These polynomials satisfy

$$\mathrm{p}'_n = \mathrm{p}_{n-1} \quad , \quad \mathrm{q}'_n = (n+2)\,\mathrm{q}_{n+1} - \mathrm{p}_{n+1} \quad , \tag{H.8}$$

and

$$\sqrt{2\pi}\,\mathrm{p}_n(z) = \mathrm{R}_{n+1}(z) + (-1)^n \mathrm{R}_{n+1}(-z) = \frac{\sqrt{2\pi}}{i^n 2^{\frac{n}{2}} n!}\mathrm{H}_n\big(i\tfrac{z}{\sqrt{2}}\big) \quad , \tag{H.9}$$

where H_n are the Hermite polynomials (see [38]).

Values at zero are

$$\mathrm{R}_\nu(0) = 2^{\frac{\nu}{2}} \frac{\Gamma(\frac{\nu}{2}+1)}{\Gamma(\nu+1)} = \frac{1}{2} \frac{\sqrt{2\pi}}{2^{\frac{\nu-1}{2}} \Gamma(\frac{\nu-1}{2}+1)} = \begin{cases} \frac{1}{(\nu-1)!!} & \text{for } \nu \text{ natural and even} \\ \frac{1}{\nu!!}\sqrt{\frac{\pi}{2}} & \text{for } \nu \text{ natural and odd} \end{cases} \quad , \tag{H.10}$$

$$\mathrm{p}_n(0) = \begin{cases} \frac{1}{n!!} & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd} \end{cases} \quad , \qquad \mathrm{p}'_n = \begin{cases} 0 & \text{for } n \text{ even} \\ \frac{1}{(n-1)!!} & \text{for } n \text{ odd} \end{cases} \quad , \tag{H.11}$$

$$\mathrm{q}_n(0) = \begin{cases} \frac{1}{(n+1)!!} & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd} \end{cases} \quad , \qquad \mathrm{q}'_n = \begin{cases} 0 & \text{for } n \text{ even} \\ \frac{1}{n!!} - \frac{1}{(n+1)!!} & \text{for } n \text{ odd} \end{cases} \quad . \tag{H.12}$$

The behavior for small z can be found for natural ν with help of relations (H.5) and

$$\begin{aligned} \mathrm{R}_0(z) &= \sum_{k\in\mathbb{N}_0} \frac{(-1)^k}{(2k)!!} z^{2k} \quad , \\ \mathrm{R}_1(z) &= \sqrt{\frac{\pi}{2}} + \sum_{k\in\mathbb{N}_0} \frac{(-1)^k}{(2k+1)\,(2k)!!} z^{2k+1} \quad . \end{aligned} \tag{H.13}$$

The behavior for $|z| \gg 1$ and $n \in \mathbb{N}_0$ is

$$\mathrm{R}_{n+1}(z) = \sqrt{2\pi}\,\mathrm{p}_n(z)\,\theta(z) + \exp\Big(-\frac{1}{2}z^2\Big)\,\mathcal{O}\Big(\frac{1}{z^{n+1}}\Big) \quad , \tag{H.14}$$

where $\theta(z)$ is the step function.

Now we can write down results of some integrals in terms of these functions. For $n \in \mathbb{N}_0$ we have

$$\frac{1}{n!} \int_{\mathbb{R}} dx\, x^n \exp\Big(-\frac{1}{2}(x-z)^2\Big) = \sqrt{2\pi}\,\mathrm{p}_n(z) \quad . \tag{H.15}$$

Further for $k, l \in \mathbb{N}_0$ we have

$$\begin{aligned} \frac{1}{l!} \int_{\langle -\infty, x\rangle} dx\, \xi^l \mathrm{R}_k(x) &= \sum_{m=0,\dots,l} \frac{(-1)^{l+m}}{m!} x^m \mathrm{R}_{k+l-m+1}(x) = \\ &= \sqrt{2\pi}(-1)^l \mathrm{p}_{k+l}(0) + \frac{\sqrt{2\pi}}{l!\,(k-1)!} \sum_{\substack{m\in\mathbb{N} \\ 2m\leqslant k-1}} \frac{(2m-1)!!}{k+l-2m} \binom{k-1}{2m} x^{k+l-2m} - \\ &\qquad - \sum_{m=0,\dots,l} \frac{1}{m!} x^m \mathrm{R}_{k+l-m+1}(-x) \quad , \end{aligned} \tag{H.16}$$

$$\begin{aligned} \frac{1}{l!} \int_{\langle 0, x\rangle} dx\, \xi^l \mathrm{R}_k(x) &= \\ &= (-1)^k \mathrm{R}_{k+l+1}(0) + \frac{\sqrt{2\pi}}{l!\,(k-1)!} \sum_{\substack{m\in\mathbb{N} \\ 2m\leqslant k-1}} \frac{(2m-1)!!}{k+l-2m} \binom{k-1}{2m} x^{k+l-2m} - \\ &\qquad - \sum_{m=0,\dots,l} \frac{1}{m!} x^m \mathrm{R}_{k+l-m+1}(-x) \quad . \end{aligned} \tag{H.17}$$

Finally for $m, k, l \in \mathbb{R}^+$ and $n = m + k + l$ we have

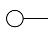
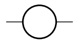
$$\frac{1}{n!} \int_{\xi,\zeta\in\mathbb{R}^+} d\xi\, d\zeta\, \frac{\xi^{m+k}\zeta^{m+l}}{(\xi+\zeta)^m} \exp\Big(-\frac{1}{2}(\xi+\zeta)^2\Big) = \sqrt{2\pi}\, 2^{-\frac{n+1}{2}} \frac{\Gamma(m+k+1)\,\Gamma(m+l+1)}{\Gamma(b+m+1)\,\Gamma(\frac{n+1}{2})} \quad . \tag{H.18}$$

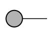
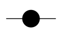
I Diagrammatic notation

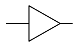
In this appendix we make some comments about the diagrammatic notation. A well-known application of this notation are Feynman diagrams used in field theory (a modification of which we use in the text). But in general, this notation is nothing other then a graphical representation of algebra of tensor objects. See for example [27] for an application to the spacetime tensors and spinors.

The main idea is to represent tensors by geometrical objects with "legs" which correspond to tensor indices. Different kind of tensor indices should be represented by different kind of legs. The contraction of tensor indices is represented by connection of corresponding legs. We can add the diagrams with the same leg structure and multiply them to obtain a diagram with more complicated leg structure which represents the tensor product of the component.

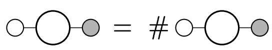
The only difference from the usual algebra is that we associate with each diagram a *symmetry factor* and we include the reciprocal of this numerical factor with the diagram. The symmetry factor is the number of ways in which the diagram can be re-arranged to obtain the identical diagram. If we want to use the diagram without the symmetry factor, we precede it with a # sign. To illustrate this convention we give some examples. Let a, b, k, H, and O be tensors represented by following diagrams

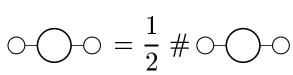
$a^n \quad \leftrightarrow$  ; $k_{mn} \quad \leftrightarrow$  , $k_{mn} = k_{nm}$,

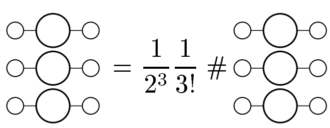
$b^n \quad \leftrightarrow$  ; $H^{mn} \quad \leftrightarrow$  , $H^{mn} = H^{nm}$, (I.1)

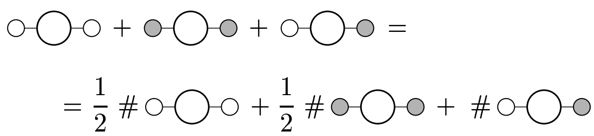
$\mathrm{O}^m_n \quad \leftrightarrow$  .

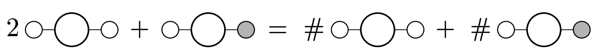
We can write

$a^m k_{mn} b^n \quad \leftrightarrow$  , (I.2)

$\frac{1}{2} a^m k_{mn} a^n \quad \leftrightarrow$  , (I.3)

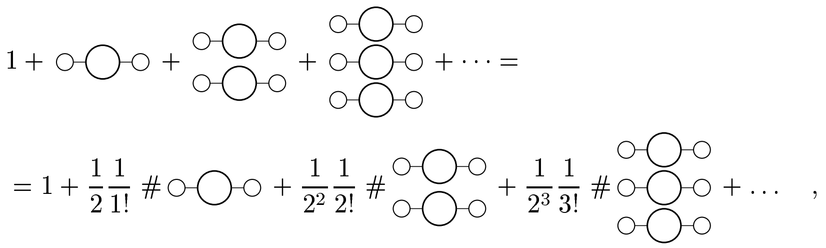
$\frac{1}{2^3}\frac{1}{3!}(a^m k_{mn} a^n)^3 \quad \leftrightarrow$  , (I.4)

$\frac{1}{2}(a^m + b^m) k_{mn} (a^n + b^n) \quad \leftrightarrow$  ,

$(a^m + b^m) k_{mn} a^n \quad \leftrightarrow$  . (I.6)

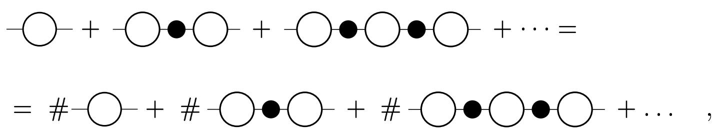
Power expansion of some functions gives

$$\exp\Big(\frac{1}{2}a^m k_{mn} a^n\Big) \quad \leftrightarrow$$



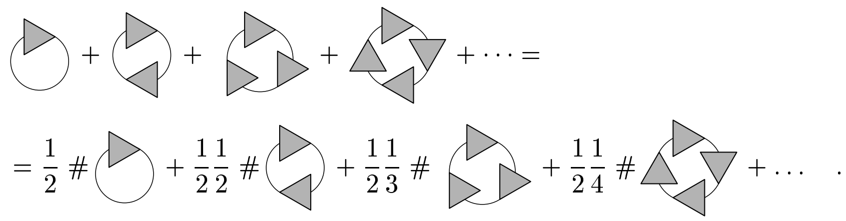
(I.7)

$$\Big(k^{-1} - H\Big)^{-1}{}_{mn} \quad \leftrightarrow$$



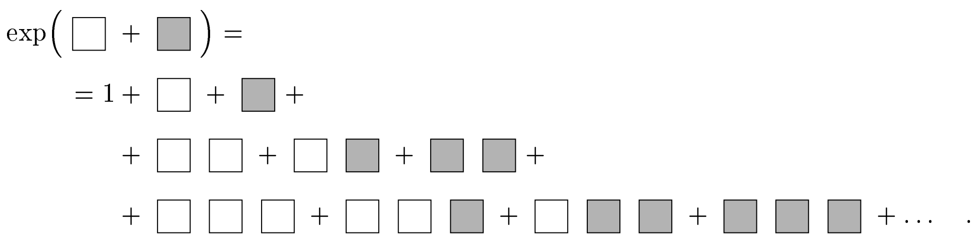
(I.8)

$$-\frac{1}{2}\,\mathrm{tr}\ln\big(\delta - \mathrm{O}\big) \quad \leftrightarrow$$



(I.9)

There are some common operation which have a nice graphical interpretation. Let have some set of elementary connected diagrams (i.e. diagrams which are not explicit product of other diagrams) without free legs. The sum of all diagrams composed of an arbitrary number of these connected diagrams is the exponential of the sum of the diagrams. For example

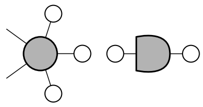


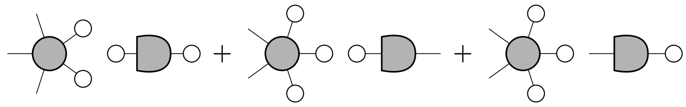
(I.10)

This fact is powerful in an opposite direction — if an expression is given by the sum of all possible products of elementary connected components, the sum of these connected components is given by logarithm of the expression.

In combination with (I.9) we also find that $\det(\delta - \mathrm{O})^{-\frac{1}{2}}$ is given by the sum of all possible products of loops formed using the diagram of the operator O.

Next, let us have an expression given by the product of elementary diagrams which contains the diagram representing a vector a. We can understand it as an analytical tensor-valued function of the vector a. The derivation with respect of its argument is graphically represented as sum of graphs which we get by "tearing out" the diagram a from all possible symmetrically non-equivalent positions. E.g.

$F_{\boldsymbol{mn}}(a) \quad \leftrightarrow$  ,

$\mathrm{d}_{\boldsymbol{k}} F_{\boldsymbol{mn}}(A) \quad \leftrightarrow$  . (I.11)

Note that the numerical factors above are correct thanks to symmetry factors included in the diagrams.

Notes

1 To define the "velocity" — an inner space derivative of the history — we need some additional structure on the fibre bundle $\boldsymbol{\mathcal{H}}$, for example a connection on this bundle. There can exist a natural connection (for example if we can identify fibres of the bundle) or a choice of the connection is equivalent to specification of a external field (e.g., a gauge field for the Yang-Mills theories). In the following we will not need to specify the exact nature of this structure. We will only assume that velocities $\mathcal{D}\mathrm{h}$ have a vector bundle structure over the inner manifold M so we can define the derivative of the Lagrangian density with respect of the velocities $\frac{\partial \mathcal{L}}{\partial \mathcal{D}\mathrm{h}}$. For the definition of the derivative of the Lagrangian density with respect of boundary value we need also some additional structure (see appendix C for discussion of similar questions for tangent bundles) which we also will not specify becacause we are not interested in an exact form of the equations of motion at this moment.

2 $[\xi_1, \xi_2]$ are Lie brackets of the tangent vectors ξ_1, ξ_2.

3 We should be careful to distinguish the spaces $\boldsymbol{\mathcal{P}}$ and $\boldsymbol{\mathcal{S}}$. We have $\boldsymbol{\mathcal{S}} \subset \boldsymbol{\mathcal{P}}$ but it is not true for duals $\boldsymbol{\mathcal{S}}^\star \not\subset \boldsymbol{\mathcal{P}}^\star$. We can only define a natural restriction $\boldsymbol{\mathcal{P}}^\star \mapsto \boldsymbol{\mathcal{S}}^\star$. Similar comments apply for $\boldsymbol{\mathcal{B}}$ and $\boldsymbol{\mathcal{S}}$. Therefore, if we will work with tensors intrinsic to $\boldsymbol{\mathcal{S}}$ we use the tensor indices $_{A}, _{B}, \dots$ and we use $\circ$ for the contraction operation. But for vector objects we sometimes use the natural identification $\boldsymbol{\mathcal{S}} \subset \boldsymbol{\mathcal{P}}$ or $\boldsymbol{\mathcal{S}} \subset \boldsymbol{\mathcal{B}}$, for example for $\phi_1, \phi_2 \in \boldsymbol{\mathcal{S}}$

$$\phi_1 \circ \overleftrightarrow{\omega} \circ \phi_2 = \phi_1 \bullet \partial\mathcal{F}[\Sigma] \bullet \phi_2 = \phi_1 \diamond \left(\underline{\pi}_{\mathrm{i}} \cdot \underline{\varphi}_{\mathrm{i}} - \underline{\varphi}_{\mathrm{i}} \cdot \underline{\pi}_{\mathrm{i}}\right) \diamond \phi_2 \quad ,$$

where in the former term the symplectic form lives on $\boldsymbol{\mathcal{S}}$, in the second one in $\boldsymbol{\mathcal{P}}$ and in the last one in $\boldsymbol{\mathcal{B}}$.

4 We have $\mathbf{T}\,\Sigma \subset \mathbf{T}\,M$, so there is a unique meaning in writing a space vector with a spacetime index (e.g. $\vec{N}^{\boldsymbol{\alpha}}$). It is not well defined for covectors. To write $q_{\boldsymbol{\alpha\beta}}$ we have to specify that we are using an orthogonal projection from $\mathbf{T}\,M$ to $\mathbf{T}\,\Sigma$ in sense of the metric $g_{\boldsymbol{\alpha\beta}}$.

5 We are using the following convention for operators

$$\begin{aligned} \pi \cdot \mathsf{p} \cdot \varphi &= \pi_{\mathbf{x}}\, \mathsf{p}^{\mathbf{x}}_{\mathbf{y}}\, \varphi^{\mathbf{y}} \quad , \\ \varphi \cdot \mathsf{p} \cdot \pi &= \varphi^{\mathbf{y}}\, \mathsf{p}^{\mathbf{x}}_{\mathbf{y}}\, \pi_{\mathbf{x}} \quad . \end{aligned}$$

This means that in the first case the operator p acts to the right, in the latter case to the left. The order is determined by the fact that φ is vector and π is covector. This convention simulates contraction of vector indices, and it is necessary to be careful in some cases. For example if $A, B \in \boldsymbol{\mathcal{S}}^1_1$ are operators on $\boldsymbol{\mathcal{S}}$ we can write

$$(A \circ \overleftrightarrow{\omega} \circ G_c \circ B)^{\boldsymbol{x}}_{\boldsymbol{y}} = A^{\boldsymbol{u}}_{\boldsymbol{y}}\, \overleftrightarrow{\omega}_{\boldsymbol{uz}}\, G_c^{\boldsymbol{zv}}\, B^{\boldsymbol{x}}_{\boldsymbol{v}} = -A^{\boldsymbol{u}}_{\boldsymbol{y}}\, \delta_{\boldsymbol{\mathcal{S}}}{}^{\boldsymbol{v}}_{\boldsymbol{u}}\, B^{\boldsymbol{x}}_{\boldsymbol{v}} = -(B \circ A)^{\boldsymbol{x}}_{\boldsymbol{y}} \quad .$$

Note the reverse order of the operators in the last term. To get used to the convention, we give another example. Let J be an operator on $\boldsymbol{\mathcal{S}}$ satisfying $\mathsf{J} \circ \overleftrightarrow{\omega} = -\overleftrightarrow{\omega} \circ \mathsf{J}$. We can write

$$\mathsf{J} \circ \overleftrightarrow{\omega} = -\overleftrightarrow{\omega} \circ \mathsf{J} = \overleftrightarrow{\omega}^{\top} \circ \mathsf{J} = (\mathsf{J} \circ \overleftrightarrow{\omega})^{\top}$$

or, using indices,

$$(\mathsf{J} \circ \overleftrightarrow{\omega})_{\boldsymbol{xy}} = \mathsf{J}^{\boldsymbol{z}}_{\boldsymbol{x}}\, \overleftrightarrow{\omega}_{\boldsymbol{zy}} = -\overleftrightarrow{\omega}_{\boldsymbol{xz}}\, \mathsf{J}^{\boldsymbol{z}}_{\boldsymbol{y}} = \overleftrightarrow{\omega}_{\boldsymbol{zx}}\, \mathsf{J}^{\boldsymbol{z}}_{\boldsymbol{y}} = \mathsf{J}^{\boldsymbol{z}}_{\boldsymbol{y}}\, \overleftrightarrow{\omega}_{\boldsymbol{zx}} = (\mathsf{J} \circ \overleftrightarrow{\omega})_{\boldsymbol{yx}} = (\mathsf{J} \circ \overleftrightarrow{\omega})^{\top}_{\boldsymbol{xy}} \quad .$$

6 On any manifold M we can define a vector bundle of tangent densities of a weight α which we denote $\tilde{\mathbb{R}}^\alpha\, M$ or $\tilde{\mathbb{C}}^\alpha\, M$ if the densities are real or complex. The space of sections will be denoted $\tilde{\mathfrak{F}}^\alpha\, M$. The standard fiber of this bundles are vector space of real or complex numbers. As for any tangent bundle, the density bundle can be defined by a map from bases e_a in tangent

vector spaces to the standard fiber which is a representation of the linear group on the bases. The map tells by what factor is a density μ is different from the coordinate density ϵ given by the base e_a

$$\mu[e_a] = \mu\epsilon^{-1} \quad , \quad \epsilon[e_a] = 1 \quad .$$

The representation for densities of the weight α is

$$\mu[A^b_a e_b] = (\det A)^\alpha \, \mu[e_a] \quad .$$

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

Beside the linear operation we can define also multiplication and constant powers of densities. Of course, these operations map densities of some weight to densities of a different weight. Let us note that complex conjugation maps the densities of a weight α to densities of the weight α^* and therefore “the absolute value” belongs to densities of weight $\operatorname{Re}\alpha$.

[7] Polar decomposition is a decomposition of an operator in a Hilbert space into its absolute value and signum. We will use it for a real Hilbert space, i.e. a real vector space with a scalar product defined by a symmetric positive quadratic form h

$$\begin{aligned} &(a,b) = a^{\mathbf{T}} \cdot b = a \cdot h \cdot b && a, b \text{ vectors} \quad , \\ &A^{\mathbf{T}} = h^{-1} \cdot A \cdot h && A \text{ an operator} \quad . \end{aligned}$$

There exists unique left and right decomposition of an operator O

$$O = |O|_l \cdot \operatorname{sign}_l O = \operatorname{sign}_r O \cdot |O|_r$$

to a positive definite symmetric operator $|O|_l$ or $|O|_r$ and an orthogonal operator $\operatorname{sign}_l O$ or $\operatorname{sign}_r O$

$$\begin{gathered} |O|^{\mathbf{T}}_{l,r} = |O|_{l,r} \quad , \quad |O|_{l,r} \quad \text{positive definite} \quad , \\ (\operatorname{sign}_{l,r} O)^{\mathbf{T}} = (\operatorname{sign}_{l,r} O)^{-1} \quad , \end{gathered}$$

and these operators are given by

$$\begin{gathered} |O|_l = \left(O \cdot O^{\mathbf{T}}\right)^{\frac{1}{2}} \quad , \quad |O|_r = \left(O^{\mathbf{T}} \cdot O\right)^{\frac{1}{2}} \quad , \\ \operatorname{sign}_l O = |O|_l^{-1} \cdot O \quad , \quad \operatorname{sign}_r O = O \cdot |O|_r^{-1} \quad . \end{gathered}$$

If O commutes with $O^{\mathbf{T}}$ both decompositions coincide.

[8] Let us remember that in our convention

$$\langle \phi, \mathbf{u} \rangle_p^{\boldsymbol{m}} = \prod_{\mathrm{k} \in \mathcal{I}} \langle \phi, u_{\mathrm{k}} \rangle_p^{m_{\mathrm{k}}}$$

and

$$\big[\mathbf{u} \circ \mathrm{d}\big]^{\boldsymbol{m}} F = \Big[\prod_{\mathrm{k} \in \mathcal{I}} \big[u_{\mathrm{k}} \circ \mathrm{d}\big]^{m_{\mathrm{k}}}\Big] F \quad .$$

[9] Filled circles correspond to disconnected transition amplitudes and empty circles to connected ones. As with usual Feynman diagrams, numerical prefactors computable from the symmetry of diagrams are included in diagrams. See more appendix I and chapter 15 for more details on diagrammatic notation.

[10] We use the proper normalization of the position bases and choose the density weight of the base equal to $(\frac{1}{2} - i\gamma_{\mathrm{f}})$ and $(\frac{1}{2} - i\gamma_{\mathrm{i}})$, where γ_{f} and γ_{i} are the order parameters as defined in (5.9). I.e. we do not need to choose any volume element on $\mathcal{V}[\Sigma_{\mathrm{f}}]$ or $\mathcal{V}[\Sigma_{\mathrm{i}}]$ and it makes sense to write, for example

$$\hat{\mathsf{F}}_{\mathrm{f}\, f} = \int\limits_{\mathrm{x_f} \in \mathcal{V}[\Sigma_{\mathrm{f}}]} |\mathrm{f}\, pos : \mathrm{x_f}\rangle\langle \mathrm{f}\, pos : \mathrm{x_f}| \quad .$$

[11] More precisely, in the Heisenberg picture which we are using, the physical state $|phys)$ is a fixed dynamically independent state, and the dynamics is hidden in the relations of basic observables $\hat{\mathsf{F}}_f$, $\hat{\mathsf{G}}_a$ to this state. But we will be a bit vague and will speak about determination of the physical state $|phys)$ because it is more intuitive and does not influence any computation.

[12] We will use $\phi, \ldots$ for elements of $\mathcal{B}$ instead of more appropriate $\partial\phi, \ldots$ to simplify the notation. It can be also understood as a representative from $\mathcal{P}$ of the element in $\mathcal{B}$. Of course, only the value and the normal derivative on the boundary is important for the boundary phase space $\mathcal{B}$.

[13] Here we use the same letter for a general momentum $\pi \in \tilde{\mathcal{V}}$ and the constant $\pi = 3.1415\ldots$ in the normalization of the measure for momenta. It is left to an intelligent reader to distinguish the meaning from the context.

[14] The Euclidian action is used here because it includes all necessary numerical factors. As discussed in appendix D, we can use both Euclidian or physical actions regardless of which version of the theory we are working. They are related by

$$-I(\mathrm{h}) = \nu S(\mathrm{h}) \quad .$$

The version of the theory is determined by actual value of the factor ν — whether it is real or imaginary.

[15] In this part we use the Lorentzian (i.e. physical) convention in the sense of appendix D with an exception that we use the Euclidian action I. It cannot lead to confusion, because we have denoted it by a different symbol than the physical action S.

[16] The factor n, which governs the signature of the spacetime metric, is chosen here for convenience and reflects that we are using Lorentzian convention for volume element. I.e., the physical amplitude is $\frac{1}{n}K$, but the quantity K will have nicer properties in language of Lorentzian quantities. Similarly, for the Green function the physical amplitude is $\frac{1}{n}G^F$, but we will use often the quantity G^F to express properties of the amplitude.

[17] Again, we factorize out the prefactor n motivated by the fact that J is a density, i.e. proportional to volume element $\mathfrak{g}^{\frac{1}{2}}$.

[18] We do not lose any generality — all the following could be done with respect to some general b-boundary conditions, only instead of $\underset{\sim}{\varphi}$, $\underset{\sim}{\pi}$, γ and related quantities we would have to use $\underset{\sim}{\varphi}_{\sim b}$, $\underset{\sim}{\pi}_{\sim b}$, $\gamma_{\sim b}$, etc..

[19] Here, the standard fiber $\mathbf{T}_{\mathrm{h}}\,\mathbf{H}$ is equal to the standard fiber of the tangent space of the fiber manifold $\mathbf{H}$.

[20] Here we mean that q is a non-degenerate metric on Σ_t if restricted on tangent space $\mathbf{T}\,\Sigma_t$. But we use here identification of tangent spaces to Σ_t with tangent spaces of the manifold assuming orthogonal projections for covectors using metric g.

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