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Sum-over-histories quantization of relativistic particle

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Abstract

Sum-over-histories quantization of particle-like theory in curved space is discussed. It is reviewed that the propagator and the related Green function satisfy the Schrödinger equation and wave equation with a Laplace-like operator, respectively. The exact dependence of the operator on the choice of measure is shown. Modifications needed for a manifold with a boundary are then introduced, and the exact form of the equation for the propagator is derived. It is shown that the Laplace-like operator contains some distributional terms localized on the boundary. These terms define boundary conditions for the propagator. Such a choice of boundary conditions is explained as a consequence of a measurement of particles on the boundary. Finally, the interaction with sources inside the domain and sources on the boundary are also discussed.

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1. Introduction

The main goal of this work is to investigate a quantization of a spinless relativistic particle in a general curved spacetime using the sum-over-histories approach. We have the following motivations to do such a study.

The usual approach to how to quantize a spinless relativistic particle is the scalar field theory. 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 a 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 give 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. The classical explanation of this approach for non-relativistic physics can be found in [1] and more technically in [2–4]. A nice non-technical overview for a relativistic theory can be found in [5]. Besides these classical introductions, this approach has received considerable attention in recent years, see, for example, [6]. The new development has led to a generalization of this method called *generalized quantum mechanics* (see [6–8]).

In this approach, the transition amplitudes associated with the chosen criteria are computed by summing over amplitudes of all possible histories which meet the criteria. It is known that some of these amplitudes computed for a relativistic particle lead in the special cases (namely, in flat spacetime) to quantities which can also be obtained from scalar field theory. The goal of our work is to investigate this correspondence in more detail.

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 to try to quantize such a simplified system. These reduced theories are called minisuperspace models. It is well known that such reduced systems are 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 key feature of our investigation is that we study the particle theory on a bounded domain of spacetime, and that we pay attention to the exact form of boundary conditions. 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 behaviour at infinities. In flat spacetime, such an approach is justifiable because there exists a preferred behaviour at infinities, but in a general curved spacetime we have to be more careful. The question of boundary conditions is usually completely ignored in definitions of the path integral. We try to formulate the theory in a more careful way and identify its boundary-condition dependence.

The plan of the work is as follows. In section 2, we review sum-over-histories approach to the quantization of the spinless particle in curved spacetime without boundary. Equations for key amplitudes (the propagator and Feynman Green function) are derived and their exact dependence on the definition of the path integral is shown.

In section 3, we investigate the theory in a bounded domain. In such a domain, we have to modify our definition of the path integral. The new definition leads to a modification of the equations for physical amplitudes. Some additional distributional terms localized on the boundary appear in these equations and we find that they specify the exact form of boundary conditions for the amplitudes. It is shown that the exact form of the boundary conditions depends on the details of the definition of the path integral.

Finally, we discuss briefly a physical meaning of the boundary conditions. We argue that boundary conditions can serve as a phenomenological description of apparatuses measuring particles on the boundary of the domain.

Sections 2 and 3 contain the main line of arguments; an outline of computations can be found in appendix A with some technical material in appendix C. Appendix B contains a general overview of the geodesic theory necessary for the computations, including the geodesic theory near a boundary. We review a generalization of standard $3+1$ splitting into a general dimension and signature of the metric, introduce parametrization of points in a neighbourhood of the boundary using geometrical quantities on the boundary and investigate covariant expansion of a tensor field in terms of directions tangent to the boundary and geodesical distance from the boundary. We also study the reflected geodesics and compute covariant expansion of several important geometrical quantities which play a role parallel to that of the world function and Van Vleck–Morette determinant. The material in appendix B is highly independent of the main text and can also be useful outside the scope of the paper.

Let us note that our study can accommodate a wider range of theories than merely quantization of relativistic particle. The theory will be parametrized by two signature factors. One of them (the factor n) characterizes a signature of a target space metric (the metric of space in which a particle lives), and another (the factor ν) describes whether the theory is physical or Euclidean. For real n and imaginary ν, we obtain the theory of a non-relativistic particle in Riemanian curved space, for n and ν both imaginary we obtain a relativistic particle in curved Lorentzian spacetime. For both signature factors real we get a mathematically better behaving, but non-physical *Euclidean version* of the theory. Usually most quantities are well defined in the Euclidean sector and the definition for physical signature is obtained by an analytical continuation in the signature factors.

We use abstract tensor indices but we do not write tensor indices when possible. To abbreviate formulae, we employ different dots to indicate contraction in different vector spaces. Namely, we use '$\cdot$' for contractions of tangent tensor indices, i.e., $g_{\alpha\beta}a^\beta = (g \cdot a)_\alpha$. To distinguish the metric with covariant and contravariant position of indices, we write the inversion of the metric g explicitly as g^{-1}. We use '$\bullet$' for contraction in functional vector spaces of functions and densities on the spacetime, i.e., the bullet means an integration over spacetime (or an action of a distribution on a test function—a formal integration): $\phi \bullet \alpha = \int_M \phi\alpha$. Similarly, a square dot '$\cdot$' indicates integration over a hypersurface Σ or a boundary $\partial\Omega$ of a spacetime domain. Finally, it is convenient to represent differential operators on the manifold M as bi-distributions. We use arrows $\leftsquigarrow$ and $\rightsquigarrow$ to indicate the direction of derivatives. Thus, for example, $\psi \bullet (\overleftarrow{\mathrm{d}}_\alpha a^\alpha) \bullet \omega = \omega \bullet (a^\alpha \overrightarrow{\mathrm{d}}_\alpha) \bullet \psi = \int \omega a^\alpha \, \mathrm{d}_\alpha \psi$ for a test function ψ, a test density ω and a vector field a.

2. Particle in a curved space without boundary

2.1. Space of histories, action and amplitudes

In this section, we briefly formulate the sum-over-histories approach to a quantization of a particle-like theory. A similar calculation has been done, for example, in [9, 10]. We present our derivation here because we generalize this line of reasoning in the following section to the case when a particle is moving in a domain with a boundary.

As usual in the sum-over-histories approach, the theory is characterized by a space of histories and by an action. An elementary history in our case is a *trajectory*—an imbedding of a one-dimensional manifold N (called the *inner space*) to a d-dimensional *spacetime manifold* M—and an *inner space metric* h on the inner manifold N. M is equipped with a fixed spacetime metric g and scalar potential V.

In the Euclidean version of the theory, the inner metric h is positive definite; in the physical version it is negative definite. We allow the spacetime metric to be also positive definite—depending on the (in general, complex) factor n. Namely, near a hypersurface Σ, the spacetime metric g and associated volume element $\mathfrak{g}^{\frac{1}{2}}$ can be written using the factor n in the following way:

$$g_{\alpha\beta} = n^2 \mathrm{n}_\alpha \mathrm{n}_\beta + q_{\alpha\beta}, \qquad \mathfrak{g}^{\frac{1}{2}} = \frac{1}{n} (\mathrm{Det}\, g)^{\frac{1}{2}}, \tag{2.1}$$

with n being the 1-form normal to Σ and q being the 'spatial' metric positive definite on Σ. Vector $\vec{\mathrm{n}}$ normal to Σ and the projector $\mathfrak{d}$ on space tangent to Σ then are

$$\vec{\mathrm{n}}^\alpha = n^2 \mathrm{n}_\mu g^{-1\mu\alpha}, \qquad \mathfrak{d}^\beta_\alpha = \delta^\beta_\alpha - \vec{\mathrm{n}}^\beta \mathrm{n}_\alpha. \tag{2.2}$$

The whole theory is invariant under diffeomorphisms of the inner manifold N. As usual (e.g., [11]), we factorize over this symmetry. If we fix a coordinate $\eta : N \to \langle 0, 1 \rangle$ on the inner manifold N, we can characterize a class of equivalent histories using a pair $[\tau, \boldsymbol{x}]$, where $\boldsymbol{x}$ is a map $\boldsymbol{x} : \langle 0, 1\rangle \to M$ and τ is a total *inner time* or a total *inner length* of N measured using the inner metric h.

The Euclidean action in these variables has the form

$$I(\tau, \boldsymbol{x}) = \frac{1}{2}\int_{\langle 0,1\rangle} \left(\frac{1}{\nu\tau}\dot{\boldsymbol{x}}^\alpha \dot{\boldsymbol{x}}^\beta g_{\alpha\beta}(\boldsymbol{x}) + \nu\tau V(\boldsymbol{x})\right) \mathrm{d}\eta. \tag{2.3}$$

Here ν is the discussed constant signature factor distinguishing Euclidean and physical versions of the theory. In the former case we use $\nu = 2$, in the latter $\nu = 2\mathrm{i}$. The Euclidean action I is related to the physical action S by $\nu S = -|\nu| I$.

In the sum-over-histories approach to quantum theory, we can define an amplitude $A(\mathrm{H})$ for any set of histories H by 'summing' over amplitudes of elementary histories in the set. The quantum amplitude is not directly a physical measurable quantity. 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 a measure on histories. This means that we will always be 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 (e.g., [11]). In the factorized integral, we are summing only over variables $[\tau, \boldsymbol{x}]$:

$$A(\mathrm{H}) = \int_{[\tau,\boldsymbol{x}]\in\mathrm{H}} \mathfrak{M}_{\mathrm{red}}(\tau, \boldsymbol{x}) \exp(-I(\tau, \boldsymbol{x})), \tag{2.4}$$

with a reduced, renormalized measure $\mathfrak{M}_{\mathrm{red}}$.

2.2. *Propagator*

It is useful to compute an amplitude $\frac{1}{n}K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$—called the *propagator* or *heat kernel*—for the set of histories restricted only by the positions of the end points of the trajectory x_{f} and x_{i} in the spacetime M and by fixing an inner time to a particular value τ:

$$\frac{1}{n}K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}}) = \int_{\boldsymbol{x}\in\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})} \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}] \exp(-I(\tau, \boldsymbol{x})), \tag{2.5}$$

where $\boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})$ is a set of trajectories $\boldsymbol{x} : \langle 0, 1\rangle \to M$ with $\boldsymbol{x}(0) = x_{\mathrm{i}}$ and $\boldsymbol{x}(1) = x_{\mathrm{f}}$. The factor n is chosen here for convenience[1] and reflects that we are using Lorentzian convention for volume element (2.1).

Because the set of histories $[\tau, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})] \overset{\mathrm{def}}{=} \{\tau\} \times \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})$ is a lower dimensional subset of the space of all histories, $K(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ is essentially an amplitude 'density' on the space $\mathbb{R}^+ \times M \times M$ of values $[\tau, x_{\mathrm{f}}, x_{\mathrm{i}}]$. Therefore, we have to expect that the restriction $\mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$ of the measure $\mathfrak{M}_{\mathrm{red}}$ to the space $[\tau, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})]$—which we call the *Feynman measure*—depends on τ and end points x_{f} and x_{i}; maybe only in a 'trivial' way.

In other words, an amplitude density of an elementary history on the space $[\tau, \boldsymbol{\mathcal{T}}(x_{\mathrm{f}}|x_{\mathrm{i}})]$ is

$$A(\tau, \boldsymbol{x}) = \mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})[\boldsymbol{x}] \exp(-I(\tau, \boldsymbol{x})). \tag{2.6}$$

It is well known [2, 6, 9, 10] that with the right choice of the measure $\mathfrak{M}^F(\tau, x_{\mathrm{f}}|x_{\mathrm{i}})$, the propagator satisfies the equation

$$-\dot{K}(\tau) = \frac{\nu}{2}\mathrm{F} \bullet K(\tau), \qquad K(0) = \mathcal{G}^{-1}, \tag{2.7}$$

[1] That is, the physical amplitude is $\frac{1}{n}K$, but the quantity K will have nicer properties in the language of Lorentzian quantities. Similarly, for the Green function the physical amplitude is $\frac{1}{n}G^F$, but we will often use the quantity G^F to express properties of the amplitude.

where F is a wave operator fixed by the action and the measure (see below), and $\mathcal{G} = \mathfrak{g}^{\frac{1}{2}}\delta$ is a delta distribution[2] on M normalized to the metric volume element $\mathfrak{g}^{\frac{1}{2}}$. In other words, K is the exponential of F

$$K(\tau) = \exp\left(-\frac{\nu\tau}{2}\mathrm{F}\right) \bullet \mathcal{G}^{-1}. \tag{2.8}$$

We have not yet specified the 'right choice' of the measure. 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 by equation (2.13) and the latter is given by equation (2.22).

The idea of the proof of the relations (2.7) is in inspecting the key properties of the exponential,

$$K(\tau_\mathrm{f}) \bullet \mathcal{G} \bullet K(\tau_\mathrm{i}) = K(\tau_\mathrm{f} + \tau_\mathrm{i}), \tag{2.9}$$

$$\mathcal{G} \bullet K(\tau) \bullet \mathcal{G} = \mathcal{G} - \frac{\nu\tau}{2}\mathcal{F} + \mathcal{O}(\tau^2), \tag{2.10}$$

where $\mathcal{F} = \mathcal{G} \bullet \mathrm{F}$ is the quadratic form of the differential operator F.

2.3. Composition law

The first condition (2.9) is a composition law for the amplitude K. This law reflects the possibility of decomposition of a history $[\tau, \boldsymbol{x}]$ into histories $[\tau_\mathrm{i}, \boldsymbol{x}_\mathrm{i}]$ during an initial amount of inner time τ_i and $[\tau_\mathrm{f}, \boldsymbol{x}_\mathrm{f}]$ during a final amount of inner time τ_f. We say that a history $[\tau, \boldsymbol{x}] = [\tau_\mathrm{f}, \boldsymbol{x}_\mathrm{f}] \odot [\tau_\mathrm{i}, \boldsymbol{x}_\mathrm{i}]$ is given by *joining* of histories $[\tau_\mathrm{f}, \boldsymbol{x}_\mathrm{f}]$ and $[\tau_\mathrm{i}, \boldsymbol{x}_\mathrm{i}]$ if

$$\tau = \tau_\mathrm{f} + \tau_\mathrm{i}, \qquad \boldsymbol{x}_\mathrm{f}(0) = \boldsymbol{x}_\mathrm{i}(1), \qquad \boldsymbol{x}_\mathrm{f} = \boldsymbol{x}\left(\frac{\tau_\mathrm{i} + \eta\tau_\mathrm{f}}{\tau}\right), \qquad \boldsymbol{x}_\mathrm{i} = \boldsymbol{x}\left(\frac{\eta\tau_\mathrm{i}}{\tau}\right). \tag{2.11}$$

The action is additive with respect to joining histories.

We have a natural 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 $[\tau_\mathrm{f}, \boldsymbol{\mathcal{T}}(x_\mathrm{f}|x_\mathrm{o})] \times [\tau_\mathrm{i}, \boldsymbol{\mathcal{T}}(x_\mathrm{o}|x_\mathrm{i})]$

$$[\tau, \boldsymbol{\mathcal{T}}(x_\mathrm{f}|x_\mathrm{i})] = \bigcup_{x_\mathrm{o}\in M} [\tau_\mathrm{f}, \boldsymbol{\mathcal{T}}(x_\mathrm{f}|x_\mathrm{o})] \times [\tau_\mathrm{i}, \boldsymbol{\mathcal{T}}(x_\mathrm{o}|x_\mathrm{i})]. \tag{2.12}$$

If the measures on these sets are related by

$$\mathfrak{M}^F(\tau, x_\mathrm{f}|x_\mathrm{i})[\boldsymbol{x}] = \mathfrak{M}^F(\tau_\mathrm{f}, x_\mathrm{f}|x_\mathrm{o})[\boldsymbol{x}_\mathrm{f}] n\mathfrak{g}^{\frac{1}{2}}(x_\mathrm{o})\mathfrak{M}^F(\tau_\mathrm{i}, x_\mathrm{o}|x_\mathrm{i})[\boldsymbol{x}_\mathrm{i}], \tag{2.13}$$

we get (2.9) by a straightforward calculation.

The condition (2.13) represents a reasonable assumption of the locality of the measure $\mathfrak{M}^F$. Together with the additivity of the action it reflects the rule 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 leads us to an investigation of the short time behaviour of the heat kernel.

[2] A volume element $\mathfrak{g}^{\frac{1}{2}}$ on spacetime defines a bi-distribution $\mathcal{G} = \mathfrak{g}^{\frac{1}{2}}\delta$—a delta function normalized to the volume element, i.e., $\phi \bullet \mathcal{G} \bullet \psi = \int \phi\psi\mathfrak{g}^{\frac{1}{2}}$. Inverse bi-distribution $\mathcal{G}^{-1} = \mathfrak{g}^{-\frac{1}{2}}\delta$ acts similarly on test densities. Clearly, for a smooth function f we can also define a distribution $f\mathcal{G}$.

2.4. Short time amplitude

Now we turn to prove equation (2.10). It can be found in the literature (e.g., [9, 10]), but we present it here to show how the measure is actually determined and how the operator $\mathcal{F}$ depends on this choice.

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 behaviour for the propagator.

First we write an expansion of the action for small τ

$$I(\tau, \boldsymbol{x}) = \frac{1}{\tau} I_{-1}(\boldsymbol{x}) + I_0(\boldsymbol{x}) + \tau I_1(\boldsymbol{x}) + \cdots. \tag{2.14}$$

For the action we are using it means

$$I_{-1}(\boldsymbol{x}) = \frac{1}{2\nu} \int_{\eta\in\langle 0,1\rangle} \dot{\boldsymbol{x}}^\alpha \dot{\boldsymbol{x}}^\beta g_{\alpha\beta}(\boldsymbol{x})\, \mathrm{d}\eta, \tag{2.15}$$

$$I_0(\boldsymbol{x}) = 0, \tag{2.16}$$

$$I_1(\boldsymbol{x}) = \frac{\nu}{2} \int_{\eta\in\langle 0,1\rangle} V(\boldsymbol{x})\, \mathrm{d}\eta. \tag{2.17}$$

We assume that the measure is slowly changing in τ compared to the leading term in the action.

The dominant contribution to the integral (2.5) 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 (2.15) is clearly a geodesic of the metric g. We expand all expressions around this extremum

$$\boldsymbol{x} = \bar{\boldsymbol{x}}(x_\mathrm{f}|x_\mathrm{i}) + \sqrt{\tau}\vec{\boldsymbol{x}}, \tag{2.18}$$

where $\vec{\boldsymbol{x}}$ is a vector tangent to the space of trajectories $\boldsymbol{\mathcal{T}}(x_\mathrm{f}|x_\mathrm{i})$ at the extremum $\bar{\boldsymbol{x}}(x_\mathrm{f}|x_\mathrm{i})$. We actually need to specify what the addition in equation (2.18) means. It is done more carefully in a similar situation in appendix A (see equation (A.5)). Now we are more interested in a qualitative answer, so we skip these details here. The expanded integral (2.5) has the structure

$$\frac{1}{n} K(\tau, x_\mathrm{f}|x_\mathrm{i}) = \exp(-I(\bar{\boldsymbol{x}}(x_\mathrm{f}|x_\mathrm{i}))) \int_{\vec{\boldsymbol{x}}\in\mathbf{T}_{\bar{\boldsymbol{x}}}\boldsymbol{\mathcal{T}}} \mathfrak{M}^F_*(\tau, x_\mathrm{f}|x_\mathrm{i}) \exp\left(-\frac{1}{2}\vec{\boldsymbol{x}}\cdot\delta^2 I_{-1}(\bar{\boldsymbol{x}}(x_\mathrm{f}|x_\mathrm{i}))\cdot\vec{\boldsymbol{x}}\right)$$
$$\times (1 + \sqrt{\tau}(\vec{\boldsymbol{x}}^{\mathrm{odd}}\text{-terms}) + \tau(\vec{\boldsymbol{x}}^{\mathrm{even}}\text{-terms}) + \cdots). \tag{2.19}$$

Here $\mathfrak{M}^F_*(\tau, x_\mathrm{f}|x_\mathrm{i})$ is a leading term in the τ and $\vec{\boldsymbol{x}}$-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 tangent 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 tangent space, which is infinite.

'$\vec{\boldsymbol{x}}$-terms' in the last equation represent 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,

$$\sigma(x_\mathrm{f}|x_\mathrm{i}) = \nu I_{-1}(\bar{\boldsymbol{x}}(x_\mathrm{f}|x_\mathrm{i})) = \frac{1}{2}\int_{\langle 0,1\rangle} \dot{\bar{\boldsymbol{x}}}(x_\mathrm{f}|x_\mathrm{i})\cdot g(\bar{\boldsymbol{x}}(x_\mathrm{f}|x_\mathrm{i}))\cdot\dot{\bar{\boldsymbol{x}}}(x_\mathrm{f}|x_\mathrm{i})\,\mathrm{d}\eta. \tag{2.20}$$

We also use the notation

$$\bar{V}(x_f|x_i) = \frac{2}{\nu} I_1(\bar{\boldsymbol{x}}(x_f|x_i)) = \int_{\langle 0,1\rangle} V(\bar{\boldsymbol{x}}(x_f|x_i))\, d\eta. \tag{2.21}$$

The integral (2.19) 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. If the measure $\mathfrak{M}^F_*(\tau)$ has the already mentioned τ-dependence, the result can be written as

$$K(\tau, x_f|x_i) = \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \Delta(x_f|x_i) \left(\alpha_0(x_f|x_i) - \tau\frac{\nu}{2}\alpha_1(x_f|x_i) + \mathcal{O}(\tau^2)\right)$$
$$\times \exp\left(-\frac{1}{\nu\tau}\sigma(x_f|x_i) - \frac{\nu\tau}{2}\bar{V}(x_f|x_i)\right), \tag{2.22}$$

where $\alpha_0(x_f|x_i)$ should satisfy

$$\alpha_0(x|x) = 1. \tag{2.23}$$

Here $\Delta(x_f|x_i)$ is Van Vleck–Morette determinant (see (B.13)).

The terms proportional to $\sqrt{\tau}$ disappeared during integration thanks to the odd power of $\vec{\boldsymbol{x}}$. The particular behaviour of a coincidence limit of the coefficient α_0 will be needed for a proper normalization in (2.7). To obtain this behaviour, we need the mentioned τ-dependence of the measure, which can be expressed by the condition

$$\mathfrak{M}^F_*(\tau, x|x)\, \mathrm{Det}\left(\frac{\delta^2 I_{-1}(\bar{\boldsymbol{x}}(x|x))}{2\pi\nu\tau}\right)^{-\frac{1}{2}} = \frac{1}{(2\pi\nu\tau)^{\frac{d}{2}}}. \tag{2.24}$$

That is, the measure must satisfy this condition to conclude the proof of equation (2.10).

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 yet specify the measure precisely, we can do it now by fixing these coefficients. That is, we can define the measure $\mathfrak{M}^F$ by choosing functions $\alpha_0(x_f|x_i)$ and $\alpha_1(x_f|x_i)$.

In the following, we will prove that a form of the operator $\mathcal{F}$ in (2.10) 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 equation (2.22). As discussed before, equations (2.10) together with composition law (2.9) determine the propagator K, i.e., also all important information hidden in the measure $\mathfrak{M}^F$. This means that knowledge of the mentioned coincidence limits concludes our definition of the measure and path integral itself.

Let us note that this argument is some kind of justification of the usual time-discretization of the path integral and of the *a priori* choice of the short time amplitude in the form (2.22). But, in principle, it would be possible to define the measure $\mathfrak{M}^F$ in a more compact way and to compute exactly the form of the functions α_0 and α_1 in terms of variation of the action and the measure.

2.5. *Short time behaviour of the heat kernel*

Now we continue with the proof of equation (2.10). We show that for small τ, the amplitude (2.22) has the desired behaviour in a distributional sense. Most of the technical work is done in appendix A where it is shown that for small τ, the following expansion holds (equation (A.8)):

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int_{x,z\in M} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z) \exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right)\varphi(x)\psi(z)$$
$$= \varphi \bullet \mathcal{G} \bullet \psi - \tau\frac{\nu}{2}\varphi \bullet \mathcal{L} \bullet \psi + \mathcal{O}(\tau^2). \tag{2.25}$$

Here φ and ψ are smooth test functions, and $\mathcal{L}$ is the Laplace operator quadratic form

$$\varphi \bullet \mathcal{L} \bullet \psi = \int_M \mathfrak{g}^{\frac{1}{2}} (\mathrm{d}\varphi) \cdot g^{-1} \cdot (\mathrm{d}\psi) = -\int_M \mathfrak{g}^{\frac{1}{2}} \varphi(\nabla^2 \psi) = -\int_M \mathfrak{g}^{\frac{1}{2}} \psi(\nabla^2 \varphi). \tag{2.26}$$

Let us recall that at this moment we are discussing the case of a manifold without boundary. We thus 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 the propagator smoothed by test functions φ, ψ reads

$$\begin{aligned}
\varphi \bullet \mathcal{G} \bullet K(\tau) \bullet \mathcal{G} \bullet \psi = \frac{n}{(2\pi \nu\tau)^{\frac{d}{2}}} \int_{x,z\in M} & \mathfrak{g}^{\frac{1}{2}}(x) \mathfrak{g}^{\frac{1}{2}}(z) \Delta(x|z) \left(\alpha_0(x|z) - \tau \frac{\nu}{2} \alpha_1(x|z) + \mathcal{O}(\tau^2)\right) \\
& \times \exp\left(-\frac{1}{\nu\tau}\sigma(x|z) - \frac{\nu\tau}{2}\bar{V}(x|z)\right) \varphi(x)\psi(z) \\
= \varphi \bullet \mathcal{G} \bullet \psi & - \tau \frac{\nu}{2} \varphi \bullet (\mathcal{L} + (V\, \mathcal{G}) + (g^{-1\mu\nu}[\mathrm{d}_{\mathrm{l}\mu} \mathrm{d}_{\mathrm{r}\nu} \alpha_0]\mathcal{G}) + ([\alpha_1]\mathcal{G})) \bullet \psi \\
& - \tau \frac{\nu}{2} \varphi \bullet ((\overleftrightarrow{\mathrm{d}}_\mu g^{-1\mu\nu}[\mathrm{d}_{\mathrm{l}\nu}\alpha_0]) \bullet \mathcal{G} + \mathcal{G} \bullet ([\mathrm{d}_{\mathrm{r}\mu}\alpha_0] g^{-1\mu\nu} \overrightarrow{\mathrm{d}}_\nu)) \bullet \psi + \mathcal{O}(\tau^2),
\end{aligned}$$

where we used $[\bar{V}] = V$ and $[\alpha_0] = 1$. Here $[A]$ denotes a coincidence limit of a bitensor A, $\mathrm{d}_{\mathrm{r}}A$ and $\mathrm{d}_{\mathrm{l}}A$ are derivatives with respect to the right and left arguments, and the bi-distributions $\overleftarrow{\mathrm{d}}$ and $\overrightarrow{\mathrm{d}}$ are derivatives acting to the left and to the right (see footnote 2).

If the condition

$$[\mathrm{d}_{\mathrm{r}}\alpha_0] = [\mathrm{d}_{\mathrm{l}}\alpha_0] = 0, \tag{2.27}$$

is satisfied, we see that the propagator $K(\tau)$ has really the form (2.10) with

$$\mathcal{F} = \mathcal{L} + \mathcal{V}, \tag{2.28}$$

$$\mathcal{V} = (V + [\alpha_1] + g^{-1\mu\nu}[\mathrm{d}_{\mathrm{l}\mu}\mathrm{d}_{\mathrm{r}\nu}\alpha_0])\mathcal{G}. \tag{2.29}$$

That is, $\mathcal{F}$ is a Laplace operator with a potential term which includes 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

$$\alpha_0 = \Delta^{-p}, \tag{2.30}$$

which satisfies the condition (2.27). It leads to an additional part in the potential,

$$g^{-1\mu\nu}[\mathrm{d}_{\mathrm{l}\mu}\mathrm{d}_{\mathrm{r}\nu}\Delta^{-p}] = \frac{p}{3}R, \tag{2.31}$$

where R is a scalar curvature of the metric g.

The condition (2.27) is actually a consequence of (2.23) and an assumption of the symmetry of α_0

$$\alpha_0(x|z) = \alpha_0(z|x). \tag{2.32}$$

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. But we will not discuss such a situation and in the following we will assume that the conditions (2.32) and (2.27) are satisfied.

In summary, we have seen that for small τ, the propagator $K(\tau)$ has the behaviour given by (2.10). If the measure is defined using the decomposition property (2.9) and the short time amplitude (2.22), the operator $\mathcal{F}$ is fixed by knowledge of the coincidence limits of α_1 and the first two derivatives of α_0.

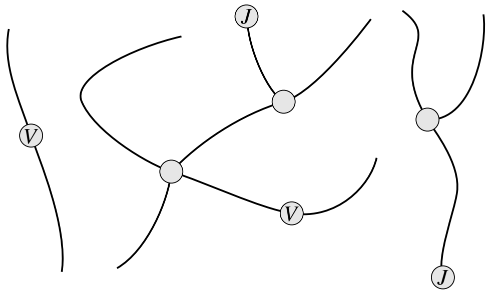

Figure 1. An example of the elementary history of the interacting theory. The elementary history of the many particle interacting theory is formed by one-particle histories which can be glued in interaction vertices. The simplest interactions are sources—one-leg J-vertices—and a potential interaction—two-leg V-vertices.

2.6. Feynman Green function

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 called the *Feynman Green function* $\frac{1}{n}G^F(x_\mathrm{f}|x_\mathrm{i})$ associated with the set of histories restricted only by the initial and final points x_f, x_i. 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 $\frac{\nu}{2}\,\mathrm{d}\tau$

$$\frac{1}{n}G^F(x_\mathrm{f}|x_\mathrm{i}) = \int_{\mathbb{R}^+} \frac{1}{n}K(\tau, x_\mathrm{f}|x_\mathrm{i})\frac{\nu}{2}\,\mathrm{d}\tau. \tag{2.33}$$

Using equation (2.8), we immediately get that the Feynman Green function is the inverse of the wave operator $\mathcal{F}$.

2.7. Interacting theory

Until now we computed only *one particle amplitudes*—amplitudes associated with sets of histories of one particle. We could also study an *interacting theory*—a many particle theory in which particles can be created and annihilated, or they can interact with each other. Such a theory can be built from the free theory using general ideas of the sum-over-histories approach: an elementary history of the interacting theory is given by an arbitrary number of copies of one-particle free histories, endpoints of which are glued in interaction vertices (see, e.g., figure 1). The amplitude of such a multiple particle history is given by a product of amplitudes of all one particle histories and of amplitudes associated with each interaction. The amplitude of a set of histories is then given by the sum of amplitudes of elementary histories in the set.

The simplest interactions 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). These two interactions do not change substantially the character of the free theory. One-leg vertices allow us to introduce the amplitude of propagation of the particle from a given source, see equation (3.32). Taking into account two-leg vertices leads only to modification of the potential term (see, e.g., [5, 11] for discussion in flat spacetime or [12] for details in the current context).

A non-trivial interaction is introduced using vertices of higher order. The amplitude corresponding to a multiple particle history with such an interaction can be computed by an integration over all possible positions of interaction where propagation between interactions is given by free Feynman Green function computed above. This is analogous to the methods used in the interacting scalar field theory. The difference between sum-over-histories and field theory approach lies only in the method of obtaining the Feynman Green function. Therefore, in the following, we will concentrate on the derivation of the Feynman Green function of the free theory and on the analysis of its boundary condition, and we will not discuss a non-trivial interacting theory in more detail.

2.8. Boundary conditions

In this section, we completely ignored the question of boundary conditions using the 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. But a problem arises for the relativistic particle when the manifold M is Lorentzian and operators $\mathcal{L}, \mathcal{F}$ 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 special situations (e.g., the existence of a timelike 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 a special choice, and we have to address the question of the boundary conditions. To deal with this problem, in the following section we investigate the theory in a bounded domain Ω of the manifold M.

3. Particle in a curved space with boundary

3.1. General considerations

In this section, our goal is a better understanding of the physical meaning of boundary conditions for the differential operators in the equation for the propagator and Green function. Therefore, we restrict ourselves to a domain Ω which is bounded 'in all physically interesting directions', because we want to investigate the boundary conditions on boundaries at a *finite* region not at the infinity.

If the target space metric is positive definite (i.e., in the Euclidean and non-relativistic version of the theory) we restrict to a compact domain. In the case of a relativistic particle (which we are mostly interested in), we allow domains which do not have to be compact: we allow the domain Ω to be unbounded if we know that its infinity is 'safe'. The situation we have in mind is the Lorentzian globally hyperbolic manifold with asymptotically flat spatial infinity. In this case, we can ignore spatial infinity because we can restrict ourselves to situations in which spacetime is 'empty' sufficiently far in spatial directions. However, 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.

Therefore, in the case of a Lorentzian globally hyperbolic manifold, the typical choice of the domain will thus be a sandwich domain between two Cauchy surfaces. The discussion is, however, also valid for the Euclidean version of the theory restricted to a compact domain.

3.2. Restriction to a domain—naive approach

Let us start with a straightforward restriction to a domain Ω. We want to compute an amplitude $K_{\rm o}(\tau, x_{\rm f}|x_{\rm i})$ which corresponds to a set of histories with inner time equal to τ, endpoints $x_{\rm i}$, $x_{\rm f}$ and which wholly belong to the domain Ω. We can repeat the derivation of the short time amplitude (2.22), at least for x_{f}, x_{i} sufficiently far from the boundary, because for small τ only trajectories near the geodesic between x_{f} and x_{i} contribute to the amplitude.

If we do this calculation, we find that a new term can appear in the expansion for endpoints *near* the boundary. As can be seen from equation (A.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 with boundary the integration of odd powers of Z disappears. However, in the case of a domain with a boundary, the Gauss integration is not over the whole tangent space if a point x is near the boundary, and therefore the integral of odd powers of Z does not disappear. As shown in appendix A (equation (A.25)), the correct asymptotic expansion of the leading term of the short time amplitude (equivalent of (2.25)) is given by

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\int_{x,z\in M}\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z)\exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right)\varphi(x)\psi(z)$$
$$=\varphi\bullet\left(\mathcal{G}+\sqrt{\tau}\left(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\right)\mathcal{Q}-\tau\frac{\nu}{2}\overleftrightarrow{\mathcal{L}}+\mathcal{O}\big(\tau^{\frac{3}{2}}\big)\right)\bullet\psi, \tag{3.1}$$

where $\mathcal{Q}[\partial\Omega]$ is a delta bi-distribution localized on the boundary $\partial\Omega$ normalized to the boundary volume element $\mathfrak{q}^{\frac{1}{2}}$ understood as a distribution on spacetime,

$$\varphi\bullet\mathcal{Q}\bullet\psi=\int_{\partial\Omega}\varphi\psi\mathfrak{q}^{\frac{1}{2}}, \tag{3.2}$$

and $\overleftrightarrow{\mathcal{L}}$ is a particular ordering of the Laplace operator given by

$$\overleftrightarrow{\mathcal{L}}=\frac{1}{2}(\overleftarrow{\mathcal{L}}+\overrightarrow{\mathcal{L}}), \tag{3.3}$$

$$\varphi\bullet\overrightarrow{\mathcal{L}}\bullet\psi=-\int_{\Omega}\varphi(\nabla^2\psi)\mathfrak{g}^{\frac{1}{2}}. \tag{3.4}$$

Using this result it is easy to show that the expansion of the propagator K_{o} is

$$\mathcal{G}\bullet K_{\mathrm{o}}(\tau)\bullet\mathcal{G}=\mathcal{G}+\sqrt{\tau}\left(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\right)\mathcal{Q}-\tau\frac{\nu}{2}\overleftrightarrow{\mathcal{F}}+\mathcal{O}\big(\tau^{\frac{3}{2}}\big), \tag{3.5}$$

where $\overleftrightarrow{\mathcal{F}}$ is a Laplace-like quadratic form with potential,

$$\overleftrightarrow{\mathcal{F}}=\tfrac{1}{2}(\overleftarrow{\mathcal{F}}+\overrightarrow{\mathcal{F}})=\overleftrightarrow{\mathcal{L}}+\mathcal{V}, \tag{3.6}$$

$$\overleftarrow{\mathcal{F}}^{\top}=\overrightarrow{\mathcal{F}}=\overrightarrow{\mathcal{L}}+\mathcal{V}. \tag{3.7}$$

The corrected potential $\mathcal{V}$ is given again by the expression (2.29) and we have assumed that the condition (2.27) 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 (2.22). 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.

3.3. Boundary correction term

The short time amplitude (2.22) 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

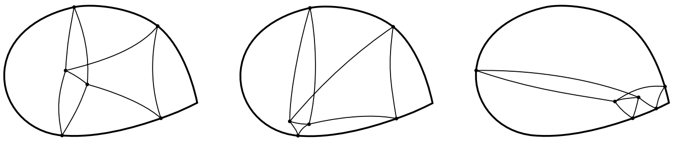

Figure 2. Examples of extremal trajectories. Dominant terms to sum over trajectories are given by trajectories near extreme trajectories, possibly reflected from the boundary. If close endpoints are sufficiently far from the boundary, the reflected geodesics are longer then the straight geodesic. If the endpoints are near the boundary, there is a reflected geodesic with length comparable to the length of the straight one. Near the corner there are more reflected geodesics with comparable length.

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, and any trajectory with a reflection on the boundary is too long (see figure 2 left).

But for endpoints near 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 2 middle).

The *reflected extreme trajectory* $\bar{\boldsymbol{x}}_\mathrm{b}(x|z)$ is an extremum of the leading term of the action (2.15) with the additional condition that the trajectory reflects on the boundary. Let us denote the *point of reflection* $b(x|z)$ and the *parameter for which the reflection occurs* $\lambda_\mathrm{r}(x|z)$ and its complement $\lambda_\mathrm{l}(x|z)$. Clearly the trajectory is a joining of two geodesics

$$[\tau, \bar{\boldsymbol{x}}_\mathrm{b}(x|z)] = [\lambda_\mathrm{l}(x|z)\tau, \bar{\boldsymbol{x}}(x|b(x|z))] \odot [\lambda_\mathrm{r}(x|z)\tau, \bar{\boldsymbol{x}}(b(x|z)|z)]. \tag{3.8}$$

Using additivity of the action, we get the value of its leading term

$$\sigma_\mathrm{b}(x|z) \stackrel{\mathrm{def}}{=} \nu I_{-1}(\bar{\boldsymbol{x}}_\mathrm{b}(x|z)) = \frac{\sigma_\mathrm{l}(x|z)}{\lambda_\mathrm{l}(x|z)} + \frac{\sigma_\mathrm{r}(x|z)}{\lambda_\mathrm{r}(x|z)}, \tag{3.9}$$

where, following the convention (B.77),

$$\sigma_\mathrm{l}(x|z) = \sigma(x|b(x|z)), \qquad \sigma_\mathrm{r}(x|z) = \sigma(b(x|z)|z). \tag{3.10}$$

The extremum requirement gives us conditions on b and λ_r, λ_l,

$$\frac{\mathrm{D}\sigma(x|b(x|z))}{\lambda_\mathrm{l}(x|z)} + \frac{\mathrm{D}\sigma(b(x|z)|z)}{\lambda_\mathrm{r}(x|z)} = 0, \qquad \frac{\sigma_\mathrm{l}}{\lambda_\mathrm{l}^2} = \frac{\sigma_\mathrm{r}}{\lambda_\mathrm{r}^2}, \tag{3.11}$$

where D denotes the orthogonal projection of the gradient on the boundary (the gradient with respect to the argument on the boundary). See appendix B for more details and other quantities defined on the boundary.

Now we can estimate the contribution from the trajectories near the reflected geodesic $\bar{\boldsymbol{x}}_\mathrm{b}(x|z))$. Using reasoning similar to that used for deriving (2.22), we can write an approximation of the short time amplitude associated with the reflected geodesic as

$$K_\mathrm{b}(\tau, x_\mathrm{f}|x_\mathrm{i}) = \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \Delta_\mathrm{b}^{1-p}(x_\mathrm{f}|x_\mathrm{i})\beta(\tau, x_\mathrm{f}|x_\mathrm{i}) \exp\left(-\frac{1}{\nu\tau}\sigma_\mathrm{b}(x_\mathrm{f}|x_\mathrm{i})\right), \tag{3.12}$$

where Δ_b is the Van Vleck–Morette determinant associated with the reflected geodesic (see (B.89)). The coefficient β is an analogue of the coefficients α_0, α_1; only in this case we have to expect an expansion in powers of $\sqrt{\tau}$:

$$\beta(\tau, x|z) = \beta_0(x|z) + \sqrt{\tau}\beta_{\frac{1}{2}}(x|z) + \mathcal{O}(\tau). \tag{3.13}$$

As we will see, the right normalization relative to the leading term K_o requires

$$\beta_0(x|x) = 1. \tag{3.14}$$

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 A. We also already anticipated an arbitrary power of the Van Vleck–Morette determinant, similar to the choice (2.30).

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 (2.22) concludes the definition of the path integral in the domain with a smooth boundary.

3.4. Short time behaviour of the heat kernel

Next, we proceed to derive the short time behaviour of the propagator. Again, the technical work is done in appendix A, where it is shown that for small τ we have the expansion (see equation (A.45))

$$\begin{aligned}\varphi \bullet \mathcal{G} \bullet K_b(\tau) \bullet \mathcal{G} \bullet \psi = \sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\varphi \bullet \mathcal{Q} \bullet \psi - \tau\frac{\nu}{2}\frac{1}{2}\varphi \bullet (\overleftrightarrow{\mathrm{d}}\mathcal{F}_{\tilde{n}} + \overrightarrow{\mathrm{d}}\mathcal{F}_{\tilde{n}}) \bullet \psi \\ - \tau\frac{\nu}{2}\varphi \bullet \left(\frac{1+p}{3}k + \beta\text{-terms}\right)\mathcal{Q} \bullet \psi + \mathcal{O}\big(\tau^{\frac{3}{2}}\big).\end{aligned} \tag{3.15}$$

The β-terms contain coincidence limits of the first two derivatives of the coefficient β on the boundary, and the exact form can be found in (A.55). k is the trace of the external curvature (B.50) and $\overleftrightarrow{\mathrm{d}}\mathcal{F}_{\tilde{n}}$, $\overrightarrow{\mathrm{d}}\mathcal{F}_{\tilde{n}}$ are defined in (3.24). The normalization (3.14) ensures that the $\sqrt{\tau}$-term in K_b cancels exactly with such a term in K_o.

So, if we add both dominant terms we get

$$K_k(\tau) = K_o(\tau) + K_b(\tau), \tag{3.16}$$

$$\mathcal{G} \bullet K_k(\tau) \bullet \mathcal{G} = \mathcal{G} - \tau\frac{\nu}{2}\mathcal{F}_{\tilde{k}} + \mathcal{O}\big(\tau^{\frac{3}{2}}\big), \tag{3.17}$$

where $\mathcal{F}_{\tilde{k}}$ is the quadratic form of the Laplace-like operator with the boundary conditions given by the choice of β coefficients[3]

$$\mathcal{F}_{\tilde{k}} = \mathcal{F}_{\tilde{n}} - \Theta_k, \tag{3.18}$$

$$\mathcal{F}_{\tilde{n}} = \overleftrightarrow{\mathrm{d}}_\alpha \bullet (\chi g^{-1\alpha\beta}\mathcal{G}) \bullet \overrightarrow{\mathrm{d}}_\beta + (\chi\mathcal{V}), \tag{3.19}$$

$$\Theta_k \stackrel{\text{def}}{=} -\left(\frac{1+p}{3}k + \beta\text{-terms}\right)\mathcal{Q}, \tag{3.20}$$

where χ is the characteristic function of the domain Ω. Here $\mathcal{F}_{\tilde{n}}$ is the standard quadratic form which appears in the action for a non-interacting scalar field with a potential evaluated on the domain Ω and Θ_k is a bi-distribution localized on the boundary.

[3] Here, the subscript k labels particular boundary conditions which are satisfied by the propagator, as discussed below. More precisely, it labels a choice of notion of *generalized values* and *momenta* at hypersurface Σ which are fixed by bi-distribution $\overrightarrow{\mathrm{d}}\mathcal{F}_{\tilde{k}}$—see [12]. Specifically, the subscript n corresponds to the standard value and momentum at Σ, cf equation (3.27). The meaning of the tilde in the index of the quadratic form $\mathcal{F}_{\tilde{k}}$ will not be discussed in this paper—it can be safely ignored here. It is used only for consistency with [12].

The short time behaviour (3.17) together with the composition law again proves the heat equation for the propagator:

$$-\mathcal{G} \bullet \dot{K}_{\mathrm{k}}(\tau) = \frac{\nu}{2} \mathcal{F}_{\tilde{\mathrm{k}}} \bullet K_{\mathrm{k}}(\tau). \tag{3.21}$$

The quadratic form $\mathcal{F}_{\tilde{\mathrm{k}}}$ identifies what kind of boundary conditions the propagator K_{k} satisfies. If we compare $\mathcal{F}_{\tilde{\mathrm{k}}}$ with the operator $\overset{\rightsquigarrow}{\mathcal{F}}$ (all derivatives act to the right) we find

$$\mathcal{F}_{\tilde{\mathrm{k}}} = \overset{\rightsquigarrow}{\mathcal{F}} + \overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{k}}}, \tag{3.22}$$

$$\overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{k}}} = \overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{n}}} - \Theta_{\mathrm{k}}, \tag{3.23}$$

where the bi-distribution $\overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{n}}}$ is essentially the integration of a value of the left argument and a momenta of the right argument over the boundary of the domain

$$\varphi \bullet \overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{n}}} \bullet \psi = \int_{\partial\Omega} \varphi \vec{\mathrm{n}}^{\alpha} \mathrm{d}_{\alpha} \psi \mathrm{q}^{\frac{1}{2}}. \tag{3.24}$$

To see clearly what kind of boundary conditions the propagator satisfies, we write the heat equation in the following way:

$$-\mathcal{G} \bullet \dot{K}_{\mathrm{k}}(\tau) = \frac{\nu}{2} \overset{\rightsquigarrow}{\mathcal{F}} \bullet K_{\mathrm{k}}(\tau) + \frac{\nu}{2} \overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{k}}} \bullet K_{\mathrm{k}}(\tau). \tag{3.25}$$

The solution of the heat equation is smooth for non-zero time τ. Therefore, the left-hand side, as well as the first term on the right-hand side is smooth. The second term is localized on the boundary and therefore it has to vanish. So we find

$$\overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{k}}} \bullet K_{\mathrm{k}}(\tau) = 0. \tag{3.26}$$

Or, if we define maps $\underline{\varphi}$ and $\underline{\pi}$ which assign a value $\varphi = \underline{\varphi} \bullet \phi$ and a momenta $\pi = \underline{\pi} \bullet \phi$ on the boundary to a spacetime function ϕ, we can write[4]

$$\overset{\rightsquigarrow}{\mathrm{d}\mathcal{F}}_{\tilde{\mathrm{n}}} = \underline{\varphi} \cdot \underline{\pi}, \tag{3.27}$$

$$\Theta_{\mathrm{k}} = -\underline{\varphi} \cdot \left(\left(\tfrac{1+p}{3} k + \beta\text{-terms} \right) \mathrm{q}^{\frac{1}{2}} \delta \right) \cdot \underline{\varphi}, \tag{3.28}$$

and the boundary conditions get the form

$$\left(\underline{\pi} + \left(\tfrac{1+p}{3} k + \beta\text{-terms} \right) \underline{\varphi} \right) \bullet K_{\mathrm{k}}(\tau) = 0. \tag{3.29}$$

We see that K_{k} satisfies Robin-like boundary conditions.

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 (3.12). In general, they are Robin-like conditions with a non-degenerate coefficient in front of the momentum.

3.5. Green function and sources

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 compute the amplitude associated with the set of histories with fixed

[4] As mentioned at the end of section 1, the square dot '$\cdot$' indicates spatial integration over Σ.

endpoints but without a restriction on the inner time. As before, we will call this amplitude the Feynman Green function

$$\frac{1}{n} G^F_{\rm k}(x|z) = \int_{\tau\in\mathbb{R}^+} \frac{1}{n} K_{\rm k}(\tau, x|z) \frac{\nu}{2}\, {\rm d}\tau\,. \tag{3.30}$$

Using the heat equation and initial conditions for the heat kernel, the integration gives

$$\mathcal{F}_{\bar{\rm k}} \bullet G^F_{\rm k} = \delta. \tag{3.31}$$

So, $G^F_{\rm k}$ is the inverse of $\mathcal{F}_{\bar{\rm k}}$ and restricted to smooth sources it satisfies the same boundary conditions as the propagator $K_{\rm k}$.

Let us also compute the amplitude $Z^{(1)}_{\rm k}(J)$ of a set of histories which end at a given point x and are emitted by a source described by a spacetime dependent amplitude[5] nJ. We will call it the *one-particle amplitude*. Clearly, it is given by the solution $\bar{\phi}_{\rm k}(J)$ of the non-homogeneous wave equation with source J:

$$Z^{(1)}_{\rm k}(J) = \bar{\phi}_{\rm k}(J) = G^F_{\rm k} \bullet J. \tag{3.32}$$

It satisfies the same boundary conditions as the Feynman Green function.

3.6. Interpretation of boundary conditions

We can interpret the boundary conditions for $Z^{(1)}_{\rm k}(J)$ 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 have the meaning that no particles are emitted from the boundary. What about different boundary conditions? Why is the choice of the above conditions special? We are facing a question of what kind of particles we are dealing with. What does it mean that no particles are emitted or absorbed[6]?

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 apparatus 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 a 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. All necessary information about experimental devices can thus be phenomenologically characterized by the choice of boundary conditions of the type we encountered above.

However, the Robin-like boundary conditions obtained above are not the most general. Particularly, they do not cover typical boundary conditions for the Feynman Green function obtained in the standard scalar field theory, as can be seen, e.g., from the fact that the boundary conditions of the field theory are intrinsically complex whereas the conditions above are real, see [12]. It is discussed in [12] that boundary conditions different from those derived above can be obtained by assuming an additional interaction of particles with the boundary and

[5] Again, we factorize out the prefactor n motivated by the fact that J is a density, i.e., it is proportional to volume element $\mathfrak{g}^{\frac{1}{2}}$.

[6] For scalar particle, the meanings of 'emitted' and 'absorbed' are interchangeable if we do not distinguish initial and final parts of the boundary.

within the boundary, an interaction which phenomenologically describes more complicated measurement of particles on the boundary.

3.7. Emission from the boundary

We will not discuss such an interaction here. But we ask what is the amplitude 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 on the boundary manifold, which we call the *boundary source*. The amplitude $Z_{\mathrm{k}}^{(1)}(\tau; j)$ 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* $K_{\mathrm{k}}^{\dashv}$

$$Z_{\mathrm{k}}^{(1)}(\tau; j) = K_{\mathrm{k}}^{\dashv}(\tau) \cdot j. \tag{3.33}$$

The boundary propagator propagates between points inside 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 (2.9)

$$K_{\mathrm{k}}^{\dashv}(\tau) = K_{\mathrm{k}}(\tau - \epsilon) \bullet \mathcal{G} \bullet K_{\mathrm{k}}^{\dashv}(\epsilon). \tag{3.34}$$

We can take a limit $\epsilon \to 0$ and get

$$K_{\mathrm{k}}^{\dashv}(\tau) = K_{\mathrm{k}}(\tau) \bullet \overleftrightarrow{K}_{\mathrm{k}}, \tag{3.35}$$

$$\overleftrightarrow{K}_{\mathrm{k}} \stackrel{\text{def}}{=} \mathcal{G} \bullet K_{\mathrm{k}}^{\dashv}(0). \tag{3.36}$$

We see that the amplitude is given by the propagator $K_{\mathrm{k}}(\tau)$ with no emission from the boundary, and by the boundary term $\overleftrightarrow{K}_{\mathrm{k}}$ 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

$$Z_{\mathrm{k}}^{(1)}(j) = G_{\mathrm{k}}^{F} \bullet \overleftrightarrow{K}_{\mathrm{k}} \cdot j. \tag{3.37}$$

The boundary term $\overleftrightarrow{K}_{\mathrm{k}}$ is a zero-time amplitude, so it is straightforward to estimate it. The short time amplitude approximation similar to (2.22) for the boundary propagator is

$$\begin{aligned}\phi \bullet \mathcal{G} \bullet K_{\mathrm{k}}^{\dashv}(\tau) \cdot j &= \frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int_{\substack{x\in\Omega\\ \hat{y}\in\partial\Omega}} \mathfrak{g}^{\frac{1}{2}}(x)\phi(x)j(\hat{y})\Delta(x|\hat{y}) \exp\left(-\frac{1}{\nu\tau}\sigma(x|\hat{y})\right)(1+\mathcal{O}(\sqrt{\tau}))\\ &= \int_{\hat{y}\in\partial\Omega} \phi(\hat{y})j(\hat{y})\,(1+\mathcal{O}(\sqrt{\tau})) = \phi \bullet \underline{\varphi} \cdot j\,(1+\mathcal{O}(\sqrt{\tau})).\end{aligned} \tag{3.38}$$

Therefore, for zero inner time we get

$$\overleftrightarrow{K}_{\mathrm{k}} = \underline{\varphi}. \tag{3.39}$$

It means that the emission from the boundary is equivalent to the emission of particles inside the domain but with a distributional source $\partial J = j \cdot \underline{\varphi}$ with support on the boundary.

Allowing both boundary sources and sources inside the domain, we find that the one-particle amplitude is

$$Z_{\mathrm{k}}^{(1)}(J, \partial J) = G_{\mathrm{k}}^{F} \bullet (J + \partial J) = \bar{\phi}_{\mathrm{k}}(J + \partial J). \tag{3.40}$$

A careful discussion of the distributional character of introduced boundary sources, differential operators and Green functions shows (see [12]) that it satisfies the equation of motion in the expected form

$$\mathcal{F}_{\bar{\mathrm{k}}} \bullet \bar{\phi}_{\mathrm{k}}(J + \partial J) = J + \partial J, \tag{3.41}$$

with boundary conditions fixed by the boundary source

$$\partial J = \overleftrightarrow{\mathrm{d}\mathcal{F}}_{\bar{\mathrm{k}}} \bullet \bar{\phi}_{\mathrm{k}}(J + \partial J). \tag{3.42}$$

4. Summary

We studied sum-over-histories quantization of relativistic particle on a bounded domain of the spacetime. We modified the definition of the path integral by adding terms corresponding to paths reflected on the boundary of the domain. Such contributions can be dominant in the short time approximation near the boundary in addition to the usual dominant contributions from the straight geodesic. These contributions compensate other terms localized on the boundary which arise from restriction of non-reflected paths into the interior of the domain. They also specify the exact form of the boundary conditions for the propagator and Green functions. We found that boundary conditions have Robin-like form and their exact form depends on the details of the definition of the path integral—a non-uniqueness is hidden in the specification of β-coefficients in the short time amplitude (3.12).

We interpreted the specific boundary conditions as a consequence of an interaction with apparatus (localized on the boundary) which define a notion of particles. Because of the non-uniqueness of the definition of the path integral, we do not have a uniqueness in the definition of particles. The boundary condition can thus be viewed as a phenomenological description of the specific kind of particles—the different boundary conditions correspond to different types of detection of particles on the boundary.

The boundary conditions obtained by a sum-over-histories quantization of a relativistic particle, however, do not correspond to the boundary conditions of the quantum field theory in curved spacetime. The boundary condition (satisfied, e.g., by a Green function) in the field theory approach is related to the choice of the vacuum state. They also have Robin-like form (they are given by a condition on a linear combination of field values and momenta on the boundary), however, they are intrinsically complex (they actually specify the splitting of a solution of a wave equation into positive and negative frequency parts). To obtain such boundary conditions in sum-over-histories quantization of a relativistic particle, it would be necessary to assume an additional interaction of particles on the boundary. Different choices of such an interaction would then lead to Green functions corresponding to different choices of vacuum state. We leave, however, a detailed discussion of such a correspondence to another work (cf also [12]).

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Appendix A. Asymptotic expansion of the leading term in the heat kernel

A.1. Vector space

In a vector space V equipped with a positive non-degenerate quadratic form g, an expansion in $\sqrt{\tau}$ and a simple Gaussian integration gives

$$\frac{1}{(2\pi\nu\tau)^{\frac{d}{2}}}\int_{X,Z\in V}\mathfrak{g}^{\frac{1}{2}}(X)\mathfrak{g}^{\frac{1}{2}}(Z)\varphi(X)\psi(Z)\exp\left(-\frac{1}{2\nu\tau}(X-Z)\cdot g\cdot(X-Z)\right)$$
$$=\sum_{m\in\mathbb{N}_0}\frac{1}{m!}\left(-\frac{\nu\tau}{2}\right)^m\varphi\bullet\mathcal{L}^m\bullet\psi. \qquad \text{(A.1)}$$

Here φ, ψ are test functions, $\mathfrak{g}^{\frac{1}{2}}$ is the constant volume element of the metric g, ν is a constant $\big(\mathrm{Re}\,\frac{1}{\nu} \geqslant 0\big)$ and $\mathcal{L}^m$ represents a bi-distribution

$$\varphi \bullet \mathcal{L}^m \bullet \psi = \int_V \mathfrak{g}^{\frac{1}{2}} \varphi[(g^{-1\alpha\beta}\partial_\alpha\partial_\beta)^m \psi] = \int_V \mathfrak{g}^{\frac{1}{2}} \psi[(g^{-1\alpha\beta}\partial_\alpha\partial_\beta)^m \varphi]. \tag{A.2}$$

It can be viewed as an 'mth' power of the Laplace quadratic form $\mathcal{L}$ associated with the metric g on the vector space V. We can thus write the asymptotic expansion for small τ as

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \mathfrak{g}^{\frac{1}{2}}(X)\mathfrak{g}^{\frac{1}{2}}(Z) \exp\left(-\frac{1}{2\nu\tau}(X-Z)\cdot g\cdot(X-Z)\right) = \sum_{m\in\mathbb{N}_0} \frac{1}{m!}\left(-\frac{\tau\nu}{2}\right)^m \mathcal{L}^m. \tag{A.3}$$

We allow the metric g to be Lorentzian—this case can be obtained by analytical continuation in the phase factor n which characterizes the signature of the metric.

In the case of the vector space, the expression on the left side of equation (A.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., [13] for more details.

A.2. 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

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \Delta(x|z)\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z) \exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right), \tag{A.4}$$

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 neighbourhood of x. In this neighbourhood we can change variables $z \to Z$ with

$$z = \boldsymbol{u}_x(\sqrt{\tau}Z) \approx x + \sqrt{\tau}Z, \tag{A.5}$$

where $\boldsymbol{u}_x(\epsilon Z)$ is a geodesic with an origin x and initial tangent vector Z (see (B.1)). This is the exact meaning of 'adding' a vector to a point questioned after equation (2.18).

The Jacobian associated with this change of variables is given by the Van Vleck–Morette determinant (see (B.43))

$$\big(\boldsymbol{u}_x^{-1\star}\mathfrak{g}^{\frac{1}{2}}\big)(\sqrt{\tau}Z) = \tau^{\frac{d}{2}}\mathfrak{g}^{\frac{1}{2}}(x)[Z]\Delta^{-1}(x|z), \tag{A.6}$$

where $\mathfrak{g}^{\frac{1}{2}}(x)[Z]$ is understood as a constant measure on the target vector space $\mathbf{T}_x M$. After a change of variables, using (B.16), expanding ψ and performing a Gaussian integration, we get

$$\begin{aligned}\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} &\int_{x,z\in M} \Delta(x|z)\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\varphi(x)\psi(z) \exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right)\\ &= \int_M \mathfrak{g}^{\frac{1}{2}}\varphi\left(\psi + \frac{\nu\tau}{2}g^{-1\alpha\beta}\psi_{2\alpha\beta} + \mathcal{O}(\tau^2)\right).\end{aligned} \tag{A.7}$$

Here ψ_2 is the second coefficient in covariant expansion (B.26). Thanks to (B.27) we have $\psi_2 = \nabla\,\mathrm{d}\psi$ and we get

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \Delta(x|z)\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z) \exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right) = \mathcal{G} - \frac{\nu\tau}{2}\mathcal{L} + \mathcal{O}(\tau^2). \tag{A.8}$$

A.3. 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

$$\mu = \mathrm{d}\eta, \qquad \mathcal{M} = \mu\delta, \qquad \partial = \frac{\partial}{\partial\eta}. \tag{A.9}$$

We define bi-distributions of the mth derivative

$$\omega \bullet \overrightarrow{\partial}^{\langle m\rangle} \bullet \varphi = \omega \bullet (\partial^m \varphi) = \int_{\mathbb{R}^+} \omega(\partial^m\varphi), \qquad \overleftarrow{\partial}^{\langle m\rangle} = \overrightarrow{\partial}^{\langle m\rangle\top}, \tag{A.10}$$

and

$$\overrightarrow{\partial} = \overrightarrow{\partial}^{\langle 1\rangle}, \qquad \overleftarrow{\partial} = \overleftarrow{\partial}^{\langle 1\rangle}. \tag{A.11}$$

We can also define a boundary delta bi-distribution $\mathcal{D}$ (the boundary is one point now) as

$$\varphi \bullet \mathcal{D} \bullet \psi = (\varphi\psi)|_{\text{boundary}}. \tag{A.12}$$

Integration by parts can be expressed by the relation

$$\begin{aligned} &\overleftarrow{\partial} \bullet \mathcal{M} + \mathcal{M} \bullet \overrightarrow{\partial} = -\mathcal{D}, \\ &\overleftarrow{\partial}^{\langle m+1\rangle} \bullet \mathcal{M} + (-1)^m \mathcal{M} \bullet \overrightarrow{\partial}^{\langle m+1\rangle} = -\sum_{k=0,\ldots,m} \overleftarrow{\partial}^{\langle m-k\rangle} \bullet \mathcal{D} \bullet \overrightarrow{\partial}^{\langle k\rangle}. \end{aligned} \tag{A.13}$$

Next we define quadratic forms of powers of the Laplace operator

$$\begin{aligned} &\overrightarrow{\mathcal{L}} = -\mathcal{M} \bullet \overrightarrow{\partial}^{\langle 2\rangle}, && \overrightarrow{\mathcal{L}}^{\langle m\rangle} = (-1)^m \mathcal{M} \bullet \overrightarrow{\partial}^{\langle 2m\rangle}, \\ &\overleftarrow{\mathcal{L}} = -\overleftarrow{\partial}^{\langle 2\rangle} \bullet \mathcal{M}, && \overleftarrow{\mathcal{L}}^{\langle m\rangle} = (-1)^m \overleftarrow{\partial}^{\langle 2m\rangle} \bullet \mathcal{M}, \\ &\overleftrightarrow{\mathcal{L}} = \tfrac{1}{2}(\overrightarrow{\mathcal{L}} + \overleftarrow{\mathcal{L}}), && \overleftrightarrow{\mathcal{L}}^{\langle m\rangle} = \tfrac{1}{2}(\overleftarrow{\mathcal{L}}^{\langle m\rangle} + \overrightarrow{\mathcal{L}}^{\langle m\rangle}), \\ &\mathcal{L} = \overleftarrow{\partial} \bullet \mathcal{M} \bullet \overrightarrow{\partial}. \end{aligned} \tag{A.14}$$

The symplectic form on the boundary is

$$\partial\mathcal{L} = \overrightarrow{\mathcal{L}} - \overleftarrow{\mathcal{L}} = -\overleftarrow{\partial} \bullet \mathcal{D} + \mathcal{D} \bullet \overrightarrow{\partial}. \tag{A.15}$$

It is straightforward to check that

$$\overrightarrow{\mathcal{L}}^{\langle m\rangle} - \overleftarrow{\mathcal{L}}^{\langle m\rangle} = (-1)^m \sum_{\substack{k,l\in\mathbb{N}_0 \\ k+l+1=2m}} \overleftarrow{\partial}^{\langle k\rangle} \bullet \mathcal{D} \bullet \overrightarrow{\partial}^{\langle l\rangle}. \tag{A.16}$$

Now we prove the following expansion for small τ:

$$\begin{aligned} &\frac{1}{\sqrt{2\pi\tau\nu}} \exp\left(-\frac{1}{2\tau\nu}(\xi-\zeta)^2\right) \mu(\xi)\mu(\zeta) \\ &\quad = \sum_{m\in\mathbb{N}_0} \frac{1}{\Gamma\left(\frac{m}{2}+1\right)} \left(\frac{\tau\nu}{2}\right)^{\frac{m}{2}} \frac{1}{2}(\overleftarrow{\partial}^{\langle m\rangle} \bullet \mathcal{M} + \mathcal{M} \bullet \overrightarrow{\partial}^{\langle m\rangle}) \\ &\quad = \sum_{m\in\mathbb{N}_0} \frac{(-1)^m}{m!} \left(\frac{\tau\nu}{2}\right)^m \overleftrightarrow{\mathcal{L}}^{\langle m\rangle} \\ &\qquad + \sum_{m\in\mathbb{N}_0} \frac{(-1)^{m+1}}{\Gamma\left(m+\frac{3}{2}\right)} \left(\frac{\tau\nu}{2}\right)^{m+\frac{1}{2}} \frac{1}{2} \sum_{\substack{k,l\in\mathbb{N}_0 \\ k+l=2m}} (-1)^{\frac{k-l}{2}} \overleftarrow{\partial}^{\langle k\rangle} \bullet \mathcal{D} \bullet \overrightarrow{\partial}^{\langle l\rangle}. \end{aligned} \tag{A.17}$$

Here ν is a complex constant such that $\frac{1}{\nu}$ has a 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 a limiting procedure. Because only a combination of $\tau\nu$ appears in the equation, we drop ν in the following derivation—it can be easily restored by inspecting the τ-dependence.

Clearly, the second equality follows from integration by parts (A.13). To prove the first one we smooth it with test functions φ and ψ and get

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi\tau}}\int_{\xi,\zeta\in\mathbb{R}^+}\exp\left(-\frac{1}{2\tau}(\xi-\zeta)^2\right)\varphi(\xi)\psi(\zeta)\mu(\xi)\mu(\zeta)\\
&\quad=\frac{1}{\sqrt{2\pi\tau}}\int_{\xi\in\langle 0,\epsilon\rangle}\mathrm{d}\xi\int_{\zeta\in\mathbb{R}^+}\mathrm{d}\zeta\,\varphi(\xi)\psi(\zeta)\exp\left(-\frac{1}{2\tau}(\xi-\zeta)^2\right)\\
&\quad\quad+\frac{1}{\sqrt{2\pi\tau}}\int_{\xi\in\langle \epsilon,\infty\rangle}\mathrm{d}\xi\int_{\zeta\in\mathbb{R}^+}\mathrm{d}\zeta\,\varphi(\xi)\psi(\zeta)\exp\left(-\frac{1}{2\tau}(\xi-\zeta)^2\right),
\end{aligned}\tag{A.18}$$

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 we obtain

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi\tau}}\int_{\xi\in\langle 0,\epsilon\rangle}\mathrm{d}\xi\int_{\zeta\in\mathbb{R}^+}\mathrm{d}\zeta\,\varphi(\xi)\psi(\zeta)\exp\left(-\frac{1}{2\tau}(\xi-\zeta)^2\right)\\
&\quad=\frac{1}{\sqrt{2\pi}}\sum_{k,l\in\mathbb{N}_0}\tau^{\frac{k+l+1}{2}}\varphi^{\langle k\rangle}(0)\psi^{\langle l\rangle}(0)\frac{1}{k!}\int_{\xi\in\langle 0,\frac{\epsilon}{\sqrt{\tau}}\rangle}\mathrm{d}\xi\,\xi^k\mathrm{R}_{l+1}(\xi),
\end{aligned}\tag{A.19}$$

where we have used the definition (C.1) of special functions R_l. Properties of these special functions are summarized in appendix C. Using equations (C.17), (C.10) and (C.14), the last expression can be rewritten as

$$\begin{aligned}
&-\sum_{m\in\mathbb{N}}\frac{\tau^m}{(2m)!!}\frac{1}{2}\sum_{l=0,\ldots,2m-1}(-1)^l\varphi^{\langle 2m-l-1\rangle}(0)\psi^{\langle l\rangle}(0)\\
&\quad+\sum_{m\in\mathbb{N}_0}\frac{\tau^{m+\frac{1}{2}}}{(2m+1)!!}\frac{-1}{\sqrt{2\pi}}\sum_{l=0,\ldots,2m}(-1)^l\varphi^{\langle 2m-l\rangle}(0)\psi^{\langle l\rangle}(0)\\
&\quad+\sum_{m\in\mathbb{N}_0}\frac{\tau^m}{(2m)!!}\sum_{k,l\in\mathbb{N}_0}\frac{\epsilon^{k+l+1}}{k!l!(k+l+1)}\varphi^{\langle k\rangle}(0)\psi^{\langle l+2m\rangle}(0)+\exp\left(-\frac{1}{2}\frac{\epsilon^2}{\tau}\right)\mathcal{O}(\tau).
\end{aligned}\tag{A.20}$$

In the second term of the expression (A.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 with the help of (C.15), (C.11), (C.16) and (C.14) we obtain

$$\begin{aligned}
&\sum_{m=\mathbb{N}_0}\frac{\tau^m}{(2m)!!}\int_{\xi\in\mathbb{R}^+}\mathrm{d}\xi\,\varphi(\xi)\psi^{\langle 2m\rangle}(\xi)-\sum_{m=\mathbb{N}_0}\frac{\tau^m}{(2m)!!}\int_{\xi\in\langle 0,\epsilon\rangle}\mathrm{d}\xi\,\varphi(\xi)\psi^{\langle 2m\rangle}(\xi)\\
&\quad+\exp\left(-\frac{1}{2}\frac{\epsilon^2}{\tau}\right)\mathcal{O}(\tau).
\end{aligned}\tag{A.21}$$

For small ϵ we can expand φ and $\psi^{\langle 2m\rangle}$ about zero in the second term. Also performing an integration by parts in the first term (A.21) transforms to

$$\sum_{m\in\mathbb{N}_0}\frac{\tau^m}{(2m)!!}\frac{1}{2}\int_{\xi\in\mathbb{R}^+}\mathrm{d}\xi\,(\varphi^{\langle 2m\rangle}(\xi)\psi(\xi)+\varphi(\xi)\psi^{\langle 2m\rangle}(\xi))$$
$$+\sum_{m\in\mathbb{N}}\frac{\tau^m}{(2m)!!}\frac{1}{2}\sum_{l=0,\dots,2m-1}(-1)^l\varphi^{\langle 2m-l-1\rangle}(0)\psi^{\langle l\rangle}(0)$$
$$-\sum_{m\in\mathbb{N}_0}\frac{\tau^m}{(2m)!!}\sum_{k,l\in\mathbb{N}_0}\frac{\epsilon^{k+l+1}}{k!l!(k+l+1)}\varphi^{\langle k\rangle}(0)\psi^{\langle l+2m\rangle}(0)+\exp\left(-\frac{1}{2}\frac{\epsilon^2}{\tau}\right)\mathcal{O}(\tau). \tag{A.22}$$

Substituting equations (A.20) and (A.22) to equation (A.18) and ignoring exponentially suppressed terms $\exp\left(-\frac{1}{2}\frac{\epsilon^2}{\tau}\right)\mathcal{O}(\tau)$, we obtain the desired relation (A.17).

It is also possible to write down another expansion for small τ

$$\frac{1}{\sqrt{2\pi\nu\tau}}\omega\left(\frac{\xi\zeta}{\xi+\zeta}\right)\exp\left(-\frac{1}{2\nu\tau}(\xi+\zeta)^2\right)\mu(\xi)\mu(\zeta)$$
$$=\sum_{n\in\mathbb{N}_0}\left(\frac{\tau\nu}{2}\right)^{\frac{n+1}{2}}\frac{1}{\Gamma\left(\frac{n+1}{2}\right)}\sum_{\substack{m,k,l\in\mathbb{N}_0\\ k+l+m=n}}\frac{\omega^{\langle m\rangle}(0)}{n+m+1}\frac{\binom{m+k}{k}\binom{m+l}{l}}{\binom{n+m}{m}}\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}, \tag{A.23}$$

where ω is a smooth function. It can be proved, if we smooth the relation with test functions φ and ψ—only small values of ξ and ζ contribute to the integrals, thanks to the exponential suppression, and we can thus rescale ξ and ζ by $\sqrt{\tau}$, expand φ, ψ and ω about zero, and using (C.18) we obtain the desired result.

As a corollary, for $\omega = 1$ we get

$$\frac{1}{\sqrt{2\pi\nu\tau}}\exp\left(-\frac{1}{2\nu\tau}(\xi+\zeta)^2\right)\mu(\xi)\mu(\zeta)$$
$$=\sum_{k,l\in\mathbb{N}_0}\frac{1}{\Gamma\left(\frac{k+l+1}{2}+1\right)}\left(\frac{\tau\nu}{2}\right)^{\frac{k+l+1}{2}}\frac{1}{2}\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}$$
$$=\sum_{m\in\mathbb{N}}\frac{1}{m!}\left(\frac{\tau\nu}{2}\right)^m\frac{1}{2}\sum_{\substack{k,l\in\mathbb{N}_0\\ k+l+1=2m}}\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}$$
$$+\sum_{m\in\mathbb{N}_0}\frac{1}{\Gamma\left(m+\frac{3}{2}\right)}\left(\frac{\tau\nu}{2}\right)^{m+\frac{1}{2}}\frac{1}{2}\sum_{\substack{k,l\in\mathbb{N}_0\\ k+l=2m}}\overleftarrow{\partial}^{\langle k\rangle}\bullet\mathcal{D}\bullet\overrightarrow{\partial}^{\langle l\rangle}. \tag{A.24}$$

A.4. 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

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z)\exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right)=\mathcal{G}+\sqrt{\tau}\left(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\right)\mathcal{Q}-\tau\frac{\nu}{2}\overleftrightarrow{\mathcal{L}}+\mathcal{O}\left(\tau^{\frac{3}{2}}\right). \tag{A.25}$$

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 in the 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 neighbourhood $U \subset \Omega$ of the boundary with topology $\mathbb{R} \times \partial\Omega$ on which the geodesics normal to the boundary do not cross. In such a neighbourhood, we can use the method described in appendix B and change the integration over a neighbourhood to integration over the boundary $\partial\Omega$ and geodesic distance from the boundary (see (B.60))

$$\begin{aligned} x &\to \hat{x}, \xi, \qquad x = \hat{\boldsymbol{w}}(\hat{x}, \xi), \\ z &\to \hat{z}, \zeta, \qquad y = \hat{\boldsymbol{w}}(\hat{z}, \zeta). \end{aligned} \tag{A.26}$$

The Jacobian $\hat{j}(\hat{x}, \xi)$ associated with this change of variables is

$$\mathfrak{g}^{\frac{1}{2}}(\hat{x}) = \mathrm{d}\xi\, \hat{\mathfrak{q}}^{\frac{1}{2}}(\hat{x}, \xi) = \mathrm{d}\xi\, \hat{j}(\hat{x}, \xi)\mathfrak{q}^{\frac{1}{2}}. \tag{A.27}$$

Here we use the convention (B.62)—we denote a spacetime dependent object $A(x)$ expressed in variables $\hat{x}$, ξ and with tensor indices moved to the boundary as $\hat{A}(\hat{x}, \xi)$. Changing variables we get

$$\begin{aligned} &\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int_{x,z\in\Omega} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\Delta(x|z) \exp\left(-\frac{1}{\nu\tau}\sigma(x|z)\right)\varphi(x)\psi(z) \\ &\quad = \int_{\hat{x}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\hat{x}) \frac{n}{(2\pi\nu\tau)^{\frac{d+1}{2}}} \int_{\xi,\zeta\in\mathbb{R}^+} \mathrm{d}\xi\,\mathrm{d}\zeta\; \hat{\varphi}(\hat{x}, \xi) \\ &\qquad \times \int_{\hat{z}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\hat{z}) \triangle(\hat{x}|\hat{z})\, \hat{\psi}(\hat{z}, \zeta) \exp\left(-\frac{1}{\nu\tau}\,\hat{\sigma}(\hat{x}, \xi|\hat{z}, \zeta) + \hat{l}(\hat{x}, \xi|\hat{z}, \zeta)\right). \end{aligned} \tag{A.28}$$

Here we have defined

$$\hat{l}(\hat{x}, \xi|\hat{z}, \zeta) = \ln\left(\hat{j}(\hat{x}, \xi) \frac{\hat{\Delta}(\hat{x}, \xi|\hat{z}, \zeta)}{\triangle(\hat{x}|\hat{z})} \hat{j}(\hat{z}, \zeta)\right), \tag{A.29}$$

where $\triangle(\hat{x}|\hat{z})$ (small symbol '$\triangle$'!) is the Van Vleck–Morette determinant of the metric q on the boundary manifold.

Exponential suppression ensures again that the only contribution comes from $\hat{x} \approx \hat{z}$. So we can change variables $\hat{x}, \hat{z} \to \hat{y}, Y$

$$\hat{y} = \hat{x}\,, \qquad Y \in \mathbf{T}_{\hat{y}}\partial\Omega, \qquad \hat{z} = \boldsymbol{v}_{\hat{y}}(\sqrt{\tau}Y), \tag{A.30}$$

with the exponential map $\boldsymbol{v}_{\hat{y}}(Y)$ defined as in (B.1) but on the boundary manifold. The Jacobian for this change of variables is given by an equation similar to (B.43), only with the Van Vleck–Morette determinant $\triangle(\hat{x}, \hat{y})$ defined using the metric q on the boundary manifold. We use covariant expansions

$$\hat{\sigma}(\hat{y}, \xi|\hat{y}, \sqrt{\tau}Y, \zeta) = \tau n^2 \frac{1}{2}(\xi - \zeta)^2 + \sum_{k=2,3,\ldots} \tau^{\frac{k}{2}} \frac{1}{k!} \hat{\sigma}_{0,k\mu_1\ldots\mu_k}(\hat{y}; \xi, \zeta) Y^{\mu_1} \ldots Y^{\mu_k}, \tag{A.31}$$

$$\hat{l}(\hat{y}, \xi|\hat{y}, \sqrt{\tau}Y, \zeta) = \sum_{k=\mathbb{N}_0} \tau^{\frac{k}{2}} \frac{1}{k!} \hat{l}_{0,k\mu_1\ldots\mu_k}(\hat{y}; \xi, \zeta) Y^{\mu_1} \ldots Y^{\mu_k}, \tag{A.32}$$

$$\hat{\psi}(\hat{y}, \sqrt{\tau}Y, \zeta) = \sum_{k=\mathbb{N}_0} \tau^{\frac{k}{2}} \frac{1}{k!} \hat{\psi}_{k\mu_1\ldots\mu_k}(\hat{y}; \zeta) Y^{\mu_1} \ldots Y^{\mu_k}, \tag{A.33}$$

with coefficients given by expressions (B.99)–(B.103), (B.104)–(B.106), and (B.27). Expanding the exponential, gathering all terms up to order $\mathcal{O}(\tau)$, and performing a Gaussian integration over Y lead to

$$\int_{\widehat{y}\in\partial\Omega} \frac{n}{(2\pi\nu\tau)^{\frac{1}{2}}} \int_{\xi,\zeta\in\mathbb{R}^+} \mathrm{d}\xi\,\mathrm{d}\zeta\,\exp\left(-\frac{n^2}{2\nu\tau}(\zeta-\xi)^2\right) \times \tilde{j}(\widehat{y};\xi,\zeta)(\omega_0(\widehat{y};\xi,\zeta)+\tau\omega_1(\widehat{y};\xi,\zeta)+\mathcal{O}(\tau^2)), \tag{A.34}$$

with

$$\tilde{j}(\widehat{y};\xi,\zeta) = \widehat{j}(\widehat{y},\xi)\widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\widehat{j}(\widehat{y},\zeta)\mathfrak{q}^{\frac{1}{2}}(\widehat{y})(\mathrm{Det}_{\shortparallel}\widehat{\sigma}_{0,2}(\widehat{y};\xi,\zeta))^{-\frac{1}{2}} = (\widehat{j}(\widehat{y},\xi)\widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\widehat{j}(\widehat{y},\zeta))^{\frac{1}{2}}, \tag{A.35}$$

$$\omega_0(\widehat{y};\xi,\zeta) = \widehat{\varphi}(\widehat{y},\xi)\widehat{\psi}(\widehat{y},\zeta), \tag{A.36}$$

$$\begin{aligned}\omega_1(\widehat{y};\xi,\zeta) = {}& \nu\widehat{\varphi}(\widehat{y},\xi)\widehat{\psi}(\widehat{y},\zeta)\big(-\tfrac{1}{8}\widehat{\sigma}_{0,4\mu\nu\kappa\lambda}\widehat{\sigma}_{0,2}^{-1\mu\nu}\widehat{\sigma}_{0,2}^{-1\kappa\lambda}+\tfrac{1}{2}\widehat{l}_{0,2\mu\nu}\widehat{\sigma}_{0,2}^{-1\mu\nu}\\ &+\tfrac{1}{8}\widehat{\sigma}_{0,3\mu\nu\alpha}\widehat{\sigma}_{0,3\kappa\lambda\beta}\widehat{\sigma}_{0,2}^{-1\mu\nu}\widehat{\sigma}_{0,2}^{-1\alpha\beta}\widehat{\sigma}_{0,2}^{-1\kappa\lambda}-\tfrac{1}{2}\widehat{l}_{0,1\mu}\widehat{\sigma}_{0,3\kappa\lambda\nu}\widehat{\sigma}_{0,2}^{-1\mu\nu}\widehat{\sigma}_{0,2}^{-1\kappa\lambda}\\ &+\tfrac{1}{12}\widehat{\sigma}_{0,3\mu\kappa\alpha}\widehat{\sigma}_{0,3\nu\lambda\beta}\widehat{\sigma}_{0,2}^{-1\mu\nu}\widehat{\sigma}_{0,2}^{-1\alpha\beta}\widehat{\sigma}_{0,2}^{-1\kappa\lambda}+\tfrac{1}{2}\widehat{l}_{0,1\mu}\widehat{l}_{0,1\nu}\widehat{\sigma}_{0,2}^{-1\mu\nu}\big)(\widehat{y};\xi,\zeta)\\ &+\nu\widehat{\varphi}(\widehat{y};\xi)\widehat{\psi}_{1\mu}(\widehat{y};\zeta)\widehat{\sigma}_{0,2}^{-1\mu\nu}\big(\widehat{l}_{0,1\nu}-\tfrac{1}{2}\widehat{\sigma}_{0,3\kappa\lambda\nu}\widehat{\sigma}_{0,2}^{-1\kappa\lambda}\big)(\widehat{y};\xi,\zeta)\\ &+\nu\widehat{\varphi}(\widehat{y};\xi)\widehat{\psi}_{2\mu\nu}(\widehat{y};\zeta)\widehat{\sigma}_{0,2}^{-1\mu\nu}(\widehat{y};\xi,\zeta).\end{aligned} \tag{A.37}$$

The equality in (A.35) is proved in (B.76). Applying the expansion in (A.17) in (A.34) and using (A.6) we get

$$\begin{aligned}&\int_{y\in\Omega}\mathfrak{g}^{\frac{1}{2}}(y)\varphi(y)\psi(y)+\sqrt{\tau}\left(-\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\right)\int_{\widehat{y}\in\Omega}\mathfrak{q}^{\frac{1}{2}}(\widehat{y})\varphi(\widehat{y})\psi(\widehat{y})\\ &\quad+\tau\int_{\substack{\widehat{y}\in\partial\Omega\\ \eta\in\mathbb{R}^+}}\mathrm{d}\eta\,\mathfrak{q}^{\frac{1}{2}}(\widehat{y})\widehat{j}(\widehat{y};\eta)\Big(\frac{\nu}{4n^2}\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathfrak{l}\prime\mathfrak{l}\prime}+\frac{\nu}{4n^2}\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathfrak{r}\prime\mathfrak{r}\prime}+\omega_1\Big)(\widehat{y};\eta,\eta)\\ &\quad+\mathcal{O}\big(\tau^{\frac{3}{2}}\big),\end{aligned} \tag{A.38}$$

where $f^{\mathfrak{l}\prime}(\xi,\zeta)$ (or $f^{\mathfrak{r}\prime}(\xi,\zeta)$) means derivative of a function f with respect to the left (or right) argument (i.e., 'left prime' and 'right prime').

We see that we have already proved 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 (B.101))

$$[\widehat{\sigma}_{0,2}] = \widehat{q}, \tag{A.39}$$

where by a coincidence limit $[f](\eta)$ of a function $f(\xi,\zeta)$ depending on two real parameters we mean $[f](\eta) = f(\eta,\eta)$. Using (B.107) and (B.108) we get

$$\begin{aligned}&\frac{1}{n}[(\ln\tilde{j})^{\mathfrak{r}\prime}] = \frac{1}{2}n\widehat{k},\\ &\frac{1}{n^2}[(\ln\tilde{j})^{\mathfrak{r}\prime\mathfrak{r}\prime}] = \frac{1}{2n^2}(\ln\widehat{j})^{\mathfrak{r}\prime\mathfrak{r}\prime}+\frac{1}{2n^2}[(\ln\widehat{\Delta})^{\mathfrak{r}\prime\mathfrak{r}\prime}] = -\frac{n^2}{6}\widehat{\mathrm{K}}^2+\frac{1}{3}\widehat{k}',\end{aligned} \tag{A.40}$$

and therefore

$$\frac{1}{n^2}[\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathfrak{r}\prime\mathfrak{r}\prime}] = \frac{1}{n^2}\widehat{\varphi}\widehat{\psi}''+\widehat{k}\widehat{\varphi}\widehat{\psi}'+\left(\frac{1}{3}\widehat{k}'-\frac{1}{6}n^2\widehat{\mathrm{K}}^2+\frac{1}{4}\widehat{k}^2\right)\widehat{\varphi}\widehat{\psi}. \tag{A.41}$$

Here $\widehat{k}$ is a trace of extrinsic curvature and $\widehat{\mathrm{K}}^2$ is a square of the extrinsic curvature (equation (B.51)). Next, using (B.27), (B.105) and (B.102), transforming the connection ∇ to $\widehat{\nabla}$ (equation (B.64)) and performing an integration by parts give

$$\frac{\nu}{2}\int_{\partial\Omega} \mathfrak{q}^{\frac{1}{2}}\widehat{j}\widehat{\varphi}\left(\widehat{q}^{-1\mu\nu}\widehat{\psi}_{2\mu\nu}+\widehat{\psi}_{1\mu}\widehat{q}^{-1\mu\nu}\left([\widehat{l}_{0,1\nu}]-\frac{1}{2}[\widehat{\sigma}_{0,3\kappa\lambda\nu}]\widehat{q}^{-1\kappa\lambda}\right)\right)$$
$$=-\frac{\nu}{2}\int_{\partial\Omega}\widehat{\mathfrak{q}}^{\frac{1}{2}}\mathrm{D}_\mu\widehat{\varphi}\widehat{q}^{-1\mu\nu}\mathrm{D}_\nu\widehat{\psi}. \tag{A.42}$$

Substituting for $[\widehat{\sigma}_{0,k}]$ and $[\widehat{l}_{0,k}]$ in the remaining terms of $[\omega_1]$, a straightforward long calculation gives

$$-\frac{1}{8}[\widehat{\sigma}_{0,4\mu\nu\kappa\lambda}]\widehat{q}^{-1\mu\nu}\widehat{q}^{-1\kappa\lambda}+\frac{1}{2}[\widehat{l}_{0,2\mu\nu}]\widehat{q}^{-1\mu\nu}+\frac{1}{8}[\widehat{\sigma}_{0,3\mu\nu\alpha}][\widehat{\sigma}_{0,3\kappa\lambda\beta}]\widehat{q}^{-1\mu\nu}\widehat{q}^{-1\alpha\beta}\widehat{q}^{-1\kappa\lambda}$$
$$+\frac{1}{2}[\widehat{l}_{0,1\mu}][\widehat{l}_{0,1\nu}]\widehat{q}^{-1\mu\nu}+\frac{1}{12}[\widehat{\sigma}_{0,3\mu\kappa\alpha}][\widehat{\sigma}_{0,3\nu\lambda\beta}]\widehat{q}^{-1\mu\nu}\widehat{q}^{-1\alpha\beta}\widehat{q}^{-1\kappa\lambda}$$
$$-\frac{1}{2}[\widehat{l}_{0,1\mu}][\widehat{\sigma}_{0,3\kappa\lambda\nu}]\widehat{q}^{-1\mu\nu}\widehat{q}^{-1\kappa\lambda}$$
$$=\nu\left(-\frac{1}{6}\widehat{k}'+\frac{n^2}{12}\widehat{\mathrm{K}}^2-\frac{n^2}{8}\widehat{k}^2\right). \tag{A.43}$$

Putting together (A.41)–(A.43), and integrating by parts we find

$$\int_{\substack{\widehat{y}\in\partial\Omega\\ \eta\in\mathbb{R}^+}}\mathrm{d}\eta\,\mathfrak{q}^{\frac{1}{2}}(\widehat{y})\widehat{j}(\widehat{y};\eta)\left(\frac{\nu}{4n^2}\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathrm{1}/\mathrm{1}'}+\frac{\nu}{4n^2}\tilde{j}^{-1}(\tilde{j}\omega_0)^{\mathrm{r}/\mathrm{r}'}+\omega_1\right)(\widehat{y};\eta,\eta)$$
$$=\frac{\nu}{2}\int_{\mathbb{R}^+}\mathrm{d}\eta\int_{\partial\Omega}\widehat{\mathfrak{q}}^{\frac{1}{2}}\left(\frac{1}{2n^2}(\widehat{\varphi}''\widehat{\psi}+\widehat{\varphi}\widehat{\psi}''+n^2\widehat{k}(\widehat{\varphi}'\widehat{\psi}+\widehat{\varphi}\widehat{\psi}'))-\mathrm{D}_\mu\widehat{\varphi}\,\widehat{q}^{-1\mu\nu}\,\mathrm{D}_\nu\widehat{\psi}\right)$$
$$=-\frac{\nu}{2}\int_\Omega\mathfrak{g}^{\frac{1}{2}}\;\mathrm{d}_\mu\varphi\,g^{-1\mu\nu}\,\mathrm{d}_\nu\psi-\frac{\nu}{4n^2}\int_{\partial\Omega}\mathfrak{q}^{\frac{1}{2}}(\psi\,\vec{\mathrm{n}}^\mu\,\mathrm{d}_\mu\varphi+\varphi\,\vec{\mathrm{n}}^\mu\,\mathrm{d}_\mu\psi)$$
$$=-\frac{\nu}{2}\varphi\bullet\overset{\leftrightsquigarrow}{\mathcal{L}}\bullet\psi. \tag{A.44}$$

This concludes the proof of the expansion in (A.25).

A.5. Manifold with boundary—reflection contribution

Finally, we prove the last expansion used in the main text:

$$\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}}\Delta_{\mathrm{b}}^{1-p}(x|z)\beta(\tau,x|z)\exp\left(-\frac{1}{\nu\tau}\sigma_{\mathrm{b}}(x|z)\right)$$
$$=\sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\mathcal{Q}-\tau\frac{\nu}{2}\frac{1}{2}(\overset{\leftsquigarrow}{\mathrm{d}}\mathcal{F}_{\tilde{\mathrm{n}}}+\overset{\rightsquigarrow}{\mathrm{d}}\mathcal{F}_{\tilde{\mathrm{n}}})-\tau\frac{\nu}{2}\left(\frac{1+p}{3}k+\beta\text{-terms}\right)+\mathcal{O}\big(\tau^{\frac{3}{2}}\big). \tag{A.45}$$

Similarly to the previous section, we smooth this expression with test functions, perform a change of variables (A.26) and consequently (A.30), and use the covariant expansions (A.33),

$$\widehat{\beta}(\tau,\widehat{x},\xi|\widehat{z},\zeta)=\widehat{\beta}_0(\widehat{x},\xi|\widehat{z},\zeta)+\sqrt{\tau}\widehat{\beta}_{\frac{1}{2}}(\widehat{x},\xi|\widehat{z},\zeta)+\mathcal{O}(\tau),$$
$$\widehat{\beta}_0(\widehat{y},\xi|\widehat{y},\sqrt{\tau}Y,\zeta)=\sum_{k=\mathbb{N}_0}\tau^{\frac{k}{2}}\frac{1}{k!}\widehat{\beta}_{0;0,k\mu_1\ldots\mu_k}(\widehat{y};\xi,\zeta)Y^{\mu_1}\ldots Y^{\mu_k}, \tag{A.46}$$

similarly for $\beta_{\frac{1}{2}}(x|z)$, and

$$\widehat{\sigma}_{\mathrm{b}}(\widehat{y}, \xi|\widehat{y}, \sqrt{\tau}Y, \zeta) = \tau n^2 \frac{1}{2}(\xi+\zeta)^2 + \sum_{k=2,3,\ldots} \tau^{\frac{k}{2}} \frac{1}{k!} \widehat{\sigma}_{\mathrm{b}0,k\mu_1\ldots\mu_k}(\widehat{y}; \xi, \zeta) Y^{\mu_1}\ldots Y^{\mu_k}, \tag{A.47}$$

$$\widehat{l}_{\mathrm{b}}(\widehat{y}, \xi|\widehat{y}, \sqrt{\tau}Y, \zeta) = \sum_{k=\mathbb{N}_0} \tau^{\frac{k}{2}} \frac{1}{k!} \widehat{l}_{\mathrm{b}0,k\mu_1\ldots\mu_k}(\widehat{y}; \xi, \zeta) Y^{\mu_1}\ldots Y^{\mu_k}, \tag{A.48}$$

where

$$\widehat{l}_{\mathrm{b}}(\widehat{x}, \xi|\widehat{z}, \zeta) = \ln\left(\widehat{j}(\widehat{x}, \xi) \frac{\widehat{\Delta}_{\mathrm{b}}^{1-p}(\widehat{x}, \xi|\widehat{z}, \zeta)}{\triangle(\widehat{x}\ |\widehat{z})} \widehat{j}(\widehat{z}, \zeta)\right). \tag{A.49}$$

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

$$\begin{aligned}
&\frac{n}{(2\pi\nu\tau)^{\frac{d}{2}}} \int_{x,z\in\Omega} \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z)\varphi(x)\psi(z)\Delta_{\mathrm{b}}^{1-p}(x|z)\beta(\tau, x|z) \exp\left(-\frac{1}{\nu\tau}\sigma_{\mathrm{b}}(x|z)\right) \\
&\quad = \int_{\widehat{y}\in\partial\Omega} \frac{n}{(2\pi\nu\tau)^{\frac{1}{2}}} \mathfrak{q}^{\frac{1}{2}}(\widehat{y}) \int_{\xi,\zeta\in\mathbb{R}^+} \mathrm{d}\xi\, \mathrm{d}\zeta \exp\left(-\frac{n^2}{2\nu\tau}(\xi+\zeta)^2\right) \widehat{\varphi}(\widehat{y}, \xi)\widehat{\psi}(\widehat{y}, \zeta) \\
&\quad\quad \times \tilde{j}_{\mathrm{b}}\left(\widehat{y}; \xi, \frac{\xi\zeta}{\xi+\zeta}, \zeta\right)\left(\tilde{\beta}_0\left(\widehat{y}; \xi, \frac{\xi\zeta}{\xi+\zeta}, \zeta\right) + \sqrt{\tau}\tilde{\beta}_{\frac{1}{2}}\left(\widehat{y}; \xi, \frac{\xi\zeta}{\xi+\zeta}, \zeta\right) + \mathcal{O}(\tau)\right),
\end{aligned} \tag{A.50}$$

where

$$\begin{aligned}
\tilde{j}_{\mathrm{b}}\left(\widehat{y}; \xi, \frac{\xi\zeta}{\xi+\zeta}, \zeta\right) &= \widehat{j}(\widehat{y}, \xi)\widehat{\Delta}_{\mathrm{b}}^{1-p}(\widehat{y}; \xi|\widehat{y}, \zeta)\widehat{j}(\widehat{y}, \zeta)\mathfrak{q}^{\frac{1}{2}}(\widehat{y})(\mathrm{Det}_{\shortparallel}\widehat{\sigma}_{\mathrm{b}0,2}(\widehat{y}; \xi, \zeta))^{-\frac{1}{2}} \\
&= \left(\widehat{j}(\widehat{y}, \xi)\widehat{\Delta}_{\mathrm{b}}^{1-2p}(\widehat{y}; \xi|\widehat{y}, \zeta)\widehat{j}(\widehat{y}, \zeta)\right)^{\frac{1}{2}},
\end{aligned} \tag{A.51}$$

$$\tilde{\beta}_0\left(\widehat{y}; \xi, \frac{\xi\zeta}{\xi+\zeta}, \zeta\right) = \widehat{\beta}_0(\widehat{y}, \xi|\widehat{y}, \zeta), \tag{A.52}$$

with $\tilde{j}_{\mathrm{b}}$ and $\tilde{\beta}_0$ depending analytically on their three real arguments. $\tilde{\beta}_{\frac{1}{2}}$ is defined in a similar way to $\tilde{\beta}_0$. Here we anticipate that $\widehat{\Delta}_{\mathrm{b}}$ and $\widehat{\beta}$ can have more complicated analytical dependence on ξ and ζ. The equality in (A.51) follows from (B.98). Using the expansion (A.23) we obtain

$$\begin{aligned}
\int_{\widehat{y}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\widehat{y}) \Bigg(&\sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\tilde{\beta}_0(\widehat{y}; 0, 0, 0)\varphi(\widehat{y})\psi(\widehat{y}) \\
&+ \tau\frac{\nu}{4n^2}\tilde{\beta}_0(\widehat{y}; 0, 0, 0)\left(\widehat{\varphi}'(\widehat{y}, 0)\widehat{\psi}(\widehat{y}, 0) + \widehat{\varphi}(\widehat{y}, 0)\widehat{\psi}'(\widehat{y}, 0)\right) \\
&+ \tau\left(\frac{\nu}{4n^2}(\tilde{j}_{\mathrm{b}}\tilde{\beta}_0)^{\mathrm{l}'} + \frac{\nu}{4n^2}(\tilde{j}_{\mathrm{b}}\tilde{\beta}_0)^{\mathrm{r}'} + \frac{\nu}{12n^2}(\tilde{j}_{\mathrm{b}}\tilde{\beta}_0)^{\mathrm{m}'} + \frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\tilde{\beta}_{\frac{1}{2}}\right)(\widehat{y}; 0, 0, 0) \\
&\times \varphi(\widehat{y})\psi(\widehat{y}) + \mathcal{O}\left(\tau^{\frac{3}{2}}\right)\Bigg).
\end{aligned} \tag{A.53}$$

Using the expansion (B.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

$$\int_{\hat{y}\in\partial\Omega} \mathfrak{q}^{\frac{1}{2}}(\hat{y})\Bigg(\sqrt{\tau}\frac{1}{n}\sqrt{\frac{\nu}{2\pi}}\beta(0,\hat{y}|\hat{y})\varphi(\hat{y})\psi(\hat{y})$$
$$+\tau\frac{\nu}{4n^2}\beta(0,\hat{y}|\hat{y})(\hat{\varphi}'(\hat{y},0)\hat{\psi}(\hat{y},0)+\hat{\varphi}(\hat{y},0)\hat{\psi}'(\hat{y},0))$$
$$+\frac{\tau\nu}{2}\Bigg(-\frac{1+6}{3}\beta(0,\hat{y}|\hat{y})k(\hat{y})+\frac{2}{n}\sqrt{\frac{1}{2\pi\nu}}\dot{\beta}(0,\hat{y}|\hat{y})$$
$$+\left(\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{l}\prime}+\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{r}\prime}+\frac{1}{6n^2}\tilde{\beta}_0{}^{\mathtt{m}\prime}\right)(\hat{y};0,0,0)\Bigg)\varphi(\hat{y})\psi(\hat{y})+\mathcal{O}\big(\tau^{\frac{3}{2}}\big)\Bigg). \quad \text{(A.54)}$$

Using the normalization condition (3.14) concludes the proof of the expansion (A.45). By inspection we see that the β-terms have the form

$$\beta\text{-terms} = -\frac{2}{n}\sqrt{\frac{1}{2\pi\nu}}\dot{\beta}(0,\hat{y}|\hat{y}) - \left(\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{l}\prime}+\frac{1}{2n^2}\tilde{\beta}_0{}^{\mathtt{r}\prime}+\frac{1}{6n^2}\tilde{\beta}_0{}^{\mathtt{m}\prime}\right)(\hat{y};0,0,0). \quad \text{(A.55)}$$

Appendix B. Geodesic theory

B.1. Basic definitions

In this appendix, we review some facts from geodesic theory and list a number of useful expansions, 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 [14–16]. The theory of expansion near a boundary is less known. Some material can be found in [17–19]. The calculations are usually straightforward but cumbersome, often treatable only with help of a computer [20]. We will present mostly only results.

We start by introducing the *covariant expansion* in a curved manifold. We would like to expand a sufficiently smooth tensor field $A^{\alpha\ldots}_{\beta\ldots}$ 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 defines a parallel transport. It allows us to transform tensors from the tangent space at point z in a normal neighbourhood of the point x to the space $\mathbf{T}_x M$ along the geodetic joining these two points. In the normal neighbourhood of x, we can parametrize a geodesic by its tangent vector at x, i.e., we can define an *exponential map* $\boldsymbol{u}_x$

$$\boldsymbol{u}_x : \mathbf{T}_x M \to M, \quad \text{(B.1)}$$

$$\frac{\nabla}{\mathrm{d}\tau}\frac{\mathrm{D}}{\mathrm{d}\tau}\boldsymbol{u}_x(\tau X) = 0, \qquad \frac{\mathrm{D}}{\mathrm{d}\tau}\boldsymbol{u}_x(\tau X)|_{\tau=0} = X. \quad \text{(B.2)}$$

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

$$\iota^{\mu}{}_{\nu}(x|z) \in \mathbf{T}_x M \otimes \mathbf{T}^{\star}_z M, \qquad \frac{\nabla}{\mathrm{d}\tau}\iota(x,\boldsymbol{u}_x(\tau X)) = 0, \quad \text{(B.3)}$$

and its version with indices up and down

$$\bar{\iota} = \iota \cdot g^{-1}, \qquad \underline{\iota} = g \cdot \iota. \tag{B.4}$$

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

$$A^{\mu\dots}_{\nu\dots}(x;\,.)\iota^{\alpha}{}_{\mu}(x|x;\,.)\dots\iota^{-1\nu}{}_{\beta}(x|x;\,.)\dots \quad : \mathbf{T}_x M \to \mathbf{T}_{x}{}^{k}_{l} M. \tag{B.5}$$

Finally, we can write the *covariant expansion*

$$A^{\mu\dots}_{\nu\dots}(x;Z)\iota^{\alpha}{}_{\mu}(x|x;Z)\cdots\iota^{-1\nu}{}_{\beta}(x|x;Z)\cdots = \sum_{k\in\mathbb{N}_0}\frac{1}{k!}A_k{}^{\alpha\dots}_{\beta\dots\mu_1\dots\mu_k}(x)Z^{\mu_1}\dots Z^{\mu_k}. \tag{B.6}$$

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 $\mu_1,\dots,\mu_k$.

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 (2.20). For timelike separated points it is negative. The *geodesic distance* is then given by

$$s(x|z) = |2\sigma(x|z)|^{\frac{1}{2}}. \tag{B.7}$$

We define *geodesic tangent vectors* $\vec{\sigma}, \overleftarrow{\sigma}$

$$\vec{\sigma}(x|z) = g^{-1}(x)\cdot \mathrm{d}_{\mathrm{l}}\sigma(x|z), \qquad \overleftarrow{\sigma}(x|z) = \mathrm{d}_{\mathrm{r}}\sigma(x|z)\cdot g^{-1}(z). \tag{B.8}$$

Here, as before, $\mathrm{d}_{\mathrm{l}} f$ or $\mathrm{d}_{\mathrm{r}} f$ 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., [15]) are that its gradient vector $\vec{\sigma}(x|z)$ is really tangent to the geodesic between x and z and it is normalized to the length of the geodesic. That is

$$-Z = \vec{\sigma}(x|x;Z). \tag{B.9}$$

We also introduce a special notation for the second derivatives of the world function

$$\vec{\vec{\sigma}} = \nabla_{\mathrm{l}}\mathrm{d}_{\mathrm{l}}\sigma, \qquad \overleftrightarrow{\sigma} = \mathrm{d}_{\mathrm{l}}\mathrm{d}_{\mathrm{r}}\sigma, \qquad \overleftarrow{\overleftarrow{\sigma}} = \nabla_{\mathrm{r}}\mathrm{d}_{\mathrm{r}}\sigma. \tag{B.10}$$

To conclude our definition, we also introduce determinants of $\iota, \underline{\iota}, \overleftrightarrow{\sigma}$. They are well-defined objects—bi-densities on M

$$\begin{aligned} \mathfrak{i}(x|z) &= \frac{1}{n^2}\,\mathrm{Det}\,\iota(x|z) = \mathfrak{g}^{-\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z),\\ \underline{\mathfrak{i}}(x|z) &= \frac{1}{n^2}\,\mathrm{Det}\,\underline{\iota}(x|z) = \mathfrak{g}^{\frac{1}{2}}(x)\mathfrak{g}^{\frac{1}{2}}(z), \end{aligned} \tag{B.11}$$

$$\mathfrak{s}(x|z) = \frac{1}{n^2}\,\mathrm{Det}\,(-\overleftrightarrow{\sigma}(x|z)). \tag{B.12}$$

Finally, we define the *Van Vleck–Morette determinant*

$$\Delta(x|z) = \mathfrak{s}(x|z)\,\underline{\mathfrak{i}}^{-1}(x|z) = \mathfrak{s}(x|z)\,\mathfrak{g}^{-\frac{1}{2}}(x)\mathfrak{g}^{-\frac{1}{2}}(z). \tag{B.13}$$

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*

$$[F](x) = F(x|x). \tag{B.14}$$

The generalized Synge's theorem (see, e.g., [21]) tells us that

$$\nabla[F] = [\nabla_{\mathrm{l}}F] + [\nabla_{\mathrm{r}}F]. \tag{B.15}$$

Here $\nabla_{\mathrm{l}}F$ and $\nabla_{\mathrm{r}}F$, similarly to $\mathrm{d}_{\mathrm{l}} f$ and $\mathrm{d}_{\mathrm{r}} f$, denote the covariant derivative of a bi-tensor $F(x|z)$ in the left and right arguments, respectively.

B.2. Coincidence limits and covariant expansions

Equation (B.9) gives

$$\sigma = \tfrac{1}{2}\mathrm{d}_{\mathtt{r}}\sigma \cdot g^{-1} \cdot \mathrm{d}_{\mathtt{r}}\sigma = \tfrac{1}{2}\mathrm{d}_{\mathtt{l}}\sigma \cdot g^{-1} \cdot \mathrm{d}_{\mathtt{l}}\sigma = \tfrac{1}{2}\overset{\rightarrow}{\sigma} \cdot g \cdot \overset{\rightarrow}{\sigma} = \tfrac{1}{2}\overset{\leftarrow}{\sigma} \cdot g \cdot \overset{\leftarrow}{\sigma}. \tag{B.16}$$

Taking repeatedly derivatives of this expression in both arguments, we can derive

$$\overset{\rightarrow}{\sigma} \cdot g = \overset{\rightarrow}{\sigma} \cdot \overset{\twoheadrightarrow}{\sigma} = \overset{\leftrightarrow}{\sigma} \cdot \overset{\leftarrow}{\sigma}, \qquad g \cdot \overset{\leftarrow}{\sigma} = \overset{\twoheadleftarrow}{\sigma} \cdot \overset{\leftarrow}{\sigma} = \overset{\rightarrow}{\sigma} \cdot \overset{\leftrightarrow}{\sigma}, \tag{B.17}$$

and following identities

$$\overset{\rightarrow}{\sigma}{}^{\mu}\mathrm{d}_{\mathtt{l}\mu}\sigma = 2\sigma, \tag{B.18}$$

$$\begin{aligned} &\overset{\rightarrow}{\sigma}{}^{\mu}\nabla_{\mathtt{l}\mu}\overset{\rightarrow}{\sigma}{}^{\alpha} = \overset{\rightarrow}{\sigma}{}^{\alpha}, \\ &\overset{\rightarrow}{\sigma}{}^{\mu}\nabla_{\mathtt{l}\mu}\overset{\leftarrow}{\sigma}{}^{\alpha} = \overset{\leftarrow}{\sigma}{}^{\alpha}, \end{aligned} \tag{B.19}$$

$$\begin{aligned} &\overset{\rightarrow}{\sigma}{}^{\mu}\nabla_{\mathtt{l}\mu}\overset{\twoheadrightarrow}{\sigma}_{\alpha\beta} = \overset{\twoheadrightarrow}{\sigma}_{\alpha\beta} - \overset{\twoheadrightarrow}{\sigma}_{\alpha\mu}\overset{\twoheadrightarrow}{\sigma}_{\beta\nu}g^{-1\mu\nu} - \mathrm{R}_{\alpha\mu\beta\nu}\overset{\rightarrow}{\sigma}{}^{\mu}\overset{\rightarrow}{\sigma}{}^{\nu}, \\ &\overset{\rightarrow}{\sigma}{}^{\mu}\nabla_{\mathtt{l}\mu}\overset{\leftrightarrow}{\sigma}_{\alpha\beta} = \overset{\leftrightarrow}{\sigma}_{\alpha\beta} - \overset{\twoheadrightarrow}{\sigma}_{\alpha\mu}g^{-1\mu\nu}\overset{\leftrightarrow}{\sigma}_{\nu\beta}, \\ &\overset{\rightarrow}{\sigma}{}^{\mu}\nabla_{\mathtt{l}\mu}\overset{\twoheadleftarrow}{\sigma}_{\alpha\beta} = \overset{\twoheadleftarrow}{\sigma}_{\alpha\beta} - g^{-1\mu\nu}\overset{\leftrightarrow}{\sigma}_{\mu\alpha}\overset{\leftrightarrow}{\sigma}_{\nu\beta}, \\ &\overset{\rightarrow}{\sigma}{}^{\mu}\nabla_{\mathtt{l}\alpha}\nabla_{\mathtt{l}\beta}\nabla_{\mathtt{l}\mu}\sigma = \overset{\twoheadrightarrow}{\sigma}_{\alpha\beta} - \overset{\twoheadrightarrow}{\sigma}_{\alpha\mu}\overset{\twoheadrightarrow}{\sigma}_{\beta\nu}g^{-1\mu\nu}. \end{aligned} \tag{B.20}$$

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 the coincidence limits of relations above and similar relations for higher derivatives and using Synge's theorem, we get

$$[\sigma] = 0, \tag{B.21}$$

$$[\mathrm{d}_{\mathtt{l}}\sigma] = [\mathrm{d}_{\mathtt{r}}\sigma] = 0, \tag{B.22}$$

$$[\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\sigma] = -[\nabla_{\mathtt{l}}\nabla_{\mathtt{r}}\sigma] = [\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\sigma] = g, \tag{B.23}$$

$$[\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\sigma] = [\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\nabla_{\mathtt{r}}\sigma] = [\nabla_{\mathtt{l}}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\sigma] = [\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\sigma] = 0, \tag{B.24}$$

$$\begin{aligned} [\nabla_{\mathtt{l}\alpha}\nabla_{\mathtt{l}\beta}\nabla_{\mathtt{l}\mu}\nabla_{\mathtt{l}\nu}\sigma] &= -[\nabla_{\mathtt{l}\beta}\nabla_{\mathtt{l}\mu}\nabla_{\mathtt{l}\nu}\nabla_{\mathtt{r}\alpha}\sigma] \\ &= [\nabla_{\mathtt{l}\mu}\nabla_{\mathtt{l}\nu}\nabla_{\mathtt{r}\beta}\nabla_{\mathtt{r}\alpha}\sigma] = -[\nabla_{\mathtt{l}\nu}\nabla_{\mathtt{r}\mu}\nabla_{\mathtt{r}\beta}\nabla_{\mathtt{r}\alpha}\sigma] \\ &= [\nabla_{\mathtt{r}\nu}\nabla_{\mathtt{r}\mu}\nabla_{\mathtt{r}\beta}\nabla_{\mathtt{r}\alpha}\sigma] = -\tfrac{1}{3}(\mathrm{R}_{\alpha\mu\beta\nu} + \mathrm{R}_{\alpha\nu\beta\mu}). \end{aligned} \tag{B.25}$$

A similar relation for the fifth and sixth derivatives can be found in [20, 21].

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 the tensor nature of f and we do not have to worry about parallel transport of tensor indices. Equation (B.6) can be rewritten using (B.9) as

$$f(z) = \sum_{k\in\mathbb{N}_0} \frac{(-1)^k}{k!} f_{k\mu_1\ldots\mu_k}(x)\overset{\rightarrow}{\sigma}{}^{\mu_1}(x,z)\ldots\overset{\rightarrow}{\sigma}{}^{\mu_k}(x,z). \tag{B.26}$$

Taking derivatives of this equation and coincidence limits, we can find that the coefficients are given by

$$f_{k\mu_1\ldots\mu_k} = \nabla_{(\mu_1}\ldots\nabla_{\mu_k)}f. \tag{B.27}$$

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

$$\overset{\rightarrow}{\sigma} = -\iota \cdot \overset{\leftarrow}{\sigma} \tag{B.28}$$

by taking derivatives and coincidence limits. We give only a list of some of them (see [16, 21] or [20]).

$$[\underline{\iota}] = g, \tag{B.29}$$

$$[\nabla_{\mathtt{l}}\underline{\iota}] = [\nabla_{\mathtt{r}}\underline{\iota}] = 0, \tag{B.30}$$

$$-[\nabla_{\mathtt{l}\beta}\nabla_{\mathtt{l}\alpha}\underline{\iota}_{\mu\nu}] = [\nabla_{\mathtt{l}\alpha}\nabla_{\mathtt{r}\beta}\underline{\iota}_{\mu\nu}] = -[\nabla_{\mathtt{r}\alpha}\nabla_{\mathtt{r}\beta}\underline{\iota}_{\mu\nu}] = \tfrac{1}{2}\mathrm{R}_{\alpha\beta\mu\nu}, \tag{B.31}$$

$$[\nabla_{\mathtt{l}\gamma}\nabla_{\mathtt{l}\beta}\nabla_{\mathtt{l}\alpha}\underline{\iota}_{\mu\nu}] = -\tfrac{1}{3}\nabla_{\gamma}\mathrm{R}_{\alpha\beta\mu\nu} - \tfrac{1}{3}\nabla_{\beta}\mathrm{R}_{\alpha\gamma\mu\nu}, \tag{B.32}$$

$$\begin{aligned}
[\nabla_{\mathtt{l}\delta}\nabla_{\mathtt{l}\gamma}\nabla_{\mathtt{l}\beta}\nabla_{\mathtt{l}\alpha}\underline{\iota}_{\mu\nu}] = {} & -\tfrac{1}{4}\nabla_{\delta}\nabla_{\gamma}\mathrm{R}_{\mu\nu\alpha\beta} - \tfrac{1}{4}\nabla_{\delta}\nabla_{\beta}\mathrm{R}_{\mu\nu\alpha\gamma} - \tfrac{1}{4}\nabla_{\gamma}\nabla_{\beta}\mathrm{R}_{\mu\nu\alpha\delta} \\
& + \tfrac{1}{8}\mathrm{R}_{\mu\nu\delta\lambda}\mathrm{R}_{\kappa\alpha\beta\gamma}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\mu\nu\gamma\lambda}\mathrm{R}_{\kappa\alpha\beta\delta}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\mu\nu\beta\lambda}\mathrm{R}_{\kappa\alpha\gamma\delta}g^{-1\kappa\lambda} \\
& + \tfrac{1}{24}\mathrm{R}_{\mu\nu\delta\lambda}\mathrm{R}_{\kappa\beta\alpha\gamma}g^{-1\kappa\lambda} + \tfrac{1}{24}\mathrm{R}_{\mu\nu\gamma\lambda}\mathrm{R}_{\kappa\beta\alpha\delta}g^{-1\kappa\lambda} + \tfrac{1}{24}\mathrm{R}_{\mu\nu\delta\lambda}\mathrm{R}_{\kappa\gamma\alpha\beta}g^{-1\kappa\lambda} \\
& + \tfrac{1}{8}\mathrm{R}_{\nu\lambda\gamma\delta}\mathrm{R}_{\kappa\mu\alpha\beta}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\nu\lambda\beta\delta}\mathrm{R}_{\kappa\mu\alpha\gamma}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\nu\lambda\beta\gamma}\mathrm{R}_{\kappa\mu\alpha\delta}g^{-1\kappa\lambda} \\
& + \tfrac{1}{8}\mathrm{R}_{\nu\lambda\alpha\delta}\mathrm{R}_{\kappa\mu\beta\gamma}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\nu\lambda\alpha\gamma}\mathrm{R}_{\kappa\mu\beta\delta}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\nu\lambda\alpha\beta}\mathrm{R}_{\kappa\mu\gamma\delta}g^{-1\kappa\lambda} \\
& + \tfrac{1}{24}\mathrm{R}_{\mu\nu\kappa\gamma}\mathrm{R}_{\alpha\beta\delta\lambda}g^{-1\kappa\lambda} + \tfrac{1}{24}\mathrm{R}_{\mu\nu\kappa\beta}\mathrm{R}_{\alpha\gamma\delta\lambda}g^{-1\kappa\lambda} + \tfrac{1}{24}\mathrm{R}_{\mu\nu\kappa\beta}\mathrm{R}_{\alpha\delta\gamma\lambda}g^{-1\kappa\lambda} \\
& + \tfrac{1}{24}\mathrm{R}_{\mu\nu\kappa\alpha}\mathrm{R}_{\beta\gamma\delta\lambda}g^{-1\kappa\lambda} + \tfrac{1}{24}\mathrm{R}_{\mu\nu\kappa\alpha}\mathrm{R}_{\beta\delta\gamma\lambda}g^{-1\kappa\lambda} + \tfrac{1}{8}\mathrm{R}_{\nu\mu\kappa\alpha}\mathrm{R}_{\beta\lambda\gamma\delta}g^{-1\kappa\lambda}.
\end{aligned} \tag{B.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 (B.6)

$$A^{\mu\dots}_{\nu\dots}(z)\iota^{\alpha}_{\mu}(x|z)\dots\iota^{-1\nu}{}_{\beta}(x|z)\dots = \sum_{k\in\mathbb{N}_0}\frac{(-1)^k}{k!}A_k{}^{\alpha\dots}_{\beta\dots\mu_1\dots\mu_k}(x)\vec{\sigma}^{\mu_1}(x|z)\dots\vec{\sigma}^{\mu_k}(x|z). \tag{B.34}$$

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 the coefficients of such an expansion $A_{k,l}(y)$. That is

$$\iota^{\star}(y|y;X)\iota^{\star}(y|y;Z)A(y;X|y;Z) = \sum_{k,l\in\mathbb{N}} A_{k,l\mu_1\dots\mu_k\nu_1\dots\nu_l}(y)X^{\mu_1}\dots X^{\mu_k}Z^{\nu_1}\dots Z^{\nu_k}, \tag{B.35}$$

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 (B.27) we can derive that

$$f_{k,l\mu_1\dots\mu_k\nu_1\dots\nu_l} = \big[\nabla_{(\mathtt{l}\mu_1}\dots\nabla_{\mathtt{l}\mu_k)}\nabla_{(\mathtt{r}\nu_1}\dots\nabla_{\mathtt{r}\nu_l)}f\big]. \tag{B.36}$$

For calculations in appendix A, 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

$$\sigma(y;X|y;Z) = \tfrac{1}{2}(X-Z)^{\mu}g_{\mu\nu}(y)(X-Z)^{\nu} - \tfrac{1}{6}X^{\mu}X^{\nu}Z^{\kappa}Z^{\lambda}\mathrm{R}_{\mu\kappa\nu\lambda}(y) + \cdots. \tag{B.37}$$

Clearly, the expansion of the world function at one of its arguments is given by equation (B.16).

Similarly, it is possible to derive (see [20, 21]) that the coincidence limits of derivatives of the Van Vleck–Morette determinant are

$$[\Delta] = 1, \tag{B.38}$$

$$[\mathrm{d}_{\mathtt{l}}\Delta] = [\mathrm{d}_{\mathtt{r}}\Delta] = 0, \tag{B.39}$$

$$[\nabla_{\mathtt{l}\mu}\nabla_{\mathtt{l}\nu}\Delta] = -[\nabla_{\mathtt{l}\mu}\nabla_{\mathtt{r}\nu}\Delta] = [\nabla_{\mathtt{r}\mu}\nabla_{\mathtt{r}\nu}\Delta] = \tfrac{1}{3}\,\mathrm{Ric}_{\mu\nu}, \tag{B.40}$$

and the covariant expansion

$$\Delta(y;\,X|y;\,Z) = 1 + \tfrac{1}{6}(X - Z)\cdot\mathrm{Ric}\cdot(X - Z) + \cdots. \tag{B.41}$$

Finally, let us note that the Jacobian associated with a map

$$\boldsymbol{u}_x^{-1} : z \to Z = -\overrightarrow{\sigma}(x|z) \tag{B.42}$$

is given by

$$\left|\mathrm{Det}\,\mathrm{D}\boldsymbol{u}_x^{-1}(z)\right| = |\mathrm{Det}(g^{-1}(x)\cdot\overleftrightarrow{\sigma}(x|z))| = \mathfrak{g}^{-1}(x)\mathfrak{s}(x|z) = \mathfrak{i}(x|z)\Delta(x|z). \tag{B.43}$$

B.3. $(d-1)+1$ *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 neighbourhood of the boundary with topology $\mathbb{R}\times\Sigma$ where Σ is part of the boundary manifold. In such a neighbourhood, we can perform a $(d-1)+1$ splitting which is discussed, for example, in [22]. 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 the notation of the 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 the domain Ω. We denote Σ_t hypersurfaces defined by conditions $t = \mathrm{const}$. We denote n and $\vec{\mathrm{n}}$ 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. That is

$$g = n^2\mathrm{nn} + q, \qquad g^{-1} = n^{-2}\vec{\mathrm{n}}\vec{\mathrm{n}} + q^{-1}, \qquad \delta = \vec{\mathrm{n}}\mathrm{n} + \mathfrak{d}, \tag{B.44}$$

where q^{-1} is the inverse of q in the tangent space of the hypersurfaces. The phase factor n governs the signature of the metric g and the character of the hypersurfaces. We will use shorthand

$$A^{\dots\shortparallel\alpha\dots\perp\dots}_{\dots\perp\dots} = A^{\dots\beta\dots\mu\dots}_{\dots\nu\dots}\mathfrak{d}^{\alpha}_{\beta}\vec{\mathrm{n}}^{\nu}\mathrm{n}_{\mu}. \tag{B.45}$$

We also use

$$\overset{\twoheadrightarrow}{\sigma}_{\shortparallel} \overset{\mathrm{def}}{=} \overset{\twoheadrightarrow}{\sigma}_{\shortparallel\shortparallel}, \qquad \overleftrightarrow{\sigma}_{\shortparallel} \overset{\mathrm{def}}{=} \overleftrightarrow{\sigma}_{\shortparallel\shortparallel}, \qquad \overset{\twoheadleftarrow}{\sigma}_{\shortparallel} \overset{\mathrm{def}}{=} \overset{\twoheadleftarrow}{\sigma}_{\shortparallel\shortparallel}. \tag{B.46}$$

Decomposition of the time flow vector $\vec{t}$ defines *lapse N* and *shift* $\vec{N}$

$$\vec{t} = N\vec{\mathrm{n}} + \vec{N}, \qquad \mathrm{d}t = N\mathrm{n}. \tag{B.47}$$

We denote D the *hypersurface gradient*—an orthogonal projection of a spacetime gradient to the hypersurfaces Σ_t

$$\mathrm{D}f = \mathfrak{d}\cdot\mathrm{d}f, \tag{B.48}$$

and $\triangledown$ the *hypersurface covariant derivative* of the metric q. It is related to the spacetime connection as

$$\triangledown A = \mathfrak{d}^{\star}\nabla A \qquad \text{for A such that} \quad A = \mathfrak{d}^{\star}A. \tag{B.49}$$

where by $\mathfrak{d}^{\star}A$, we mean orthogonal 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 the covariant derivative of the normal form

$$\mathrm{K} = \mathfrak{d} \cdot \nabla \mathrm{n}, \tag{B.50}$$

and we use shorthand

$$k = \mathrm{K}_{\mu\nu} g^{-1\mu\nu}, \qquad \mathrm{K}^2 = \mathrm{K}_{\kappa\mu}\mathrm{K}_{\lambda\nu} g^{-1\kappa\lambda} g^{-1\mu\nu}. \tag{B.51}$$

We define the *time derivative* of a tensor field A tangent to the hypersurfaces:

$$A' = \mathfrak{d}^{\star}\mathcal{L}_{\vec{t}} A \qquad \text{for A such that} \quad A = \mathfrak{d}^{\star} A. \tag{B.52}$$

Now we list a number of useful relations between spacetime quantities and 'spatial' quantities, derivations of which are straightforward and for the case $n^2 = -1$ can be mostly found, for example, in [22].

$$\begin{aligned} &\vec{\mathrm{n}} \cdot \nabla \mathrm{n} = -\mathrm{D} \ln N, \\ &\nabla \cdot \vec{\mathrm{n}} = n^2 k, \end{aligned} \tag{B.53}$$

$$\begin{aligned} &\vec{\mathrm{n}} \cdot \nabla q = n^2(\mathrm{n}(\mathrm{D}\ln N) + (\mathrm{D}\ln N)\mathrm{n}), \\ &\mathfrak{d}^{\mu}_{\gamma} \nabla_{\mu} q_{\alpha\beta} = -\mathrm{n}_{\alpha}\mathrm{K}_{\beta\gamma} - \mathrm{n}_{\beta}\mathrm{K}_{\alpha\gamma}, \end{aligned} \tag{B.54}$$

$$\begin{aligned} &\nabla \cdot \mathfrak{d} = -n^2 \mathrm{n} k + \mathrm{D} \ln N, \\ &\mathfrak{d} \cdot (\nabla \mathfrak{d}) \cdot \mathfrak{d} = -\mathrm{K}\vec{\mathrm{n}} \end{aligned} \tag{B.55}$$

$$\begin{aligned} &q' = 2n^2 N\mathrm{K} + \mathcal{L}_{\vec{N}} q, \\ &\mathrm{K}' = N(\vec{\mathrm{n}} \cdot \nabla \mathrm{K})_{\parallel\parallel} + 2n^2 N\mathrm{K} \cdot q^{-1} \cdot \mathrm{K} + \mathcal{L}_{\vec{N}}\mathrm{K}, \\ &k' = N\vec{\mathrm{n}} \cdot \mathrm{d}k + \vec{N}k. \end{aligned} \tag{B.56}$$

The curvature tensors of the spacetime metric g and of the space metric q are related by

$$\begin{aligned} \mathrm{R}_{\parallel\alpha\parallel\beta\parallel\gamma\parallel\delta} &= \mathrm{R}_{\alpha\beta\gamma\delta} + n^2(\mathrm{K}_{\alpha\delta}\mathrm{K}_{\beta\gamma} - \mathrm{K}_{\alpha\gamma}\mathrm{K}_{\beta\delta}), \\ \mathrm{R}_{\parallel\alpha\parallel\beta\gamma\perp} &= n^2(\triangledown_{\alpha}\mathrm{K}_{\beta\gamma} - \triangledown_{\beta}\mathrm{K}_{\alpha\gamma}), \\ \mathrm{R}_{\parallel\perp\parallel\perp} &= n^4(\mathrm{K}k - \mathrm{K} \cdot q^{-1} \cdot \mathrm{K}) - n^2(\triangledown\triangledown \ln N + (\mathrm{D}\ln N)(\mathrm{D}\ln N) + (\nabla \cdot (\vec{\mathrm{n}}\mathrm{K}))_{\parallel\parallel}) \\ &= n^4 \mathrm{K} \cdot q^{-1} \cdot \mathrm{K} - n^2 \left(\triangledown\triangledown \ln N + (\mathrm{D}\ln N)(\mathrm{D}\ln N) + \frac{1}{N}\mathrm{K}' - \frac{1}{N}\mathcal{L}_{\vec{N}}\mathrm{K} \right), \end{aligned} \tag{B.57}$$

$$\begin{aligned} \mathrm{Ric}_{\parallel\parallel} &= \mathrm{RIC} - \triangledown\triangledown \ln N - (\mathrm{D}\ln N)(\mathrm{D}\ln N) - (\nabla \cdot (\vec{\mathrm{n}}\mathrm{K}))_{\parallel\parallel}, \\ \mathrm{Ric}_{\parallel\perp} &= n^2(\triangledown \cdot q^{-1} \cdot \mathrm{K} - \mathrm{D}k), \\ \mathrm{Ric}_{\perp\perp} &= n^4(k^2 - \mathrm{K}^2) - n^2 \nabla \cdot (\vec{\mathrm{n}}k + q^{-1} \cdot (\mathrm{D}\ln N)) \\ &= -n^4\mathrm{K}^2 - n^2(\triangledown^2 \ln N + (\mathrm{D}\ln N) \cdot q^{-1} \cdot (\mathrm{D}\ln N) + \vec{\mathrm{n}} \cdot \mathrm{d}k) \end{aligned} \tag{B.58}$$

$$\begin{aligned} R &= \mathcal{R} + n^2(k^2 - \mathrm{K}^2) - 2\nabla \cdot (\vec{\mathrm{n}}k + q^{-1} \cdot (\mathrm{D}\ln N)) \\ &= \mathcal{R} - n^2(k^2 + \mathrm{K}^2) - 2(\vec{\mathrm{n}} \cdot \mathrm{d}k + \triangledown^2 \ln N + (\mathrm{D}\ln N) \cdot q^{-1} \cdot (\mathrm{D}\ln N)). \end{aligned} \tag{B.59}$$

B.4. 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 j, the world function, its derivatives and its determinant ρ, $\overset{\rightarrow}{\rho}$, $\overset{\leftarrow}{\rho}$, $\overset{\rightarrow\!\!\!\!\rightarrow}{\rho}$,

$\overset{\leftrightarrow}{\rho}$, $\overset{\leftarrow\!\leftarrow}{\rho}$ and $\mathfrak{r}$ and Van Vleck–Morette determinant $\triangle$. Finally, we denote $\{.\}$ the coincidence limit on the boundary.

In the neighbourhood 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 $\widehat{\boldsymbol{w}}$

$$\begin{aligned}&\widehat{\boldsymbol{w}} : \Sigma \times \mathbb{R} \to M,\\ &\widehat{\boldsymbol{w}}(x,\eta) \quad \text{is geodesic}, \qquad \widehat{\boldsymbol{w}}(x,0) = x, \qquad \widehat{\boldsymbol{w}}'(x,0) = \vec{\mathrm{n}}.\end{aligned} \tag{B.60}$$

It maps point x on the boundary 'orthogonally' to the domain Ω by the distance η. We denote as Σ_η the hypersurface which we obtain by shifting $\Sigma = \Sigma_0$ by the distance η. We also use the notation

$$\begin{aligned}&\widehat{\boldsymbol{w}}_\eta : \Sigma \to \Sigma_\eta, \qquad &&\widehat{\boldsymbol{w}}_\eta(x) = \widehat{\boldsymbol{w}}(x,\eta),\\ &\widehat{\boldsymbol{w}}_{\xi,\zeta} : \Sigma_\xi \to \Sigma_\zeta, \qquad &&\widehat{\boldsymbol{w}}_{\xi,\zeta} = \widehat{\boldsymbol{w}}_\xi\big(\widehat{\boldsymbol{w}}_\zeta^{-1}\big).\end{aligned} \tag{B.61}$$

This foliation is a 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 the 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 obtained by transformation of tensor indices of $A(\hat{x},\xi)$ to the boundary tangent bundle using $\widehat{\boldsymbol{w}}^\star_{-\xi}$

$$A(\hat{x},\xi) = A(\widehat{\boldsymbol{w}}(\hat{x},\xi)), \qquad \widehat{A}(\hat{x},\xi) = \widehat{\boldsymbol{w}}^\star_{-\xi}\, A(\widehat{\boldsymbol{w}}_\xi\ (\hat{x})), \tag{B.62}$$

where $\widehat{\boldsymbol{w}}^\star_\xi$ is the induced transformation on tangent bundles. For a bi-tensor $A(x|z)$ by the *boundary coincidence limit* we mean

$$\{A\}(\hat{y};\xi,\zeta) = A(\hat{y},\xi|\hat{y},\zeta). \tag{B.63}$$

Specially, we have a metric $\hat{q}(\hat{y},\eta)$ (generally different from $q(\hat{y})$) on the boundary manifold, volume element $\hat{\mathfrak{q}}^{\frac{1}{2}}(\hat{y},\eta)$ and associated connection $\widehat{\nabla}$. It is related to the connection ∇ by

$$\widehat{\nabla} = \nabla \oplus \hat{\gamma}. \tag{B.64}$$

The relation of corresponding curvature tensors is (see, e.g., [22])

$$\begin{aligned}\widehat{\mathrm{R}}_{\gamma\alpha}{}^{\delta}{}_{\beta} &= \mathrm{R}_{\gamma\alpha}{}^{\delta}{}_{\beta} + \widehat{\nabla}_\gamma \hat{\gamma}^\delta_{\alpha\beta} - \widehat{\nabla}_\alpha \hat{\gamma}^\delta_{\gamma\beta} + \hat{\gamma}^\delta_{\alpha\mu}\hat{\gamma}^{\ \mu}_{\gamma\beta} - \hat{\gamma}^{\ \delta}_{\gamma\mu}\hat{\gamma}^{\ \mu}_{\alpha\beta},\\ \widehat{\mathrm{RIC}}_{\alpha\beta} &= \mathrm{RIC}_{\alpha\beta} + \widehat{\nabla}_\mu \hat{\gamma}^\mu_{\alpha\beta} - \widehat{\nabla}_\alpha \hat{\gamma}^\mu_{\beta\mu} + \hat{\gamma}^\nu_{\alpha\mu}\hat{\gamma}^\mu_{\beta\nu} - \hat{\gamma}^{\ \nu}_{\mu\nu}\hat{\gamma}^{\ \mu}_{\alpha\beta}.\end{aligned} \tag{B.65}$$

From the definition of the map $\widehat{\boldsymbol{w}}$, we have

$$\{\overset{\rightarrow}{\sigma}\}(\hat{y};\xi,\zeta) = (\xi - \zeta)\vec{\mathrm{n}}(\hat{y},\xi), \tag{B.66}$$

$$\{\mathrm{D}_1\sigma\} = 0. \tag{B.67}$$

Differentiating this equation, we obtain the differential map $\mathrm{D}\widehat{\boldsymbol{w}}$

$$\begin{aligned}&\mathrm{D}\widehat{\boldsymbol{w}}_{\xi,\zeta}(x) : \mathbf{T}_x\Sigma_\xi \to \mathbf{T}_z\Sigma_\zeta, \qquad z = \widehat{\boldsymbol{w}}_{\xi,\zeta}(x),\\ &\mathrm{D}^\nu_\mu\, \widehat{\boldsymbol{w}}_{\xi,\zeta}(x) = -(\nabla_{1\mu}\nabla_{1\kappa}\sigma)(x|z)\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1\kappa\nu}(x|z).\end{aligned} \tag{B.68}$$

In the special case $\xi = 0$, we get

$$\mathrm{D}^\nu_\mu\, \widehat{\boldsymbol{w}}_\eta(\hat{y}) = -(\eta n^2 \mathrm{K}_{\mu\kappa}(\hat{y}) + \overset{\rightarrow\!\rightarrow}{\sigma}_{\shortparallel\mu\kappa}(\hat{y}|\hat{y},\eta))\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1\kappa\nu}(\hat{y}|\hat{y},\eta). \tag{B.69}$$

Here $\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1}$ is the inverse of $\overset{\leftrightarrow}{\sigma}_{\shortparallel}$ in spaces tangent to hypersurfaces Σ_η. Because $\mathrm{D}\widehat{\boldsymbol{w}}_{\xi,\zeta} = \mathrm{D}\widehat{\boldsymbol{w}}^{-1}_{\zeta,\xi}$ we have

$$\{\overset{\leftrightarrow}{\sigma}_{\shortparallel\mu\nu}\} = \{(\nabla_{1\mu}\nabla_{1\kappa}\sigma)(\nabla_{\mathrm{r}\nu}\nabla_{\mathrm{r}\lambda}\sigma)\overset{\leftrightarrow}{\sigma}{}_{\shortparallel}^{-1\kappa\lambda}\}. \tag{B.70}$$

Using this relation, the definition of the Van Vleck–Morette determinant and

$$\vec{\mathrm{n}}(x)\cdot\overset{\leftrightarrow}{\sigma}(x|z) = -\vec{\mathrm{n}}(z)\cdot g(z) \qquad \text{for} \quad z = \widehat{\boldsymbol{w}}_{\xi,\zeta}(x), \tag{B.71}$$

we get an expression for the Jacobian associated with the map $\widehat{\boldsymbol{w}}_{\xi,\zeta}$,

$$\begin{aligned}\widehat{j}(\widehat{y};\xi,\zeta) &= |\mathrm{Det}_{\shortparallel}\mathrm{D}\,\widehat{\boldsymbol{w}}_{\xi,\zeta}|(\widehat{y},\xi)\\ &= \{\Delta^{-1}\mathfrak{q}^{-1}(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\sigma)\}(\widehat{y};\xi,\zeta) = \{\Delta\mathfrak{q}(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\sigma)^{-1}\}(\widehat{y};\xi,\zeta).\end{aligned} \tag{B.72}$$

As special cases we have

$$\widehat{j}(\widehat{y},\eta) = \widehat{j}(\widehat{y};0,\eta), \qquad \widehat{j}(\widehat{y};\xi,\zeta) = \widehat{j}^{-1}(\widehat{y},\xi)\widehat{j}(\widehat{y},\zeta). \tag{B.73}$$

This also gives the expression for the Van Vleck–Morette determinant,

$$\Delta(\widehat{y},\xi|\widehat{y},\zeta) = \mathfrak{q}^{-\frac{1}{2}}(\widehat{y},\xi)\mathfrak{q}^{-\frac{1}{2}}(\widehat{y},\zeta)((\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\sigma)(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\sigma))^{\frac{1}{2}}(\widehat{y},\xi|\widehat{y},\zeta). \tag{B.74}$$

Finally we can prove that

$$\begin{aligned}\widehat{j}(\widehat{y},\xi)\widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\widehat{j}(\widehat{y},\zeta) &= \mathfrak{q}^{-1}(\widehat{y})(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{l}}\nabla_{\mathtt{l}}\widehat{\sigma})(\widehat{y},\xi|\widehat{y},\zeta)\\ &= \mathfrak{q}^{-1}(\widehat{y})(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\widehat{\sigma})(\widehat{y},\xi|\widehat{y},\zeta).\end{aligned} \tag{B.75}$$

Thanks to (B.67), (B.72) and (B.73), the function $\tilde{j}$ defined in (A.35) is

$$\begin{aligned}\tilde{j}(\widehat{y};\xi,\zeta) &= \widehat{j}(\widehat{y},\xi)\widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\widehat{j}(\widehat{y},\zeta)\mathfrak{q}^{\frac{1}{2}}(\widehat{y})(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\widehat{\sigma})^{-\frac{1}{2}}(\widehat{y},\xi|\widehat{y},\zeta)\\ &= \widehat{j}(\widehat{y},\xi)\widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\widehat{\mathfrak{q}}^{\frac{1}{2}}(\widehat{y},\zeta)(\mathrm{Det}_{\shortparallel}\widehat{\nabla}_{\mathtt{r}}\widehat{\nabla}_{\mathtt{r}}\widehat{\sigma})^{-\frac{1}{2}}(\widehat{y},\xi|\widehat{y},\zeta)\\ &= j(x)\Delta(x|z)\mathfrak{q}^{\frac{1}{2}}(z)(\mathrm{Det}_{\shortparallel}\nabla_{\mathtt{r}}\nabla_{\mathtt{r}}\sigma)^{-\frac{1}{2}}(x|z) = j(x)\Delta^{\frac{1}{2}}(x|z)\widehat{j}(\widehat{y};\xi,\zeta)^{\frac{1}{2}}\\ &= (\widehat{j}(\widehat{y},\xi)\widehat{\Delta}(\widehat{y},\xi|\widehat{y},\zeta)\widehat{j}(\widehat{y},\zeta))^{\frac{1}{2}}.\end{aligned} \tag{B.76}$$

Equation (B.75) is a straightforward consequence.

B.5. Reflection on the boundary

In section 3, we have worked with the *geodesic reflected on the boundary*. We recall its definition here and list some useful properties which allow us to prove the relation (A.51).

We will study the geodesic $\bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)$ between points x and z which is reflected on the boundary at a point $b(x|z)$—an extreme trajectory of the functional given by half of the 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

$$f_{\mathrm{l}}(x|z) = f(x|b(x|z)), \qquad f_{\mathrm{r}}(x|z) = f(b(x|z)|z). \tag{B.77}$$

If we denote the parameter at which the geodesic reflects on the boundary $\lambda_{\mathrm{r}}(x|z)$ and its complement $\lambda_{\mathrm{l}}(x|z)$

$$b(x|z) = \bar{\boldsymbol{x}}_{\mathrm{b}}(x|z)|_{\lambda_{\mathrm{r}}(x|z)} \in \partial\Omega, \qquad 1 = \lambda_{\mathrm{l}}(x|z) + \lambda_{\mathrm{r}}(x|z). \tag{B.78}$$

We can write the reflected geodesic as the joining of two geodesics

$$[\tau,\bar{\boldsymbol{x}}_{\mathrm{b}}] = [\lambda_{\mathrm{l}}\tau,\bar{\boldsymbol{x}}_{\mathrm{l}}]\odot[\lambda_{\mathrm{r}}\tau,\bar{\boldsymbol{x}}_{\mathrm{r}}]. \tag{B.79}$$

The extremum conditions on the position of the reflection point and reflection parameter are

$$\frac{(\mathrm{D}\sigma)_{\mathrm{l}}}{\lambda_{\mathrm{l}}} + \frac{(\mathrm{D}\sigma)_{\mathrm{r}}}{\lambda_{\mathrm{r}}} = 0, \qquad \frac{\sigma_{\mathrm{l}}}{\lambda_{\mathrm{l}}^2} = \frac{\sigma_{\mathrm{r}}}{\lambda_{\mathrm{r}}^2}, \tag{B.80}$$

where D acts in the argument on the boundary.

We define the *reflection world function* σ_b as

$$\sigma_b = \frac{\sigma_l}{\lambda_l} + \frac{\sigma_r}{\lambda_r} = \frac{\sigma_l}{\lambda_l^2} = \frac{\sigma_r}{\lambda_r^2}. \tag{B.81}$$

Clearly

$$\begin{aligned} \lambda_l &= \sqrt{\frac{\sigma_l}{\sigma_b}}, & \lambda_r &= \sqrt{\frac{\sigma_r}{\sigma_b}}, \\ \sqrt{\sigma_b} &= \sqrt{\sigma_l} + \sqrt{\sigma_r}, & 0 &= (\mathrm{D}\sqrt{\sigma})_l + (\mathrm{D}\sqrt{\sigma})_r, \end{aligned} \tag{B.82}$$

Using the last equation, we obtain

$$\mathrm{d}_l\sqrt{\sigma_b} = (\mathrm{d}_l\sqrt{\sigma})_l, \qquad \mathrm{d}_r\sqrt{\sigma_b} = (\mathrm{d}_r\sqrt{\sigma})_r. \tag{B.83}$$

Similarly to the case without boundary we define

$$s_b = |\sqrt{2\sigma_b}| = s_l + s_r \tag{B.84}$$

$$\overrightarrow{\sigma}_b = g^{-1}\cdot \mathrm{d}_l\sigma_b = \frac{\overrightarrow{\sigma}_l}{\lambda_l}, \qquad \overleftarrow{\sigma}_b = \mathrm{d}_r\sigma_b\cdot g^{-1} = \frac{\overleftarrow{\sigma}_r}{\lambda_r}, \tag{B.85}$$

$$\overrightarrow{\overrightarrow{\sigma}}_b = \nabla_l\nabla_l\sigma_b, \qquad \overleftrightarrow{\sigma}_b = \mathrm{d}_l\mathrm{d}_r\sigma_b, \qquad \overleftarrow{\overleftarrow{\sigma}}_b = \nabla_r\nabla_r\sigma_b. \tag{B.86}$$

Additionally, we define

$$s_\perp = -\frac{1}{\lambda_l}\vec{\mathrm{n}}(b)\cdot(\mathrm{d}_r\sigma)_l = -\frac{1}{\lambda_r}\vec{\mathrm{n}}(b)\cdot(\mathrm{d}_l\sigma)_r = \vec{\mathrm{n}}\cdot(\mathrm{d}_l\sigma_b) = \vec{\mathrm{n}}\cdot(\mathrm{d}_r\sigma_b), \tag{B.87}$$

and we denote differentials of maps $x\to b(x|z)$ and $z\to b(x|z)$ as

$$\overrightarrow{b} = \mathrm{D}_l b, \qquad \overleftarrow{b} = \mathrm{D}_r b, \tag{B.88}$$

i.e., if we displace points x and z in directions X and Z, the reflection point moves in the direction $X\cdot\overrightarrow{b}(x|z) + \overleftarrow{b}(x|z)\cdot Z$. Finally we define the *reflection Van Vleck–Morette determinant* Δ_b

$$\Delta_b = |\mathrm{Det}\,\overleftrightarrow{\sigma}_b|\,\underline{\mathrm{i}}^{-1}. \tag{B.89}$$

Some long algebra gives

$$\begin{aligned} \overrightarrow{\overrightarrow{\sigma}}_b &= -\overrightarrow{b}\cdot B\cdot\overrightarrow{b} - \frac{1}{2\sigma_b}\frac{\lambda_r}{\lambda_l}(\mathrm{d}_l\sigma_b)(\mathrm{d}_l\sigma_b) + \frac{1}{\lambda_l}\overrightarrow{\overrightarrow{\sigma}}_l, \\ \overleftrightarrow{\sigma}_b &= -\overrightarrow{b}\cdot B\cdot\overleftarrow{b} + \frac{1}{2\sigma_b}(\mathrm{d}_l\sigma_b)(\mathrm{d}_r\sigma_b), \\ \overleftarrow{\overleftarrow{\sigma}}_b &= -\overleftarrow{b}\cdot B\cdot\overleftarrow{b} - \frac{1}{2\sigma_b}\frac{\lambda_l}{\lambda_r}(\mathrm{d}_r\sigma_b)(\mathrm{d}_r\sigma_b) + \frac{1}{\lambda_r}\overleftarrow{\overleftarrow{\sigma}}_l, \end{aligned} \tag{B.90}$$

where

$$\begin{aligned} B &= 2\sqrt{\sigma_b}((\nabla_r\nabla_r\sqrt{\sigma})_l + (\nabla_l\nabla_l\sqrt{\sigma})_r) \\ &= \frac{\overleftarrow{\overleftarrow{\sigma}}_{\shortparallel l}}{\lambda_l} + \frac{\overrightarrow{\overrightarrow{\sigma}}_{\shortparallel r}}{\lambda_r} + \frac{1}{2}\frac{\sigma_b}{\sigma_l\sigma_r}(\mathrm{D}_l\sigma)_r(\mathrm{D}_r\sigma)_l + 2s_\perp\mathrm{K}(b). \end{aligned} \tag{B.91}$$

Using these relations, a more intricate calculation gives the space coincidence limits

$$\{\overleftrightarrow{\sigma}_{b\shortparallel}\} = -\{\overrightarrow{b}\cdot B\cdot\overleftarrow{b}\}, \tag{B.92}$$

$$\left\{\frac{\overleftrightarrow{\sigma}_{\shortparallel l}}{\lambda_l}\right\} = -\{\overrightarrow{b}\cdot B\}, \qquad \left\{\frac{\overleftrightarrow{\sigma}_{\shortparallel r}}{\lambda_r}\right\} = -\{B\cdot\overleftarrow{b}\}, \tag{B.93}$$

$$\{(\nabla_1\nabla_1\sigma_b)^{-1}\} = \{\overset{\leftrightarrow}{\sigma}{}^{-1}_{b_{||}} \cdot (\nabla_r\nabla_r\sigma_b)^{-1} \cdot \overset{\leftrightarrow}{\sigma}{}^{-1}_{b_{||}}\}$$
$$= \{\overset{\leftrightarrow}{\sigma}{}^{-1}_{||l} \cdot (\nabla_r\nabla_r\sigma)_l \cdot \big(\lambda_l(\nabla_r\nabla_r\sigma)^{-1}_l + \lambda_r(\nabla_1\nabla_1\sigma)^{-1}_r\big) \cdot (\nabla_r\nabla_r\sigma)_l \cdot \overset{\leftrightarrow}{\sigma}{}^{-1}_{||l}\}, \tag{B.94}$$

$$\{(\nabla_1\nabla_1\sigma_b)^{-1} \cdot \overset{\leftrightarrow}{\sigma}_{b_{||}}\} = \{\overset{\leftrightarrow}{\sigma}{}^{-1}_{b_{||}} \cdot (\nabla_r\nabla_r\sigma_b)\}. \tag{B.95}$$

Here inverses are taken in the spaces tangent to the boundary. Taking the determinant of the last equation, we find

$$\{(\mathrm{Det}_{||}\overset{\leftrightarrow}{\sigma}_{b_{||}})^2\} = \{(\mathrm{Det}_{||}\nabla_1\nabla_1\sigma_b)(\mathrm{Det}_{||}\nabla_r\nabla_r\sigma_b)\},$$
$$\Delta_b(\hat{y},\xi|\hat{y},\zeta) = \big(\mathfrak{q}^{-\frac{1}{2}}(\hat{y},\xi)\mathfrak{q}^{-\frac{1}{2}}(\hat{y},\zeta)(\mathrm{Det}_{||}\nabla_1\nabla_1\sigma_b)(\mathrm{Det}_{||}\nabla_r\nabla_r\sigma_b)\big)^{\frac{1}{2}}(\hat{y},\xi|\hat{y},\zeta). \tag{B.96}$$

and

$$\frac{j^2(x)}{\mathfrak{q}(x)}(\mathrm{Det}_{||}\nabla_1\nabla_1\sigma_b)(x|z) = \frac{j^2(z)}{\mathfrak{q}(z)}(\mathrm{Det}_{||}\nabla_r\nabla_r\sigma_b)(x|z)$$
$$= \frac{j^2(\hat{y})}{\mathfrak{q}(\hat{y})}\big(\lambda_l(\nabla_r\nabla_r\sigma)^{-1}_l + \lambda_r(\nabla_1\nabla_1\sigma)^{-1}_r\big)(x|z) \tag{B.97}$$

for $x = \hat{w}(\hat{y},\xi)$ and $z = \hat{w}(\hat{y},\zeta)$. Putting these relations together, we obtain

$$j(x)\Delta_b(x|z)j(z) = \frac{j^2(x)}{\mathfrak{q}(x)}(\mathrm{Det}_{||}\nabla_1\nabla_1\sigma_b)(x|z) = \frac{j^2(z)}{\mathfrak{q}(z)}(\mathrm{Det}_{||}\nabla_r\nabla_r\sigma_b)(x|z) \tag{B.98}$$

for $x = \hat{w}(\hat{y},\xi)$ and $z = \hat{w}(\hat{y},\zeta)$. The equality in (A.51) is a straightforward consequence of this relation.

B.6. Covariant expansions near boundary

Finally, we will write down coefficients in covariant expansions (A.31) and (A.32) of the world function σ and function l defined in (A.29). These are expansions *inside* the boundary manifold of $\hat{w}$-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 are too long and uninteresting to be included here. We list only the results. See also [17–19] 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 equation (A.31)) are

$$\hat{\sigma}_{0,0}(\hat{y};\xi,\zeta) = \tfrac{1}{2}n^2(\xi-\zeta)^2, \tag{B.99}$$

$$\hat{\sigma}_{0,1}(\hat{y};\xi,\zeta) = \hat{\sigma}_{1,0}(\hat{y};\xi,\zeta) = 0, \tag{B.100}$$

$$[\hat{\sigma}_{2,0}] = -[\hat{\sigma}_{1,1}] = [\hat{\sigma}_{0,2}] = \hat{q}, \tag{B.101}$$

$$[\hat{\sigma}_{3,0\,\alpha\beta\gamma}] = [\hat{\sigma}_{0,3\,\alpha\beta\gamma}] = 3\,\hat{\gamma}^{\mu}_{(\alpha\beta}\hat{q}_{\gamma)\mu},$$
$$[\hat{\sigma}_{2,1\,\alpha\beta\kappa}] = [\hat{\sigma}_{1,2\,\kappa\alpha\beta}] = -\,\hat{\gamma}^{\mu}_{\alpha\beta}\hat{q}_{\kappa\mu}, \tag{B.102}$$

$$[\hat{\sigma}_{4,0\,\alpha\beta\gamma\delta}] = [\hat{\sigma}_{0,4\,\alpha\beta\gamma\delta}]$$
$$= -n^2\hat{\mathrm{K}}_{(\alpha\beta}\hat{\mathrm{K}}_{\gamma\delta)} + 4(\hat{\nabla}_{(\alpha}\hat{\gamma}^{\mu}_{\beta\gamma})\hat{q}_{\delta)\mu} + 8\hat{\gamma}^{\nu}_{\mu(\alpha}\hat{\gamma}^{\mu}_{\beta\gamma}\hat{q}_{\delta)\nu} + 3\hat{\gamma}^{\mu}_{(\alpha\beta}\hat{\gamma}^{\nu}_{\gamma\delta)}\hat{q}_{\mu\nu},$$

$$[\hat{\sigma}_{3,1\alpha\beta\gamma\kappa}] = [\hat{\sigma}_{1,3\kappa\alpha\beta\gamma}] = n^2\hat{\mathrm{K}}_{(\alpha\beta}\hat{\mathrm{K}}_{\gamma)\kappa} - \big(\hat{\nabla}_{(\alpha}\hat{\gamma}^{\mu}_{\beta\gamma)}\big)\hat{q}_{\mu\kappa} - \hat{\gamma}^{\mu}_{(\alpha\beta}\,\hat{\gamma}^{\nu}_{\gamma)\mu}\hat{q}_{\nu\kappa},$$

$$[\widehat{\sigma}_{2,2\alpha\beta\kappa\lambda}] = -\tfrac{1}{3}(\mathrm{R}_{\alpha\kappa\beta\lambda} + \mathrm{R}_{\alpha\lambda\beta\kappa}) - \tfrac{1}{3}n^2\widehat{\mathrm{K}}_{\alpha\kappa}\widehat{\mathrm{K}}_{\beta\lambda} - \tfrac{1}{3}n^2\widehat{\mathrm{K}}_{\alpha\lambda}\widehat{\mathrm{K}}_{\beta\kappa} - n^2\widehat{\mathrm{K}}_{\alpha\beta}\widehat{\mathrm{K}}_{\kappa\lambda} - \widehat{\gamma}^{\ \mu}_{\alpha\beta}\ \widehat{\gamma}^{\ \nu}_{\kappa\lambda}\widehat{q}_{\mu\nu}. \tag{B.103}$$

The coefficients of the boundary covariant expansion of the function l at some general point $\widehat{y}$ (slight generalization of equation (A.32)) are

$$[\widehat{l}_{0,0}] = 2\ln\widehat{j}, \tag{B.104}$$

$$[\widehat{l}_{1,0\alpha}] = [\widehat{l}_{0,1\alpha}] = \widehat{\gamma}^{\mu}_{\alpha\mu}, \tag{B.105}$$

$$\begin{aligned}[\widehat{l}_{2,0\alpha\beta}] = [\widehat{l}_{0,2\alpha\beta}] = \tfrac{1}{3}\big(&-\widehat{\mathrm{K}}'_{\alpha\beta} + 2n^2\widehat{\mathrm{K}}_{\alpha\mu}\widehat{\mathrm{K}}_{\beta\nu}\widehat{q}^{\,-1\mu\nu} - n^2\widehat{\mathrm{K}}_{\alpha\beta}\widehat{k}\\ &+ 3\,\widehat{\nabla}_{(\mu}\widehat{\gamma}^{\mu}_{\alpha\beta)} + \widehat{\gamma}^{\ \mu}_{\alpha\nu}\ \widehat{\gamma}^{\ \nu}_{\beta\mu} + 2\,\widehat{\gamma}^{\ \mu}_{\alpha\beta}\ \widehat{\gamma}^{\ \nu}_{\mu\nu}\big),\end{aligned} \tag{B.106}$$

$$[\widehat{l}_{1,1\alpha\beta}] = \tfrac{1}{3}(\widehat{\mathrm{K}}'_{\alpha\beta} - 2n^2\widehat{\mathrm{K}}_{\alpha\mu}\widehat{\mathrm{K}}_{\beta\nu}\widehat{q}^{\,-1\mu\nu} + n^2\widehat{\mathrm{K}}_{\alpha\beta}\widehat{k})$$

Computing normal derivatives we also get

$$\frac{1}{n}(\ln\widehat{j})' = n\widehat{k}, \qquad \frac{1}{n^2}(\ln\widehat{j})'' = \widehat{k}', \tag{B.107}$$

and

$$\frac{1}{n}[(\ln\widehat{j})^{\mathbf{r}'}] = 0, \qquad \frac{1}{n^2}[(\ln\widehat{j})^{\mathbf{r}'\mathbf{r}'}] = -\frac{1}{3}(\widehat{k}' + n^2\widehat{\mathrm{K}}^2). \tag{B.108}$$

Finally, we have boundary coincidence limits

$$\{\sigma_{\mathrm{b}}\}(\widehat{y};\xi,\zeta) = \frac{1}{2}n^2(\xi+\zeta)^2, \qquad \{s_{\perp}\}(\widehat{y};\xi,\zeta) = n^2(\xi+\zeta), \tag{B.109}$$

$$\{\overrightarrow{\sigma}_{\mathrm{b}}\}(\widehat{y};\xi,\zeta) = (\xi+\zeta)\vec{\mathrm{n}}(\widehat{y},\xi), \qquad \{\overleftarrow{\sigma}_{\mathrm{b}}\}(\widehat{y};\xi,\zeta) = (\xi+\zeta)\vec{\mathrm{n}}(\widehat{y},\zeta), \tag{B.110}$$

$$\{\lambda_{\mathrm{l}}\}(\widehat{y};\xi,\zeta) = \frac{\xi}{\xi+\zeta}, \qquad \{\lambda_{\mathrm{r}}\}(\widehat{y};\xi,\zeta) = \frac{\zeta}{\xi+\zeta}. \tag{B.111}$$

Using these relations, equations (B.92), (B.93), with the help of (B.69) and

$$\{\overset{\Rightarrow}{\sigma}_{\shortparallel\mathrm{r}}\}(\widehat{y};\xi,\zeta) = q(\widehat{y}) + \mathcal{O}(\zeta^2), \qquad \{\overset{\Leftarrow}{\sigma}_{\shortparallel\mathrm{l}}\}(\widehat{y};\xi,\zeta) = q(\widehat{y}) + \mathcal{O}(\xi^2), \tag{B.112}$$

we can derive

$$-\{\overset{\Leftrightarrow}{\sigma}_{\mathrm{b}\shortparallel}\}(\widehat{y};\xi,\zeta) = q(\widehat{y}) + \left(\xi+\zeta-2\frac{\xi\zeta}{\xi+\zeta}\right)n^2\mathrm{K}(\widehat{y}) + \mathcal{O}((\xi+\zeta)^2). \tag{B.113}$$

From this follows

$$\{\widehat{\Delta}_{\mathrm{b}}\}(\widehat{y};\xi,\zeta) = 1 + \left(\xi+\zeta-2\frac{\xi\zeta}{\xi+\zeta}\right)n^2k(\widehat{y}) + \mathcal{O}((\xi+\zeta)^2). \tag{B.114}$$

Together with

$$\widehat{j}(\widehat{y},\eta) = 1 + n^2k(\widehat{y})\eta + \mathcal{O}(\eta^2), \tag{B.115}$$

and definition (A.51), it finally gives the expansion for $\tilde{j}_{\mathrm{b}}$,

$$\tilde{j}_{\mathrm{b}}(\widehat{y};\xi,\lambda,\zeta) = 1 + \left(\frac{\xi+\zeta}{2} - (1-2p)\lambda\right)n^2k(\widehat{y}) + \mathcal{O}((\xi+\zeta+\lambda)^2). \tag{B.116}$$

Appendix C. Special functions R_ν

In appendix A, we have used various integrals of exponentials of quadratic exponent and integrals of such integrals. Here we summarize the properties of these 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 [23]. The derivations of the properties below are not all simple, and we do not include them here.

We define the function $R_\nu(x)$ for positive ν as

$$R_\nu(z) = \frac{1}{\Gamma(\nu)} \int_{\mathbb{R}^+} dx\, x^{\nu-1} \exp\left(-\frac{1}{2}(x-z)^2\right). \tag{C.1}$$

It is a solution of the differential equation

$$R'_\nu(z) = \nu R_{\nu+1}(z) - z R_\nu(z), \qquad R_\nu \xrightarrow{z\to-\infty} 0. \tag{C.2}$$

In the limit $\nu \to 0$ and for $\nu = 1$ we have

$$R_0(z) = \exp\left(-\tfrac{1}{2}z^2\right), \tag{C.3}$$

$$R_1(z) = \sqrt{2\pi} - \sqrt{\frac{\pi}{2}}\, \mathrm{erfc}\left(\frac{z}{\sqrt{2}}\right). \tag{C.4}$$

We also have the recurrence relation

$$R_{\nu+2}(z) = \frac{1}{\nu+1}(z R_{\nu+1}(z) + R_\nu(z)). \tag{C.5}$$

For $\nu \in \mathbb{N}$, these functions are combinations of R_0 and R_1 with polynomial coefficients

$$R_{n+1} = p_n R_1 + q_{n-1} R_0 \qquad \text{for} \quad n \in \mathbb{N}, \tag{C.6}$$

where

$$p_{n+1}(z) = \frac{1}{n+1}(z p_n(z) + p_{n-1}(z)), \qquad p_0 = 1, \quad p_1 = z, \tag{C.7}$$

$$q_{n+1}(z) = \frac{1}{n+2}(z q_n(z) + q_{n-1}(z)), \qquad q_0 = 1, \quad q_1 = \frac{1}{2}z. \tag{C.7}$$

These polynomials satisfy

$$p'_n = p_{n-1}, \qquad q'_n = (n+2) q_{n+1} - p_{n+1}, \tag{C.8}$$

and

$$\sqrt{2\pi}\, p_n(z) = R_{n+1}(z) + (-1)^n R_{n+1}(-z) = \frac{\sqrt{2\pi}}{i^n 2^{\frac{n}{2}} n!} H_n\left(i\tfrac{z}{\sqrt{2}}\right), \tag{C.9}$$

where H_n are the Hermite polynomials (see [23]).

Values at zero are

$$R_\nu(0) = 2^{\frac{\nu}{2}} \frac{\Gamma\left(\frac{\nu}{2}+1\right)}{\Gamma(\nu+1)} = \frac{1}{2} \frac{\sqrt{2\pi}}{2^{\frac{\nu-1}{2}}\Gamma\left(\frac{\nu-1}{2}+1\right)} = \begin{cases} \dfrac{1}{(\nu-1)!!} & \text{for } \nu \text{ natural and even} \\ \dfrac{1}{\nu!!}\sqrt{\dfrac{\pi}{2}} & \text{for } \nu \text{ natural and odd,} \end{cases} \tag{C.10}$$

$$p_n(0) = \begin{cases} \dfrac{1}{n!!} & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd,} \end{cases} \qquad p'_n(0) = \begin{cases} 0 & \text{for } n \text{ even} \\ \dfrac{1}{(n-1)!!} & \text{for } n \text{ odd,} \end{cases} \tag{C.11}$$

$$\mathrm{q}_n(0) = \begin{cases} \dfrac{1}{(n+1)!!} & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd,} \end{cases} \qquad \mathrm{q}'_n(0) = \begin{cases} 0 & \text{for } n \text{ even} \\ \dfrac{1}{n!!} - \dfrac{1}{(n+1)!!} & \text{for } n \text{ odd.} \end{cases} \tag{C.12}$$

The behaviour for small z can be found for natural ν with the help of relations (C.5) and

$$\mathrm{R}_0(z) = \sum_{k\in\mathbb{N}_0} \frac{(-1)^k}{(2k)!!} z^{2k}, \qquad \mathrm{R}_1(z) = \sqrt{\frac{\pi}{2}} + \sum_{k\in\mathbb{N}_0} \frac{(-1)^k}{(2k+1)(2k)!!} z^{2k+1}. \tag{C.13}$$

The behaviour for $|z| \gg 1$ and $n \in \mathbb{N}_0$ is

$$\mathrm{R}_{n+1}(z) = \sqrt{2\pi}\,\mathrm{p}_n(z)\theta(z) + \exp\left(-\frac{1}{2}z^2\right) \mathcal{O}\left(\frac{1}{z^{n+1}}\right), \tag{C.14}$$

where $\theta(z)$ is the step function.

Now we can write down the results of some integrals in terms of these functions. For $n \in \mathbb{N}_0$ we have

$$\frac{1}{n!} \int_{\mathbb{R}} \mathrm{d}x\, x^n \exp\left(-\frac{1}{2}(x-z)^2\right) = \sqrt{2\pi}\,\mathrm{p}_n(z). \tag{C.15}$$

Further for $k, l \in \mathbb{N}_0$ we have

$$\begin{aligned} \frac{1}{l!} \int_{\langle -\infty, x\rangle} \mathrm{d}\xi\, \xi^l \mathrm{R}_k(\xi) &= \sum_{m=0,\ldots,l} \frac{(-1)^{l+m}}{m!} x^m \mathrm{R}_{k+l-m+1}(x) \\ &= \sqrt{2\pi}(-1)^l \mathrm{p}_{k+l}(0) + \frac{\sqrt{2\pi}}{l!(k-1)!} \sum_{\substack{m\in\mathbb{N} \\ 2m\leqslant k-1}} \frac{(2m-1)!!}{k+l-2m} \binom{k-1}{2m} x^{k+l-2m} \\ &\quad - \sum_{m=0,\ldots,l} \frac{1}{m!} x^m \mathrm{R}_{k+l-m+1}(-x), \end{aligned} \tag{C.16}$$

$$\begin{aligned} \frac{1}{l!} \int_{\langle 0, x\rangle} \mathrm{d}\xi\, \xi^l \mathrm{R}_k(\xi) &= (-1)^k \mathrm{R}_{k+l+1}(0) + \frac{\sqrt{2\pi}}{l!(k-1)!} \sum_{\substack{m\in\mathbb{N} \\ 2m\leqslant k-1}} \frac{(2m-1)!!}{k+l-2m} \binom{k-1}{2m} x^{k+l-2m} \\ &\quad - \sum_{m=0,\ldots,l} \frac{1}{m!} x^m \mathrm{R}_{k+l-m+1}(-x). \end{aligned} \tag{C.17}$$

Finally, for $m, k, l \in \mathbb{R}^+$ and $n = m + k + l$ we have

$$\frac{1}{n!} \int_{\xi,\zeta\in\mathbb{R}^+} \mathrm{d}\xi\, \mathrm{d}\zeta\, \frac{\xi^{m+k}\zeta^{m+l}}{(\xi+\zeta)^m} \exp\left(-\frac{1}{2}(\xi+\zeta)^2\right) = \sqrt{2\pi}\, 2^{-\frac{n+1}{2}} \frac{\Gamma(m+k+1)\Gamma(m+l+1)}{\Gamma(b+m+1)\Gamma\left(\frac{n+1}{2}\right)}. \tag{C.18}$$

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