Propagators in curved spacetimes from operator theory

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September 4, 2025

Abstract

We discuss two distinct operator-theoretic settings useful for describing (or defining) propagators associated with a scalar Klein-Gordon field on a Lorentzian manifold M. Typically, we assume that M is globally hyperbolic. The term *propagator* here refers to any Green function or bisolution of the Klein-Gordon equation pertinent to Quantum Field Theory.

The *off-shell* setting is based on the Hilbert space $L^2(M)$. It leads to the definition of the operator-theoretic Feynman and anti-Feynman propagators, which often coincide with the so-called in-out Feynman and out-in anti-Feynman propagator. On some special spacetimes, the sum of the operator-theoretic Feynman and anti-Feynman propagator equals the sum of the forward and backward propagator. This is always true on static stable spacetimes and, curiously, in some other cases as well.

The *on-shell* setting is based on the Krein space $\mathcal{W}_{\mathrm{KG}}$ of solutions of the Klein-Gordon equation. It allows us to define 2-point functions associated to two, possibly distinct, Fock states as the Klein-Gordon kernels of projectors onto maximal uniformly positive subspaces of $\mathcal{W}_{\mathrm{KG}}$.

After a general discussion, we review a number of examples. We start with static and asymptotically static spacetimes, which are especially well-suited for Quantum Field Theory. Then we discuss FLRW spacetimes, reducible by a mode decomposition to 1-dimensional Schrödinger operators. We compare various approaches to de Sitter space where, curiously, the off-shell approach gives non-physical propagators. Finally, we discuss the universal cover of anti-de Sitter spaces, where the on-shell approach may require boundary conditions, unlike the off-shell approach.

Contents

1 Introduction

1.1 Propagators and states

Let M be a Lorentzian manifold of dimension d with a *pseudometric tensor* $g_{\mu\nu}$. Let $Y(x)$ be a real-valued *scalar potential*, e.g. $Y(x) = m^2$. Consider a field on M satisfying the *Klein-Gordon equation*

$$\big(-\Box + Y(x)\big)\phi(x) = 0, \tag{1.1}$$

where $\Box := |g|^{-\frac{1}{2}}\partial_\mu |g|^{\frac{1}{2}} g^{\mu\nu}\partial_\nu$ is the *d'Alembertian*. If one wants to compute various pertinent quantities related to ϕ, and especially to its quantization $\hat{\phi}$, one needs to know several distributions on $M \times M$, often called "propagators" or "two-point functions".

These distributions fall into two categories: *Green functions* (also called *fundamental solutions*), and *bisolutions* of the Klein-Gordon equation. A *Green function* of the Klein-Gordon equation is a distribution $G^\bullet$ on $M \times M$ satisfying

$$(-\Box_x + Y(x))G^\bullet(x,y) = \delta(x,y) = (-\Box_y + Y(y))G^\bullet(x,y), \tag{1.2}$$

where $\delta(x,y)$ denotes the distributional kernel of the identity. A *bisolution* of the Klein-Gordon equation is a distribution $G^\bullet$ on $M \times M$ satisfying

$$(-\Box_x + Y(x))G^\bullet(x,y) = 0 = (-\Box_y + Y(y))G^\bullet(x,y). \tag{1.3}$$

In our paper we will colloquially use the term "propagator"[1] for various distinguished Green functions and bisolutions of (1.1) motivated by QFT: the advanced and retarded propagators, the Pauli-Jordan propagator, Feynman and anti-Feynman propagators, and Wightman and anti-Wightman two-point functions (in some situations also called positive/negative frequency bisolutions). Wightman functions serve as two-point functions of a quantum state. Hence, abusing somewhat terminology, they are often simply called *states*.

[1]This nomenclature is in accordance with the previous papers [39–41]. Note, however, that the term "propagator" is often reserved only for some of these distributions. Following the usage common in physics we will often also use the term "two-point function" for (anti-)Wightman bisolutions.

In most of our paper we assume that M is globally hyperbolic. Then one can show the existence of the *retarded* (or *forward*) and *advanced* (or *backward*) propagator $G^{\vee}(x,x')$ and $G^{\wedge}(x,x')$, which are the unique Green functions supported for x in the causal future resp. causal past of x'. The bisolution defined by

$$G^{\mathrm{PJ}}(x,x') = G^{\vee}(x,x') - G^{\wedge}(x,x') \tag{1.4}$$

is usually called the *Pauli-Jordan propagator* or the *commutator function*. It also possesses a causal support. All three propagators $G^{\vee}$, $G^{\wedge}$ and G^{PJ} are useful in the Cauchy problem of the Klein-Gordon equation. The classical field $\phi(x)$ satisfying (1.1) is equipped with the Poisson bracket

$$\{\phi(x),\phi(y)\} = -G^{\mathrm{PJ}}(x,y).$$

Therefore, following [39–41], $G^{\vee}$, $G^{\wedge}$ and G^{PJ} will be called *classical propagators*. In Quantum Field Theory one uses a few other propagators, whose operator-theoretic meaning – especially on curved spacetimes – is the main subject of this article.

Quantization of the classical field $\phi(x)$ is performed in two steps. In the first step we replace it by an operator valued distribution $\hat{\phi}(x)$, which beside the Klein-Gordon equation

$$\big(-\Box + Y(x)\big)\hat{\phi}(x) = 0 \tag{1.5}$$

satisfies the so called *Peierls relation*

$$[\hat{\phi}(x),\hat{\phi}(y)] = -\mathrm{i}G^{\mathrm{PJ}}(x,y)\mathbb{1}.$$

The fields $\hat{\phi}(x)$ generate a $*$-algebra.

In the second step one selects a representation of the fields in a Hilbert space. In practice, this is done by choosing a state ω_α on this $*$-algebra, that is, a positive and normalized linear functional. Then ω_α defines the GNS Hilbert space with a distinguished vector Ω_α. One usually considers a Fock state (a pure quasifree state), where the GNS representation has the form of a bosonic Fock space and Ω_α is its vacuum. The expectation values in this state define four important two-point functions:

$$G^{(+)}_\alpha(x,y) := \big(\Omega_\alpha|\hat{\phi}(x)\hat{\phi}(y)\Omega_\alpha\big), \tag{1.6}$$

$$G^{(-)}_\alpha(x,y) := \big(\Omega_\alpha|\hat{\phi}(y)\hat{\phi}(x)\Omega_\alpha\big), \tag{1.7}$$

$$G^{\mathrm{F}}_\alpha(x,y) := \mathrm{i}\big(\Omega_\alpha|\,\mathrm{T}\,\big(\hat{\phi}(x)\hat{\phi}(y)\big)\Omega_\alpha\big), \tag{1.8}$$

$$G^{\overline{\mathrm{F}}}_\alpha(x,y) := -\mathrm{i}\big(\Omega_\alpha|\overline{\mathrm{T}}\big(\hat{\phi}(x)\hat{\phi}(y)\big)\Omega_\alpha\big). \tag{1.9}$$

Here, T and $\overline{\mathrm{T}}$ denote the chronological, resp. anti-chronological time ordering. Note that $G^{(+)}_\alpha$ and $G^{(-)}_\alpha$ are automatically bisolutions; G^{F}_α and $G^{\overline{\mathrm{F}}}_\alpha$ are Green functions.

It is perhaps less known that it is useful to define mixed propagators corresponding to two *different* states. Suppose that they are given by vectors Ω_α and Ω_β, belonging to the same representation space, with nonzero $(\Omega_\alpha|\Omega_\beta)$. Then we set

$$G^{(+)}_{\alpha,\beta}(x,y) := \frac{\big(\Omega_\alpha|\hat\phi(x)\hat\phi(y)\Omega_\beta\big)}{\big(\Omega_\alpha|\Omega_\beta\big)}, \tag{1.10}$$

$$G^{(-)}_{\alpha,\beta}(x,y) := \frac{\big(\Omega_\alpha|\hat\phi(y)\hat\phi(x)\Omega_\beta\big)}{\big(\Omega_\alpha|\Omega_\beta\big)}, \tag{1.11}$$

$$G^{\mathrm{F}}_{\alpha,\beta}(x,y) := \mathrm{i}\frac{\big(\Omega_\alpha|\,\mathrm{T}\,\big(\hat\phi(y)\hat\phi(x)\big)\Omega_\beta\big)}{\big(\Omega_\alpha|\Omega_\beta\big)}, \tag{1.12}$$

$$G^{\overline{\mathrm{F}}}_{\alpha,\beta}(x,y) := -\mathrm{i}\frac{\big(\Omega_\alpha|\overline{\mathrm{T}}\big(\hat\phi(y)\hat\phi(x)\big)\Omega_\beta\big)}{\big(\Omega_\alpha|\Omega_\beta\big)}. \tag{1.13}$$

Again, $G^{(+)}_{\alpha,\beta}$ and $G^{(-)}_{\alpha,\beta}$ are bisolutions; the Feynman propagator $G^{\mathrm{F}}_{\alpha,\beta}$ and the anti-Feynman propagator $G^{\overline{\mathrm{F}}}_{\alpha,\beta}$ are Green functions.

We have a minor terminological problem: should $G^{\mathrm{F}}_{\alpha,\beta}$ be called the "$\alpha-\beta$ Feynman propagator" or the "$\beta-\alpha$ Feynman propagator"? The latter choice is consistent with the "time arrow": in typical applications the vacuum Ω_β is first, and Ω_α is later. This order is used e.g. in [48] (see e.g. equation (74)). In symbols we will use the former order, in names we will use the latter order. So $G^{\mathrm{F}}_{\alpha,\beta}$ will be called the *$\beta-\alpha$ Feynman propagator*.

The functions $G^{(+)}_{\alpha}(x,y)$ are used to define the GNS representation for the state ω_α and Wick-ordered product of fields. Wick ordering is a first step to renormalization, which is needed to define higher order monomials of fields. The renormalization procedure will not work for an arbitrary state. In practice one assumes that it has the so-called *Hadamard property*, and then renormalization works well. Note that this analysis can be performed on a local level, without considering the whole spacetime.

Let us now describe the application of Feynman propagators. Suppose we perturb the dynamics and we want to compute the *scattering operator* S_α in the representation given by Ω_α. By a standard argument going back to Dyson, often called the *Wick Theorem*, S_α can be expressed as a perturbation series with terms labelled by Feynman diagrams. In order to evaluate Feynman diagrams one needs to replace the lines by $G^{\mathrm{F}}_{\alpha}(x,y)$.

Often it is natural to compute the *renormalized scattering operator* $S_{\alpha,\beta}$, acting from the representation generated by Ω_β to the representation generated by Ω_α. Actually, it is then useful to divide the scattering operator by the overlap between the vacua, and compute

$$\tilde S_{\alpha,\beta} := \frac{S_{\alpha,\beta}}{\big(\Omega_\alpha|\Omega_\beta\big)}. \tag{1.14}$$

The algorithm is similar as above, except that we put $G^{\mathrm{F}}_{\alpha,\beta}$ at each line of a Feynman diagram.

We will see that $G^{\mathrm{F}}_{\alpha,\beta}$ can usually be defined even if $(\Omega_\beta|\Omega_\alpha)=0$. Therefore, we can then also compute $\tilde S_{\alpha,\beta}$. In fact, if the theory is linear, $\tilde S_{\alpha,\beta}$ will be usually a well-defined unbounded quadratic form, whose integral kernel $\tilde{S}_{\alpha\beta}(k_\alpha, k_\beta)$ can be called the "renormalized scattering amplitude". Obviously, the unitarity of $\tilde{S}_{\alpha\beta}$ is lost, hence renormalized scattering amplitudes will not have a direct probabilistic interpretation. However their ratios

$$\frac{\tilde{S}_{\alpha\beta}(k_\alpha, k_\beta)}{\tilde{S}_{\alpha\beta}(k'_\alpha, k'_\beta)} \tag{1.15}$$

have a meaning: they can be used to compute *branching ratios* of various processes.

If we want to compute $\frac{S^*_{\alpha,\beta}}{(\Omega_\beta|\Omega_\alpha)}$ we proceed similarly, except that Feynman propagators need to be replaced by anti-Feynman propagators $G^{\overline{\mathrm{F}}}_{\beta,\alpha}$.

One of the important problems of QFT on curved spacetimes is the choice of a state. In Minkowski space and with $Y(x) = m^2 \geq 0$ there is a natural state, described in all textbooks on QFT. More generally, every stationary and stable Klein-Gordon equation possesses a natural state. Stationarity means that one can identify M with $\mathbb{R} \times \Sigma$ so that $g^{\mu\nu}$ and Y are independent of $t \in \mathbb{R}$, Σ is spacelike and ∂_t is timelike. Stability means that the corresponding classical Hamiltonian is bounded from below. Again, requiring that the state is invariant under the time evolution, and in the GNS representation the dynamics is implemented by a positive quantum Hamiltonian fixes the state uniquely. The one-particle Hilbert space is then taken to be the *positive frequency space*, that is, the spectral subspace of the generator of the evolution corresponding to the positive part of the spectrum.

On generic spacetimes there are no distinguished states. There is however one class of spacetimes, particularly well adapted to QFT, where there are *two* distinguished states. These are spacetimes with asymptotically stationary and stable future and past. Such spacetimes possess two distinguished states: the *in-state* and the *out-state*, given by vectors Ω_- and Ω_+. Obviously, they define two pairs of two-point functions

$$G^{(+)}_{\pm}(x, x') = \big(\Omega_\pm|\hat{\phi}(x)\hat{\phi}(x')\Omega_\pm\big), \tag{1.16}$$

$$G^{(-)}_{\pm}(x, x') = \big(\Omega_\pm|\hat{\phi}(x')\hat{\phi}(x)\Omega_\pm\big). \tag{1.17}$$

One can use them to define two GNS representations acting on two Fock spaces.

More interesting are however the following mixed Feynman propagators: the *in-out Feynman propagator* G^{F}_{+-} and the *out-in anti-Feynman propagator* $G^{\overline{\mathrm{F}}}_{-+}$:

$$G^{\mathrm{F}}_{+-}(x, x') = \mathrm{i}\frac{\big(\Omega_+|\,\mathrm{T}\,\big(\hat{\phi}(x)\hat{\phi}(x')\big)\Omega_-\big)}{(\Omega_+|\Omega_-)}, \tag{1.18}$$

$$G^{\overline{\mathrm{F}}}_{-+}(x, x') = -\mathrm{i}\frac{\big(\Omega_-|\overline{\mathrm{T}}\big(\hat{\phi}(x)\hat{\phi}(x')\big)\Omega_+\big)}{(\Omega_-|\Omega_+)}. \tag{1.19}$$

We will see below that G^{F}_{+-} and $G^{\overline{\mathrm{F}}}_{-+}$ play an important role in applications, and possess an alternative definition that works well even if the overlap $(\Omega_-|\Omega_+)$ is formally zero.

In a generic situation, (1.18), (1.19) and (1.20) may be ill-defined because the overlap $(\Omega_+|\Omega_-)$ is zero. Fortunately, as we will see, one can define G^{F}_{+-} and $G^{\overline{\mathrm{F}}}_{-+}$ independently via operator theory, without a division by zero.

On an asymptotically stationary and stable spacetime it is natural to use for the initial, resp. final representation the Hilbert space generated by Ω_-, resp. Ω_+. Thus the main objects of interest are

$$\frac{S_{+-}}{(\Omega_+|\Omega_-)},\quad \frac{S^*_{+-}}{(\Omega_-|\Omega_+)}. \tag{1.20}$$

They can be evaluated using G^{F}_{+-} and $G^{\overline{\mathrm{F}}}_{-+}$, even if $(\Omega_+|\Omega_-)=0$.

The main topic of the present article is how to define various propagators using tools of operator theory. We will see in particular that one does not need to worry about dividing by the overlap $(\Omega_\alpha|\Omega_\beta)$. It is possible to give a purely operator theoretic definition of (1.10), (1.11), (1.12) and (1.13), which works also if $(\Omega_\alpha|\Omega_\beta)=0$.

1.2 Operator-theoretic interpretations of propagators

There are two distinct operator-theoretic settings related to the Klein-Gordon equation, which are useful in defining and computing propagators: the space of solutions to (1.1), which we denote $\mathcal{W}_{\mathrm{KG}}$, and the Hilbert space $L^2(M,|g|^{\frac12})$. The space $\mathcal{W}_{\mathrm{KG}}$ may be called the *on-shell space* and $L^2(M,|g|^{\frac12})$ the *off-shell space*.

To define the on-shell space one usually starts from the space of complex space-compact solutions to (1.1), denoted $\mathcal{W}_{\mathrm{sc}}$. This space is endowed with the so-called *Klein-Gordon charge form*—an indefinite sesquilinear form obtained by integrating the natural current over an arbitrary Cauchy surface. In the generic case, this space does not have a distinguished positive scalar product. Nevertheless, one can fix a family of equivalent positive scalar products compatible with the Klein-Gordon form. Then, for technical reasons, we extend $\mathcal{W}_{\mathrm{sc}}$ to a complete space $\mathcal{W}_{\mathrm{KG}}$, which has the structure of Krein space: a space with a Hilbertian topology equipped with a distinguished indefinite form given by a bounded self-adjoint involution. Using elements of the theory of Krein spaces one is able to give meaning to the quantities (1.10), (1.11), (1.12) and (1.13), avoiding expressions of the type $\frac{0}{0}$. This is a big advantage of the operator-theoretic viewpoint.

In practice, it is convenient to represent the space $\mathcal{W}_{\mathrm{KG}}$ in terms of Cauchy data. More precisely, we first identify $M=\mathbb{R}\times\Sigma$, where Σ has a spatial signature and ∂_t a temporal signature. Each element of $\mathcal{W}_{\mathrm{KG}}$ is uniquely determined by its value at $\{t\}\times\Sigma$ and its temporal derivative. This allows us to describe elements of $\mathcal{W}_{\mathrm{KG}}$ as pairs of functions on Σ.

The space $\mathcal{W}_{\mathrm{KG}}$ is not the only operator-theoretic setting for propagators. There is another one, provided by the Hilbert space is $L^2(M,|g|^{\frac12})$. At first many readers may protest – this space does not describe physically relevant states. However, as we will see it is very useful for the computation of propagators.

It can be easily shown that on Minkowski space the usual Feynman and anti-Feynman propagator are the boundary values of the resolvent kernel of the Klein-Gordon operator on $L^2(\mathbb{R}^{1,d-1})$:

$$G^{\mathrm{F}}(x,y) := \lim_{\epsilon\searrow 0} \frac{1}{(-\Box + m^2 + \mathrm{i}\epsilon)}(x,y), \tag{1.21}$$

$$G^{\overline{\mathrm{F}}}(x,y) := \lim_{\epsilon\searrow 0} \frac{1}{(-\Box + m^2 - \mathrm{i}\epsilon)}(x,y). \tag{1.22}$$

It is not difficult to see that an analogous statement is true on stationary stable spacetimes.

More generally, suppose we use the path integral formalism to define perturbative QFT. The usual prescription says that one should split the action in a quadratic part and the interaction, and then derive Feynman diagrams from the path integral. It is easy to see that this prescription formally yields (1.21) and (1.22) as the expressions corresponding to the lines in Feynman diagrams. This suggests an alternative definition of Feynman and anti-Feynman propagator, which we describe below.

It is clear that for real-valued $Y(x)$, $-\Box+Y(x)$ is a Hermitian operator on $C_c^\infty(M)$ in the sense of $L^2(M,|g|^{\frac{1}{2}})$. Suppose that it is essentially self-adjoint. Then its spectrum is contained in $\mathbb{R}$ and we may define the *operator-theoretic Feynman and anti-Feynman propagator* $G^{\mathrm{F}}_{\mathrm{op}}(x,y)$ and $G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,y)$ via

$$G^{\mathrm{F}}_{\mathrm{op}}(x,y) := \lim_{\epsilon\searrow 0} \frac{1}{(-\Box + Y(x) + \mathrm{i}\epsilon)}(x,y), \tag{1.23}$$

$$G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,y) := \lim_{\epsilon\searrow 0} \frac{1}{(-\Box + Y(x) - \mathrm{i}\epsilon)}(x,y), \tag{1.24}$$

provided that the distributional limits on the right-hand side exist.

Note that there is no guarantee that the limits (1.23) and (1.24) exist. For instance, if the Klein-Gordon operator has a zero eigenvalue, they fail to exist.

For static stable Klein-Gordon operators the existence of (1.23) and (1.24) is proven in [39]. There are heuristic arguments [40, 41] showing that the above definitions work on asymptotically stationary stable spacetimes and the in-out Feynman and the out-in anti-Feynman propagator coincide with the operator-theoretic Feynman propagators:

$$G^{\mathrm{F}}_{\mathrm{op}}(x,y) = G^{\mathrm{F}}_{+-}(x,y), \tag{1.25}$$

$$G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,y) = G^{\overline{\mathrm{F}}}_{-+}(x,y). \tag{1.26}$$

These identities can be viewed as a justification of the path-integral approach to QFT.

From the rigorous point of view, the definitions (1.23) and (1.24) raise difficult mathematical questions. First, the essential self-adjointness for generic spacetimes is a nontrivial problem. For asymptotically Minkowskian spacetimes satisfying some non-trapping conditions it has been proven in [71, 72, 83]. Under similar conditions one can show that (1.25) and (1.26) are true.

Propagators satisfy various identities. We already mentioned (1.4), which defines the Pauli-Jordan propagator. Another identity universally true is

$$G^{\mathrm{PJ}}(x,x') = \mathrm{i}G^{(+)}_{\alpha,\beta}(x,x') - \mathrm{i}G^{(-)}_{\alpha,\beta}(x,x'), \tag{1.27}$$

valid for any pair of Fock states $\omega_\alpha, \omega_\beta$.

On Minkowski space with $Y(x) = m^2 \geq 0$, and more generally for a stationary stable Klein-Gordon equation, we have the identity

$$G^{\mathrm{F}}_{\mathrm{op}} + G^{\overline{\mathrm{F}}}_{\mathrm{op}} = G^{\vee} + G^{\wedge}. \tag{1.28}$$

In particular, the support of $G^{\mathrm{F}}_{\mathrm{op}} + G^{\overline{\mathrm{F}}}_{\mathrm{op}}$ is causal.

Definition 1.1. We will say that the Klein-Gordon equation is *special* if one can define $G^{\mathrm{F}}_{\mathrm{op}}$ and $G^{\overline{\mathrm{F}}}_{\mathrm{op}}$ (which we expect to be true in typical situations) and the support of $G^{\mathrm{F}}_{\mathrm{op}} + G^{\overline{\mathrm{F}}}_{\mathrm{op}}$ is causal. We will then also say that the *specialty condition* is satisfied.

Special Klein-Gordon equations have the following advantage. One may expect that it is in many situations quite simple to compute the distributions $G^{\mathrm{F}}_{\mathrm{op}}$ and $G^{\overline{\mathrm{F}}}_{\mathrm{op}}$ using operator-theoretic tools. Then, splitting $G^{\mathrm{F}}_{\mathrm{op}} + G^{\overline{\mathrm{F}}}_{\mathrm{op}}$ into two distributions, one supported in the causal future and the other supported in the causal past, we may determine $G^{\vee}$ and $G^{\wedge}$.

The specialty condition is generically violated. It is however very useful if it holds. We will discuss some interesting cases when it is true.

1.3 Outline of the paper

In Section 2, we describe in detail both basic operator-theoretic settings to QFT on curved spacetimes that we outlined in the introduction: the on-shell space $\mathcal{W}_{\mathrm{KG}}$ and the off-shell space $L^2(M)$.

The remaining sections are dedicated to the discussion of various examples of spacetimes with largely different properties:

1. First we discuss stationary spacetimes. Here one can give fairly explicit formulas for the Pauli-Jordan bisolution, and the four basic Green functions: the avanced/retarded propagators, and operator-theoretic (anti-)Feynman propagators. If in addition the Klein-Gordon equation is stable, then there is a distinguished Fock state. The corresponding 2-point functions and (anti-)Feynman propagators are easy to describe. The specialty condition is fulfilled and the (anti-)Feynman propagators defined in the off-shell and on-shell formalism coincide.

   In the tachyonic case, that is, if the Hamiltonian is not positive, the speciality condition is violated, and we cannot define positive/negative frequency bisolutions. This includes the Minkowski space with imaginary mass, that is, $m^2 < 0$. Of course, this case is not very physical, but it is occasionally discussed in the literature.

2. Spacetimes asymptotically stationary and stable in the past and future form a class well suited for the formalism of QFT. After identifying M with $\mathbb{R} \times \Sigma$, where $\mathbb{R}$ describes time and Σ is a Cauchy surface with a time dependent Riemannian metric, one can give a fairly explicit description of all propagators using the time evolution of solutions, as described in [41]. Remarkably, the in-out Feynman and out-in anti-Feynman propagator are well defined—this is a non-trivial statement proven in [41]. The existence of the operator-theoretic (anti-)Feynman propagator is a difficult mathematical problem, solved only under some strong assumptions. There are heuristic arguments showing that, if they exist, they coincide with the in-out Feynman and out-in anti-Feynman propagator. As we mentioned above, the specialty condition is rarely fulfilled.

3. The Klein-Gordon operator on $1 + 0$-dimensional spacetimes essentially reduces to a one-dimensional Schrödinger operator. The corresponding propagators are well-known objects from the theory of such operators. The speciality condition is fulfilled if and only if the scattering operator is reflectionless. Obviously, it is satisfied if the potential is a constant. But curiously, as is well known, there exist potentials which are reflectionless at all energies. The best known such potential is

$$-\frac{\mu^2 - \frac{1}{4}}{\cosh^2 x} \tag{1.29}$$

for half-integer μ.

4. Spacetimes, whose pseudometric depends on time only through a conformal factor, are usually called Friedmann-Lemaître-Robertson-Walker (FLRW) spacetimes. In such spacetimes, after diagonalization of the spatial Laplacian, or in other words, after decomposing it into "modes", the Klein-Gordon equation can be reduced to the $1 + 0$-dimensional setting. Thus in principle one can write all propagators as the direct sum or integral of propagators for each mode. In particular, the Klein-Gordon equation is special if each mode is reflectionless.

5. The theory of propagators on the d-dimensional de Sitter space dS_d is especially rich and surprising.

   The de Sitter space can be interpreted as the "Wick rotated" d-dimensional sphere. Analytically continuing the Green function of the sphere in the usual spherical coordinates we obtain a certain Feynman and anti-Feynman propagator. For $m^2 \geq (\frac{d-1}{2})^2$, they can be used to write down the Wightman two-point functions of a state, as well as the classical propagators. This state is usually called the Euclidean (or Bunch-Davies) state and is believed to be the physical choice on the de Sitter space, because it is Hadamard.

   The d'Alembertian on de Sitter space is essentially self-adjoint on smooth compactly supported functions. This is a special case of a general mathematical theorem saying that invariant differential operators on maximally symmetric pseudo-Riemannian manifolds are essentially self-adjoint. In our paper we compute the integral kernel of resolvent of the d'Alembertian on dS_d. Taking its boundary values yields the operator-theoretic Feynman and anti-Feynman propagator. Curiously, they are different from the Euclidean Feynman and anti-Feynman propagator. The specialty condition is satisfied in odd dimensions; it is not true in even dimensions.

Our derivation of the formula for the resolvent is based on an argument which, while in our opinion convincing and elegant, is not fully rigorous. Alternative, more complicated proofs of our formula are possible, e.g. following the approach of [48] based on mode decompositions.

It is well-known that all de Sitter invariant states can be described and expressed in terms of Gegenbauer functions. They are usually called α-*vacua*, where α is a complex parameter that can be used to parametrize them. $\alpha = 0$ corresponds to the Euclidean vacuum. All other α-vacua are not Hadamard.

The de Sitter space is not asymptotically stationary. However, it possesses two distinguished states, which can be called the in-state and the-out state. The former has an incoming behavior in the past, the latter is outgoing in the future. The operator theoretic Feynman and anti-Feynman propagators satisfy the identitities (1.25) and (1.26). In odd dimensions the in-state coincides with the out-state. In even dimensions this is not the case. In all dimensions, the in-state and out-state are distinct from Euclidean state.

De Sitter space is a FLRW spacetime (with a conformal factor that blows up exponentially). Therefore, it is possible to decompose the Klein-Gordon equation into modes. In each mode one obtains the 1-dimensional Schrödinger operator with the potential (1.29), where μ depends on the dimension and the degree of spherical harmonics. μ is a half-integer for odd dimensions and an integer for even dimensions. This is another way to see that the Klein-Gordon equation in odd dimensions is special and in even dimension is not.

One can define retarded and advanced propagators for all values of $m^2 \in \mathbb{R}$. However, the case $m^2 < (\frac{d-1}{2})^2$ seems not physical. In fact, below $(\frac{d-1}{2})^2$ the spectrum of the d'Alembertian is discrete. Operator-theoretic Feynman and anti-Feynman propagators are well defined (and identical) outside of this spectrum. As can be expected, the specialty condition is then violated.

6. The universal cover of anti-de Sitter space $\widetilde{\mathrm{AdS}}_d$ is another maximally symmetric spacetime, where one can compute all propagators. It is a stationary spacetime, which is not globally hyperbolic: it possesses geodesics that escape to the spatial boundary in a finite proper time. One can apply two approaches to define the propagators on the universal cover of anti-de Sitter space.

   The first approach uses $L^2(\widetilde{\mathrm{AdS}}_d)$. The d'Alembertian is essentially self-adjoint—there is no need to fix boundary conditions. We compute the resolvent of the d'Alembertian and define the operator-theoretic Feynman and anti-Feynman propagators as its limits.

(Again, our computation is based on a conjecture and thus not fully rigorous.) If $m^2 > -(\frac{d-1}{2})^2$, then their sum has a causal support, so one can define the retarded and advanced propagator by splitting this sum. In particular, the specialty condition is satisfied.

Alternatively, one can use the evolution of the Cauchy data. For $m^2 \geq -(\frac{d-1}{2})^2 + 1$ this evolution is uniquely defined–one does not need to specify boundary conditions. For $m^2 < -(\frac{d-1}{2})^2 + 1$ boundary conditions are needed. For $-(\frac{d-1}{2})^2 \leq m^2 < -(\frac{d-1}{2})^2 + 1$ there exists a distinguished boundary condition (corresponding to the Friedrichs extension), which agrees with the propagators obtained from the operator-theoretic Feynman propagator. In particular, we have distinguished retarded and advanced propagators. For $m^2 < -(\frac{d-1}{2})^2$ there are no distinguished boundary conditions at spatial infinity. Thus retarded and advanced propagators are non-unique and none is distinguished.

Pertinent elements of the theory of Krein spaces are discussed in Appendix A. Propagators on de Sitter and anti-de Sitter space can be described explicitly in terms of special functions (Gegenbauer functions). We introduce their relevant properties in Appendix B.

Remark 1.2. We restrict our considerations to a real scalar field $\hat{\phi}(x)$, but they can be generalized to a complex scalar field in a fairly straightforward manner. One needs then two pairs of creation and annihilation operators. Both the real and the complex formalism are treated in [41].

1.4 Literature about the subject

Quantum Field Theory on curved spacetimes is one of the most discussed and developed areas of theoretical physics. It has enormous literature, including numerous standard textbooks [8, 12, 50, 74]. At first glance, our paper may appear to be a review article, as it presents various facts and concepts from existing literature. Surprisingly, however, many of ideas of our paper seem to be clearly articulated here for the first time. Let us in particular mention:

- the description of the two operator-theoretic setups in Section 2 and Appendix A, which is a continuation of the works [39–41] of D. Siemssen and one of the authors (JD);
- the comparison of four different approaches to the Klein-Gordon equation on de Sitter space from Section 5, where we also present a list of new formulas e.g. for correlation functions between different states;
- the discussions of the "speciality condition" throughout all sections, which provides a useful tool for computations.

We start our review of the literature with the "classical propagators", that is, the retarded and advanced propagator, and the Pauli-Jordan function. They belong to standard knowledge and are well-studied in standard references. In the massless case on the flat $\mathbb{R}^{1,3}$ the retarded and advanced propagators are well known from classical electrodynamics, and are sometimes called the *Lienard-Wiechert potentials*. In the massive flat case their expressions in terms of Hankel functions are contained in many textbooks. The Cauchy problem of the wave equation on curved spacetimes was studied already by Hadamard [56], at least locally. A recent reference to this subject on arbitrary globally hyperbolic manifolds is the book by Bär, Ginoux and Pfäffle [9]. In the introduction to this book one reads: "Tracing back the references [on the uniqueness and existence of linear wave equation on lorentzian manifolds] one typically ends at unpublished lecture notes of Leray [65] or their exposition by Choquet-Bruhat [30]."

In the literature the Pauli-Jordan function is often called the commutator function or (recently, in the mathematics oriented literature) the causal propagator, [8, 50]. Note, however, that the latter name can lead to confusion: in [16] the Feynman propagator is called the causal Green function.

Propagators on the Minkowski space, including "non-classical" ones, are well-known from various textbooks on Quantum Field Theory (especially the old-fashioned ones). For instance, Appendix 2 of Bogoliubov–Shirkov [16] and Appendix C of Bjorken–Drell [13] contain expressions for these functions in the position space in the physical case of $\mathbb{R}^{1,3}$, and discuss conventions used by various authors.

"Non-classical" propagators are expectation values of products of two fields. Those without time-ordering, sometimes called Wightman functions, are ubiquitous in the mathematical literature, since they are needed to define the GNS representation and multiplication in appropriately defined local algebras. One of major questions, which is asked in various papers is whether they satisfy the Hadamard condition.

Expectation values of time-ordered fields, that is, Feynman propagators, are needed when we want to find scattering amplitudes. They often appear in the physics literature as mixed two-point functions, typically with the out-vacuum on the left and in-vacuum on the right. For instance, in Birrell-Davies [12] in (9.13) one finds the following definition of Green functions:

$$\tau(x_1, x_2 ... x_m) = \frac{\langle \mathrm{out}, 0 | T(\phi(x_1)\phi(x_2)...\phi(x_m)|0, \mathrm{in}\rangle}{\langle \mathrm{out}, 0|0, \mathrm{in}\rangle}. \tag{1.30}$$

Then the authors write: "...unlike the case of Minkowski space where $|0, \mathrm{out}\rangle = |0, \mathrm{in}\rangle$ (up to a phase factor), the vacuum $|0, \mathrm{in}\rangle$ in curved spacetime will not in general be stable: $\langle \mathrm{out}, 0|0, \mathrm{in}\rangle \neq 1$." In particular the relationship (1.25), which says that the "in-out Feynman propagator"G^{F}_{+-} coincides with the Feynman propagator formally computed in the path-integral approach (which can be interpreted as $G^{\mathrm{F}}_{\mathrm{op}}$) is implicitly contained in [12] (and in general in the physics literature). Elements of this philosophy are also found in [78, 79].

In the more recent rigorous literature, mixed (two-state) propagators are almost absent. The majority of recent works, for example the seminal papers [23, 61], emphasize the local point of view. Their usual goal is to construct a net of local algebras, for which it is enough to fix a single state, preferably Hadamard, which can be done locally.

A systematic rigorous study of various natural propagators on curved spacetimes was undertaken in the series of papers by one of the authors (JD) with a coauthor [39–41]. In particular, the construction of the distinguished Feynman propagator by methods of Krein spaces on an asymptotically stationary stable spacetimes is contained in [41]. A construction of the same Feynman propagator on a (more narrow) class of asymptotically Minkowskian spaces by methods of pseudodifferential calculus was given by Gérard and Wrochna [50, 54].

There exist many works, especially in the PDE literature, about *parametrices* of the Klein-Gordon equations, that is, inverses modulo a *smoothing operator*. A celebrated paper with this philosophy is the work by Duistermaat and Hörmander [44], which describes four natural parametrices: retarded, advanced, Feynman and anti-Feynman. Such parametrices are enough in the study of propagation of singularities, and they do not require a global knowledge of the spacetime. Anyway, most of the literature using parametrices seems restricted to retarded and advanced propagators. See e.g. [27, 28] where parametrices involving Fourier integral operators are used as approximations of exact retarded and advanced propagators.

Similarly, it is often argued in mathematical physics papers that it is enough to know a two-point function only up to a *smooth term*. This is sufficient if we want to prove the existence of renormalized powers of fields [23]. In our paper we are interested in *exact* Green functions and bisolutions, which are needed to compute scattering amplitudes exactly.

The usefulness of the setting of Krein spaces for the Klein-Gordon equation has been known for a long time [51, 52, 69, 70, 84, 85]. Note that in some of these papers the "Klein-Gordon operator" means the "generator of the Klein-Gordon evolution", denoted in our paper by $B(t)$. For us the "Klein-Gordon" operator is the operator on $L^2(M)$ whose resolvent appears in (1.23) and (1.24).

To our knowledge the above papers miss the relevance of the Krein setting for two-state Wightman functions and in-out Feynman propagators. This seems to have been noted only in [41].

The rigorous literature about the off-shell approach to the Klein-Gordon equation seems very scarce. To the papers about self-adjointness of Klein-Gordon operators mentioned above [41, 71, 72, 83], one could add [63] about pathological examples and [11] about the Wick rotation on a background of an ADM metric.

We will discuss the literature about the examples that we present in Sections 3, 4, 5 and 6 in the respective sections.

2 Propagators in curved spacetimes

2.1 Klein-Gordon equation

In this section we will describe how to generalize the well-known propagators from $\mathbb{R}^{1,d-1}$ to generic spacetimes.

Consider a Lorentzian manifold M of dimension d with *pseudometric tensor* $g_{\mu\nu}$. Define the *d'Alembertian*

$$\Box := |g|^{-\frac{1}{2}}\partial_\mu |g|^{\frac{1}{2}} g^{\mu\nu}\partial_\nu. \tag{2.1}$$

Note that we have

$$\Box = g^{\mu\nu}\nabla_\mu\nabla_\nu, \tag{2.2}$$

where the left ∇ is the covariant derivative on covectors, and the right ∇ on scalars (which coincides with the usual derivative ∂). We also define the *Klein-Gordon operator* $-\Box + Y(x)$, where $Y(x)$ is an x-dependent, real-valued *scalar potential*. Most of the time we will assume that $Y(x) = m^2$, so that the Klein-Gordon operator is $-\Box + m^2$.

Note that the d'Alembertian (2.1) acts on scalar functions. It is sometimes more convenient to replace it by the d'Alembertian in the half-density formalism, that is

$$\Box_{\frac12} := |g|^{\frac14}\Box|g|^{-\frac14} = |g|^{-\frac14}\partial_\mu|g|^{\frac12}g^{\mu\nu}\partial_\nu|g|^{-\frac14}. \tag{2.3}$$

In the half-density formalism the space $L^2(M, |g|^{\frac12})$ is replaced by $L^2(M)$, where we just take the Lebesgue measure with respect to given coordinates. We will write $\Box$ for $\Box_{\frac12}$ when it is clear from the context that we use the half-density formalism. See e.g. [41].

2.2 Green functions and bisolutions

Suppose that we have a continuous sesquilinear form

$$C_{\rm c}^\infty(M) \times C_{\rm c}^\infty(M) \ni (f_1, f_2) \mapsto (f_1|Af_2) \in \mathbb{C}. \tag{2.4}$$

By the Schwartz Kernel Theorem there exists a distribution $A(\cdot,\cdot)$ on $M \times M$, so that (2.4) in local coordinates can be written as

$$(f_1|Af_2) = \int\int \overline{f_1(x)}|g|^{\frac12}(x)A(x,y)|g|^{\frac12}(y)f_2(y)\mathrm{d}x\mathrm{d}y. \tag{2.5}$$

The distribution $A(\cdot,\cdot)$ will be called the *integral kernel of* A. Note that we use the integral notation for distributions and that we say "integral kernel" for $A(\cdot,\cdot)$ even if it is a distribution.

Actually, the above definition applies only to the scalar formalism. If we use the half-density formalism, then the integral kernel is different:

$$A_{\frac12}(x,y) := |g|^{\frac14}(x)A(x,y)|g|^{\frac14}(y). \tag{2.6}$$

For instance, the integral kernel of the identity is in local coordinates

$$\text{in the scalar formalism} \quad |g|^{-\frac12}(x)\delta(x-y), \tag{2.7}$$

$$\text{in the half-density formalism} \quad \delta(x-y). \tag{2.8}$$

The definition of a Green function (of the Klein-Gordon operator) will have also two versions. It is a distribution on $M \times M$ satisfying

$$\text{in the scalar formalism} \quad \big(-\Box + Y(x)\big)G_\bullet(x,y) = |g|^{-\frac12}(x)\delta(x-y), \tag{2.9}$$

$$\text{in the half-density formalism} \quad \big(-\Box_{\frac12} + Y(x)\big)G_{\bullet,\frac12}(x,y) = \delta(x-y), \tag{2.10}$$

and analogous conditions with x replaced by y. We also have similar definitions of bisolutions (of the Klein-Gordon operator), where the right hand sides of (2.9) and (2.10) are zero. One can pass from the scalar formalism to the half-density formalism as in (2.6):

$$G_{\bullet,\frac{1}{2}}(x,y) := |g|^{\frac{1}{4}}(x)G_\bullet(x,y)|g|^{\frac{1}{4}}(y). \tag{2.11}$$

2.3 Classical propagators

Suppose that M is globally hyperbolic. It is well-known [9] that there exist unique fundamental solutions $G^\vee(x,y)$ and $G^\wedge(x,y)$ of the Klein-Gordon equation which have future- respectively past-directed causal support:

$$\begin{aligned} (x,y) \in \operatorname{supp} G^\vee \quad &\Rightarrow \quad \exists \text{ future oriented causal curve from } y \text{ to } x, \\ (x,y) \in \operatorname{supp} G^\wedge \quad &\Rightarrow \quad \exists \text{ future oriented causal curve from } x \text{ to } y. \end{aligned} \tag{2.12}$$

$G^\vee(x,y)$ is called the *forward* (or *retarded*) *propagator*, $G^\wedge(x,y)$ is called the *backward* (or *advanced*) *propagator*. Their difference, which obviously is a bisolution of the Klein-Gordon equation, is called the *Pauli-Jordan propagator* (or *commutator function)*

$$G^{\mathrm{PJ}}(x,y) := G^\vee(x,y) - G^\wedge(x,y). \tag{2.13}$$

These three propagators are sometimes called jointly *classical propagators* [39, 41].

Identify M with $\mathbb{R} \times \Sigma$, where for $t \in \mathbb{R}$ the metric on $t \times \Sigma$ is Riemannian and ∂_t is timelike. Such an identification is always possible for globally hyperbolic manifolds. We will then say that we fixed a *time variable on M*. (We will discuss this in more detail in Subsection 3.2). Suppose that we can multiply the distribution $G^{\mathrm{PJ}}(x,y)$ by the discontinuous function $\theta(x^0 - y^0)$. Again in Subsection 3.2, we will see a rather general setting where this is rigorously allowed. Then we can retrieve the advanced and retarded Green functions from the Pauli-Jordan propagator:

$$G^\vee(x,y) = \theta(x^0 - y^0)G^{\mathrm{PJ}}(x,y), \tag{2.14}$$

$$G^\wedge(x,y) := -\theta(y^0 - x^0)G^{\mathrm{PJ}}(x,y). \tag{2.15}$$

2.4 Quantum fields and non-classical propagators

We still assume that M is globally hyperbolic. Consider a real scalar quantum field $\hat\phi(x) = \hat\phi(x)^*$ on M satisfying

$$\begin{aligned} \big(-\Box + Y(x)\big)\hat\phi(x) &= 0, \\ [\hat\phi(x), \hat\phi(y)] &= -\mathrm{i}G^{\mathrm{PJ}}(x,y)\mathbb{1}. \end{aligned} \tag{2.16}$$

More precisely, we assume some elements of the Wightman axioms: We suppose that $\mathcal{D}$ is a complex vector space equipped with a scalar product $(\cdot|\cdot)$ such that

$$C_{\mathrm{c}}^\infty(M) \ni f \mapsto \hat\phi[f] \tag{2.17}$$

is a distribution with values in linear operators from $\mathcal{D}$ to $\mathcal{D}$ satisfying

$$\hat{\phi}\big[\big(-\Box + Y(x)\big)f\big] = 0, \tag{2.18}$$

$$\big[\hat{\phi}[f_1], \hat{\phi}[f_2]\big] = -\mathrm{i}\int\int G^{\mathrm{PJ}}(x,y)f_1(x)f_2(y)\mathrm{d}x\mathrm{d}y, \tag{2.19}$$

$$(\hat{\phi}[\overline{f}]\Phi|\Psi) = (\Phi|\hat{\phi}[f]\Psi), \tag{2.20}$$

$$C_{\mathrm{c}}^{\infty}(M) \ni f \mapsto (\Phi|\hat{\phi}[f]\Psi) \text{ is continuous for } \Phi, \Psi \in \mathcal{D}. \tag{2.21}$$

(We do not require that $\mathcal{D}$ is complete).

Consider $\Omega_\alpha, \Omega_\beta \in \mathcal{D}$ with $\|\Omega_\alpha\| = \|\Omega_\beta\| = 1$ and $(\Omega_\alpha|\Omega_\beta) \neq 0$. By the Schwartz Kernel Theorem there exist distributions $G_{\alpha,\beta}^{(+)}(\cdot,\cdot)$ and $G_{\alpha,\beta}^{(-)}(\cdot,\cdot)$ on $M \times M$ such that

$$\int\int f_1(x)G_{\alpha,\beta}^{(+)}(x,y)f_2(y)\mathrm{d}x\mathrm{d}y = \frac{\big(\Omega_\alpha|\hat{\phi}[f_1]\hat{\phi}[f_2]\Omega_\beta\big)}{(\Omega_\alpha|\Omega_\beta)}, \tag{2.22}$$

$$\int\int f_1(x)G_{\alpha,\beta}^{(-)}(x,y)f_2(y)\mathrm{d}x\mathrm{d}y = \frac{\big(\Omega_\alpha|\hat{\phi}[f_2]\hat{\phi}[f_1]\Omega_\beta\big)}{(\Omega_\alpha|\Omega_\beta)}. \tag{2.23}$$

Note that both $G_{\alpha,\beta}^{(+)}$ and $G_{\alpha,\beta}^{(-)}$ are bisolutions and they satisfy

$$G_{\alpha,\beta}^{(+)} - G_{\alpha,\beta}^{(-)} = -\mathrm{i}G^{\mathrm{PJ}}. \tag{2.24}$$

In the special case $\Omega_\alpha = \Omega_\beta$ we will write

$$G_{\alpha}^{(+)} := G_{\alpha,\alpha}^{(+)}, \tag{2.25}$$

$$G_{\alpha}^{(-)} := G_{\alpha,\alpha}^{(-)}. \tag{2.26}$$

$\hat{\phi}[f]$ are called *smeared fields*. In the physics literature one introduce $\hat{\phi}(x)$, the *field at point* $x \in M$ and one writes

$$\hat{\phi}[f] = \int \hat{\phi}(x)f(x)\mathrm{d}x, \tag{2.27}$$

so that (2.25), (2.26), (2.22) and (2.23) are rigorous versions of the heuristic definitions (1.6), (1.7), (1.10), (1.11) from the introduction.

$G_{\alpha}^{(+)}$ and $G_{\alpha}^{(-)}$ are often called *Wightman*, resp. *anti-Wightman functions* (of the state given by Ω_α). $G_{\alpha,\beta}^{(+)}$ and $G_{\alpha,\beta}^{(-)}$ can be called *2-state Wightman*, resp. *anti-Wightman functions*.

Sometimes, it is also useful to consider the symmetric two-point function

$$G_{\alpha}^{\mathrm{sym}}(x,x') := G_{\alpha}^{(+)}(x,x') + G_{\alpha}^{(-)}(x,x'). \tag{2.28}$$

For $\Omega_\alpha, \Omega_\beta$ as above, we define the Feynman and anti-Feynman propagator assocated with Ω_α and Ω_β as follows:

$$G^{\mathrm{F}}_{\alpha,\beta} = \mathrm{i}G^{(+)}_{\alpha,\beta} + G^{\wedge} \tag{2.29}$$
$$= \mathrm{i}G^{(-)}_{\alpha,\beta} + G^{\vee}, \tag{2.30}$$
$$G^{\overline{\mathrm{F}}}_{\alpha,\beta} = -\mathrm{i}G^{(+)}_{\alpha,\beta} + G^{\vee} \tag{2.31}$$
$$= -\mathrm{i}G^{(-)}_{\alpha,\beta} + G^{\wedge}. \tag{2.32}$$

Note that the equalities (2.29)=(2.30) and (2.31)=(2.32) follow from the properties of the Pauli-Jordan propagator: (2.13) and (2.24). Obviously, $G^{\mathrm{F}}_{\alpha,\beta}$ and $G^{\overline{\mathrm{F}}}_{\alpha,\beta}$ are Green functions, being sums of bisolutions and Green functions.

In the special case $\Omega_\alpha = \Omega_\beta$ we will write

$$G^{\mathrm{F}}_{\alpha} := G^{\mathrm{F}}_{\alpha,\alpha}, \tag{2.33}$$
$$G^{\overline{\mathrm{F}}}_{\alpha} := G^{\overline{\mathrm{F}}}_{\alpha,\alpha}. \tag{2.34}$$

Suppose we fix a time variable x^0 on M. Then, using (2.13), (2.24), and (2.15) we can rewrite the definitions of the Feynman and anti-Feynman propagator in a way that is not manifestly rigorous, is however more symmetric and closer to the usual treatment in textbooks:

$$G^{\mathrm{F}}_{\alpha,\beta}(x,y) := \mathrm{i}\Big(\theta(x^0-y^0)G^{(+)}_{\alpha,\beta}(x,y) + \theta(y^0-x^0)G^{(-)}_{\alpha,\beta}(x,y)\Big), \tag{2.35}$$
$$G^{\overline{\mathrm{F}}}_{\alpha,\beta}(x,y) := -\mathrm{i}\Big(\theta(x^0-y^0)G^{(-)}_{\alpha,\beta}(x,y) + \theta(y^0-x^0)G^{(+)}_{\alpha,\beta}(x,y)\Big). \tag{2.36}$$

In the usuall textbook treatment one introduces the chronological and antichronological time ordering by

$$\mathrm{T}\left(\hat\phi(x)\hat\phi(y)\right) := \begin{cases} \hat\phi(x)\hat\phi(y), & x^0 > y^0, \\ \hat\phi(y)\hat\phi(x), & y^0 > x^0, \end{cases} \tag{2.37}$$
$$\overline{\mathrm{T}}\big(\hat\phi(x)\hat\phi(y)\big) := \begin{cases} \hat\phi(y)\hat\phi(x), & x^0 > y^0, \\ \hat\phi(x)\hat\phi(y), & y^0 > x^0. \end{cases} \tag{2.38}$$

This definition extends uniquely to $M \times M \setminus \{x = y\}$ because of the Einstein causality of the field $\hat\phi(x)$. Then one defines G^{F}_{α}, $G^{\overline{\mathrm{F}}}_{\alpha}$, $G^{\mathrm{F}}_{\alpha,\beta}$ and $G^{\overline{\mathrm{F}}}_{\alpha,\beta}$ as in (1.8), (1.9), (1.12) and (1.13) from the introduction. Note that this definition does not extend to the diagonal, unlike the definition that we gave in (2.29)—(2.32).

In order to express the dependence on Ω_α and Ω_β one may call $G^{(+)}_{\alpha,\beta}$ and $G^{\mathrm{F}}_{\alpha,\beta}$, the β-α-Wightman function and the β-α-Feynman propagator, respectively— see the explanation of the inversion of symbols in the paragraph following (1.13).

Let us summarize the identities involving the propagators:

$$G^{\mathrm{F}}_{\alpha,\beta} - G^{\overline{\mathrm{F}}}_{\alpha,\beta} = \mathrm{i}\Big(G^{(+)}_{\alpha,\beta} + G^{(-)}_{\alpha,\beta}\Big), \tag{2.39a}$$

$$G^{\mathrm{PJ}} = G^{\vee} - G^{\wedge} = \mathrm{i}\Big(G^{(+)}_{\alpha,\beta} - G^{(-)}_{\alpha,\beta}\Big), \tag{2.39b}$$

$$G^{\mathrm{F}}_{\alpha,\beta} = \mathrm{i}G^{(+)}_{\alpha,\beta} + G^{\wedge} = \mathrm{i}G^{(-)}_{\alpha,\beta} + G^{\vee}, \tag{2.39c}$$

$$G^{\overline{\mathrm{F}}}_{\alpha,\beta} = -\mathrm{i}G^{(+)}_{\alpha,\beta} + G^{\vee} = -\mathrm{i}G^{(-)}_{\alpha,\beta} + G^{\wedge}. \tag{2.39d}$$

Note that in this subsection Wightman and anti-Wightman 2-point functions, as well as Feynman and anti-Feynman Green functions involved arbitrary vectors Ω_α, Ω_β in a single represention of quantum fields. In most applications in these definitions one assumes that Ω_α, Ω_β are Fock vacua, that is, vectors that yield Fock representations. In the following subsection we will give a different definition of Feynman and anti-Feynman propagators. These definitions will be restricted to Fock vacua. They will be purely operator-theoretic and not make use of quantum fields. These new definitions will have one important advantage: they will work also if Ω_α and Ω_β do not belong to the same representation, and hence $(\Omega_\alpha|\Omega_\beta) = 0$ (which is actually quite common).

2.5 Klein-Gordon charge form

Let us now develop a mathematical formalism which will yield an alternative, more satisfactory definition of non-classical propagators. It will be based entirely on operator theory, without going through quantum fields.

For $\zeta, \xi \in C^\infty(M)$, set

$$\overline{\zeta(x)}\overset{\leftrightarrow}{\nabla}_\mu\xi(x) := \big(\nabla_\mu\overline{\zeta(x)}\big)\xi(x) - \overline{\zeta(x)}\nabla_\mu\xi(x). \tag{2.40}$$

Let $\mathcal{W}_{\mathrm{sc}}$ denote the space of smooth, space-compact solutions to the Klein-Gordon equation

$$\big(-\Box + Y(x)\big)\zeta(x) = 0. \tag{2.41}$$

Using (2.2) we see that if $\zeta, \xi \in \mathcal{W}_{\mathrm{sc}}$, then

$$J_\mu[\zeta,\xi](x) := \overline{\zeta(x)}\overset{\leftrightarrow}{\nabla}_\mu\xi(x) = \big(\nabla_\mu\overline{\zeta(x)}\big)\xi(x) - \overline{\zeta(x)}\nabla_\mu\xi(x) \tag{2.42}$$

is a covariantly conserved current, which means

$$|g|^{-\frac{1}{2}}\partial_\mu|g|^{\frac{1}{2}}g^{\mu\nu}J_\nu = \nabla_\mu J^\mu = 0. \tag{2.43}$$

Therefore,

$$(\zeta|\xi)_{\mathrm{KG}} := \mathrm{i}\int_\Sigma \overline{\zeta(x)}\overset{\leftrightarrow}{\nabla}_\mu\xi(x)\mathrm{d}\Sigma^\mu(x), \tag{2.44}$$

does not depend on the choice of the Cauchy surface Σ, where $\mathrm{d}\Sigma^\mu(x)$ is the natural measure on Σ times the future-directed normal vector. (2.44) is called the Klein-Gordon charge form.

The Klein-Gordon charge form is not positive definite. We can, however, usually extend the space $\mathcal{W}_{\rm sc}$ to a larger space, denoted $\mathcal{W}_{\rm KG}$, which admits a direct sum decomposition

$$\mathcal{W}_{\rm KG} = \mathcal{Z}_\alpha^{(+)} \oplus \mathcal{Z}_\alpha^{(-)}, \quad \mathcal{Z}_\alpha^{(+)} = \overline{\mathcal{Z}_\alpha^{(-)}}, \tag{2.45}$$

where the components are orthogonal with respect to $(\cdot|\cdot)_{\rm KG}$, $\mathcal{Z}_\alpha^{(+)}$ is positive and complete wrt $\sqrt{(\cdot|\cdot)_{\rm KG}}$, and $\mathcal{Z}_\alpha^{(-)}$ is negative and complete wrt $\sqrt{-(\cdot|\cdot)_{\rm KG}}$.

Every $\zeta \in \mathcal{W}_{\rm sc}$, decomposed according to (2.45) as

$$\zeta = \zeta_\alpha^{(+)} + \zeta_\alpha^{(-)}, \quad \zeta_\alpha^{(+)} = \overline{\zeta_\alpha^{(-)}}, \tag{2.46}$$

satisfies

$$\pm(\zeta_\alpha^{(\pm)}|\zeta_\alpha^{(\pm)})_{\rm KG} \geq 0, \quad (\zeta_\alpha^{(\pm)}|\zeta_\alpha^{(\mp)})_{\rm KG} = 0. \tag{2.47}$$

Thus

$$(\zeta|\xi)_{\rm KG} = (\zeta_\alpha^{(+)}|\xi_\alpha^{(+)})_{\rm KG} + (\zeta_\alpha^{(-)}|\xi_\alpha^{(-)})_{\rm KG}. \tag{2.48}$$

The index α indicates the decomposition (2.45). We also have a positive definite scalar product

$$(\zeta|\xi)_\alpha = (\zeta_\alpha^{(+)}|\xi_\alpha^{(+)})_{\rm KG} - (\zeta_\alpha^{(-)}|\xi_\alpha^{(-)})_{\rm KG}, \tag{2.49}$$

which is however less canonical than the Klein-Gordon charge form because it depends on the decomposition (2.45). Note that $\mathcal{W}_{\rm KG}$ is complete in the topology given by (2.49), and that $\mathcal{W}_{\rm sc}$ is dense in $\mathcal{W}_{\rm KG}$. Clearly, not all elements of $\mathcal{W}_{\rm KG}$ are space-compact, but they decay at an appropriate rate in spatial directions.

Mathematically, $\mathcal{W}_{\rm KG}$ has the structure of a *Krein space*. A decomposition (2.45) is an example of a *fundamental decomposition*, see Prop. A.24. We refer to Appendix A for a discussion of Krein spaces.

Let $\Pi_\alpha^{(\pm)}$ be the orthogonal projections onto $\mathcal{Z}_\alpha^{(\pm)}$. Denoting by $\mathcal{N}$ the nullspace and by $\mathcal{R}$ the range, we thus have

$$\begin{aligned}
&\mathcal{N}(\Pi_\alpha^{(\pm)}) = \mathcal{Z}_\alpha^{(\mp)}, \quad \mathcal{R}(\Pi_\alpha^{(\pm)}) = \mathcal{Z}_\alpha^{(\pm)}, \\
&\big(\Pi_\alpha^{(\pm)}\big)^2 = \Pi_\alpha^{(\pm)}, \quad \Pi_\alpha^{(\pm)}\Pi_\alpha^{(\mp)} = 0, \\
&\big(\Pi_\alpha^{(\pm)}\zeta|\Pi_\alpha^{(\pm)}\zeta)_{\rm KG} \gtrless 0, \quad \zeta \in \mathcal{W}_{\rm KG} \\
&\quad \big(\Pi_\alpha^{(\pm)}\zeta|\xi\big)_{\rm KG} = \big(\zeta|\Pi_\alpha^{(\pm)}\xi\big)_{\rm KG}, \quad \zeta, \xi \in \mathcal{W}_{\rm KG}.
\end{aligned} \tag{2.50}$$

It is important to note that there are many decompositions of the form (2.49) with properties as above leading to the same space $\mathcal{W}_{\mathrm{KG}}$. Note that $\mathcal{W}_{\mathrm{sc}}$ is uniquely defined and the Klein-Gordon charge $(\cdot|\cdot)_{\mathrm{KG}}$ on $\mathcal{W}_{\mathrm{sc}}$ is also unique. However, there can be more then one Krein structure extending $\big(\mathcal{W}_{\mathrm{sc}}, (\cdot|\cdot)_{\mathrm{KG}}\big)$. Clearly, specifying a fundamental decomposition fixes such a structure. We expect that in typical spacetimes all physically reasonable decompositions lead to the same $\mathcal{W}_{\mathrm{KG}}$.

2.6 Klein-Gordon kernels

If $\zeta \in \mathcal{W}_{\mathrm{sc}}$, and ξ is a distributional solution of the Klein-Gordon equation which is not necessarily space compact, then the current $J_\mu[\zeta, \xi]$ defined by (2.42) is a well-defined space-compact distribution that satisfies the relation (2.43). However, for such ζ, ξ the quantity (2.44) is problematic, because it is not clear what it means to integrate a distribution on a surface Σ. Let us describe an appropriate replacement of (2.44) in that case.

We first choose a time variable x^0. Let then $j \in C^\infty(\mathbb{R})$ be a real function such that $j(t) = 0$ for $t < -\frac{1}{2}$ and $j(t) = 1$, $t > \frac{1}{2}$. We have

$$\nabla_\mu\big(J^\mu(x)j(x^0)\big) = J^0(x)j'(x^0). \tag{2.51}$$

Therefore,

$$(\zeta|\xi)_{\mathrm{KG}} := \mathrm{i}\int \Big(\overline{\zeta(x)}\overset{\leftrightarrow}{\nabla}_{x^0}\xi(x)\Big)j'(x^0)|g(x)|^{\frac{1}{2}}\mathrm{d}x \tag{2.52}$$

is well-defined for distributional ξ and does not depend on the choice of the time variable x^0 and the function j. If ξ is regular enough, it coincides with (2.44).

Suppose now that $B(x, y)$ is a bisolution of the Klein-Gordon equation, which is sufficiently regular, say C^∞. Then it is easy to see that for $\zeta_1, \zeta_2 \in \mathcal{W}_{\mathrm{sc}}$, the integral

$$\mathrm{i}\int_{\Sigma_1}\int_{\Sigma_2} \zeta_1(x)\overset{\leftrightarrow}{\nabla}_{x^\mu}B(x, y)\overset{\leftrightarrow}{\nabla}_{y^\mu}\zeta_2(y)\mathrm{d}\Sigma_1^\mu(x)\mathrm{d}\Sigma_2^\mu(y). \tag{2.53}$$

does not depend on the choice of Cauchy surfaces Σ_1, Σ_2 and defines a sesquilinear form on $\mathcal{W}_{\mathrm{sc}}$. If this form is bounded, then it defines a unique operator B on $\mathcal{W}_{\mathrm{KG}}$. We then say that $B(\cdot, \cdot)$ is the *Klein-Gordon kernel* of the operator B.

For distributional Klein-Gordon kernels one needs a different definition:

Definition 2.1. Let $B(\cdot, \cdot)$ be a (distributional) bisolution. Choose a time variable x^0 on M (see Subsection 3.2). Let j_i, $i = 1, 2$ be two functions on $\mathbb{R}$ such that $j_i(t) = 0$ for $t < -\frac{1}{2}$ and $j_i(t) = 1$, $t > \frac{1}{2}$. Then for $\zeta_1, \zeta_2 \in \mathcal{W}_{\mathrm{sc}}$

$$\mathrm{i}\int\int j_1'(x^0)\Big(\zeta_1(x)\overset{\leftrightarrow}{\nabla}_{x^0}B(x, y)\overset{\leftrightarrow}{\nabla}_{y^0}\zeta_2(y)\Big)j_2'(y^0)|g(x)|^{\frac{1}{2}}\mathrm{d}x|g(y)|^{\frac{1}{2}}\mathrm{d}y \tag{2.54}$$

does not depend on the choice of the time variable and the functions j_1, j_2. It defines a bilinear form on $\mathcal{W}_{\mathrm{sc}}$. If this form corresponds to a bounded operator B on $\mathcal{W}_{\mathrm{sc}}$, then $B(\cdot, \cdot)$ will be called the *Klein-Gordon kernel of the operator* B.

Note that if $B(\cdot,\cdot)$ is sufficiently regular, then (2.54)=(2.53). An example of a Klein-Gordon kernel that usually is of distributional nature is the Pauli-Jordan bisolution $G^{\mathrm{PJ}}(x,y)$, which is the Klein-Gordon kernel of the identity.

Let us describe the physical meaning of a fundamental decomposition (2.45). Let $\pm G_\alpha^{(\pm)}(x,y)$ be the Klein-Gordon kernel of the projection $\Pi_\alpha^{(\pm)}$, so that the sum $G_\alpha^{\mathrm{sym}}(x,y) := G_\alpha^{(+)}(x,y) + G_\alpha^{(-)}(x,y)$ is the Klein-Gordon kernel of the involution $S_\alpha := \Pi_\alpha^{(+)} - \Pi_\alpha^{(-)}$. Then there exists a Fock representation with the Fock vacuum Ω_α such that $G_\alpha^{(\pm)}(x,y)$ are the corresponding two-point functions

$$G_\alpha^{(+)}(x,y) := \big(\Omega_\alpha|\hat\phi(x)\hat\phi(y)\Omega_\alpha\big), \tag{2.55}$$
$$G_\alpha^{(-)}(x,y) := \big(\Omega_\alpha|\hat\phi(y)\hat\phi(x)\Omega_\alpha\big). \tag{2.56}$$

Let $\mathcal{W}_{\mathrm{KG}} = \mathcal{Z}_\beta^{(+)} \oplus \mathcal{Z}_\beta^{(-)}$ be another orthogonal decomposition of the Krein space $\mathcal{W}_{\mathrm{KG}}$ into a maximal uniformly positive and maximal uniformly negative subspace, defining the vacuum Ω_β. One can show [41] (see also Appendix A) that the spaces $\mathcal{Z}_\beta^{(+)}$ and $\mathcal{Z}_\alpha^{(-)}$ are complementary, so that we have a (non-orthogonal) direct sum decomposition

$$\mathcal{W}_{\mathrm{KG}} = \mathcal{Z}_\beta^{(+)} \oplus \mathcal{Z}_\alpha^{(-)}. \tag{2.57}$$

Therefore, we can define projections $\Pi_{\alpha,\beta}^{(+)}$, $\Pi_{\alpha,\beta}^{(-)}$ corresponding to this decomposition. They satisfy

$$\begin{aligned} \mathcal{N}(\Pi_{\alpha,\beta}^{(+)}) = \mathcal{R}(\Pi_{\alpha,\beta}^{(-)}) &= \mathcal{Z}_\beta^{(-)}, \\ \mathcal{R}(\Pi_{\alpha,\beta}^{(+)}) = \mathcal{N}(\Pi_{\alpha,\beta}^{(-)}) &= \mathcal{Z}_\alpha^{(+)}, \\ \Pi_{\alpha,\beta}^{(+)} + \Pi_{\alpha,\beta}^{(-)} &= \mathbb{1}. \end{aligned} \tag{2.58}$$

We may also decompose $\mathcal{W}_{\mathrm{KG}}$ the other way around,

$$\mathcal{W}_{\mathrm{KG}} = \mathcal{Z}_\alpha^{(+)} \oplus \mathcal{Z}_\beta^{(-)}. \tag{2.59}$$

The corresponding projections are denoted $\Pi_{\beta,\alpha}^{(+)}$, $\Pi_{\beta,\alpha}^{(-)}$. Then one finds

$$\big(\Pi_{\alpha,\beta}^{(\pm)}\zeta|\xi\big)_{\mathrm{KG}} = \big(\zeta|\Pi_{\beta,\alpha}^{(\pm)}\xi\big)_{\mathrm{KG}}. \tag{2.60}$$

Thus, these projections are orthogonal if and only if $\mathcal{Z}_\alpha^{(+)} = \mathcal{Z}_\beta^{(+)}$.

Let R be a bounded linear transformation on $\mathcal{W}_{\mathrm{KG}}$. The Klein-Gordon Hermitian conjugate $R^{*\mathrm{KG}}$ of R is defined by

$$(R^{*\mathrm{KG}}\zeta|\xi)_{\mathrm{KG}} := (\zeta|R\xi)_{\mathrm{KG}}, \tag{2.61}$$

and the complex conjugate $\overline{R}$ by

$$\overline{R}\,\overline{\zeta} := \overline{R\zeta}. \tag{2.62}$$

Linear transformations that preserve the structure of $\mathcal{W}_{\rm KG}$ are called *symplectic*, or (especially in the physics literature) *Bogoliubov transformations*. Here, R preserving the structure of $\mathcal{W}_{\rm KG}$ means that R is *pseudounitary* and *real*, i.e.,

$$(R\zeta|R\xi)_{\rm KG} = (\zeta|\xi)_{\rm KG} \quad \text{and} \quad R\overline{\zeta} = \overline{R\zeta}, \tag{2.63}$$

or in other words $R^{*{\rm KG}} = R^{-1}$ and $\overline{R} = R$.

2.7 Mode expansions

Many papers about QFT on curved spacetimes do not mention the word "Krein space". Instead, they introduce a decomposition of solutions to the Klein-Gordon equation into a "positive frequency part" and a "negative frequency part". This is usually done through modes, by assuming that the classical field can be written as

$$\phi(x) = \int \big(\overline{\varphi_{\alpha,k}(x)}a_{\alpha,k} + \varphi_{\alpha,k}(x)a_{\alpha,k}^*\big)\mathrm{d}k, \tag{2.64}$$

where the mode functions $\varphi_{\alpha,k}$ and $\overline{\varphi_{\alpha,k}}$ should satisfy

$$\begin{aligned}\big(\varphi_{\alpha,k}|\varphi_{\alpha,k'}\big)_{\rm KG} = -\big(\overline{\varphi_{\alpha,k}}|\overline{\varphi_{\alpha,k'}}\big)_{\rm KG} &= -\delta(k,k'),\\ \big(\varphi_{\alpha,k}|\overline{\varphi_{\alpha,k'}}\big)_{\rm KG} &= 0,\\ (-\Box_g + Y(x))\varphi_{\alpha,k}(x) &= 0.\end{aligned} \tag{2.65}$$

The variable k (and the measure $\mathrm{d}k$) may be continuous or discrete (e.g. if the Cauchy surface is compact). In Minkowski space it usually coincides with the $d-1$-momentum, which is not available on a generic spacetime.

Let us try to interpret this in a more rigorous sense. Let us assume that K is a measure set. For the sake of definiteness we will assume that $K = \mathbb{R}^n$ with the Lebesgue measure $\mathrm{d}k$, but this is not relevant. Suppose that for any "wave packets" $f \in L^2(K)$, we can interpret

$$\int \overline{\varphi_{\alpha,k}}f(k)\mathrm{d}k \quad \text{and} \quad \int \varphi_{\alpha,k}f(k)\mathrm{d}k \tag{2.66}$$

in a rigorous sense as a solution to the Klein-Gordon equation. The functions

$$\int \overline{\varphi_{\alpha,k}}f_1(k)\mathrm{d}k + \int \varphi_{\alpha,k}\overline{f_2(k)}\mathrm{d}k \tag{2.67}$$

with $f_1, f_2 \in L^2(K)$ with the sesquilinear form defined by (2.65) form a Krein space.

Thus by introducing the modes satisfying (2.65) we automatically fix a Krein space. The positive/negative frequency modes span maximal uniformly positive/negative subspaces of this Krein space in the sense of "wave packets"–so we have a distinguished fundamental decomposition (and the corresponding Fock representation). Hence the idea of a Krein spaces is introduced in many papers “through the back door”.

After quantization, we obtain

$$\hat{\phi}(x) = \int \big(\overline{\varphi_{\alpha,k}(x)}\hat{a}_{\alpha,k} + \varphi_{\alpha,k}(x)\hat{a}^*_{\alpha,k}\big)\mathrm{d}k, \tag{2.68}$$
$$[\hat{a}_{\alpha,k}, \hat{a}^*_{\alpha,k'}] = \delta(k,k'), \quad [\hat{a}_{\alpha,k}, \hat{a}_{\alpha,k'}] = 0.$$

Then

$$G^{(+)}_{\alpha}(x,y) = \int \overline{\varphi_{\alpha,k}(x)}\varphi_{\alpha,k}(y)\mathrm{d}k, \tag{2.69}$$
$$G^{(-)}_{\alpha}(x,y) = \int \varphi_{\alpha,k}(x)\overline{\varphi_{\alpha,k}(y)}\mathrm{d}k.$$

Mode decompositions are convenient, because they allow us to represent operators on the Krein space in terms of integral kernels on $K \times K$. As an illustration, assume that we have another state Ω_β with a decomposition analogous to (2.68), whose modes generate the same Krein space $\mathcal{W}_{\mathrm{KG}}$ and use the same measure space K:

$$\phi(x) = \int \big(\overline{\varphi_{\beta,k}(x)}a_{\beta,k} + \varphi_{\beta,k}(x)a^*_{\beta,k}\big)\mathrm{d}k. \tag{2.70}$$

Assume further, that the two decompositions are related by a Bogoliubov transformation

$$\varphi_{\beta,k}(x) = N(k)\varphi_{\alpha,k}(x) + \int \Lambda(k,k')\overline{\varphi_{\alpha,k'}(x)}\mathrm{d}k'. \tag{2.71}$$

The pseudounitarity of (2.71) is equivalent to

$$N(k')\Lambda(k,k') = \Lambda(k',k)N(k), \tag{2.72}$$
$$\int \overline{\Lambda(k,p)}\Lambda(k',p)\mathrm{d}p = \big(|N(k)|^2 - 1\big)\delta(k-k').$$

Therefore, the transformation inverse to (2.71) is

$$\varphi_{\alpha,k}(x) = \overline{N(k)}\varphi_{\beta,k}(x) - \int \Lambda(k',k)\overline{\varphi_{\beta,k'}(x)}\mathrm{d}k'. \tag{2.73}$$

On the level of $a_{\alpha,k}$ and $a_{\beta,k}$, or their quantized versions, we have

$$\hat{a}_{\beta,k} = N(k)\hat{a}_{\alpha,k} - \int \Lambda(k',k)\hat{a}^*_{\alpha,k'}\mathrm{d}k', \tag{2.74}$$

$$\hat{a}_{\alpha,k} = \overline{N(k)}\hat{a}_{\beta,k} + \int \Lambda(k,k')\hat{a}^*_{\beta,k'}\mathrm{d}k'. \tag{2.75}$$

Thus, the fields can be written as

$$\hat{\phi}(x) = \int \bigg(\varphi_{\alpha,k}(x) \hat{a}^*_{\alpha,k} + \frac{\overline{\varphi_{\alpha,k}(x)}}{N(k)} \int \Lambda(k',k) \hat{a}^*_{\alpha,k'} \mathrm{d}k' + \frac{\overline{\varphi_{\alpha,k}(x)}}{N(k)} \hat{a}_{\beta,k} \bigg) \mathrm{d}k \tag{2.76}$$

$$= \int \bigg(\overline{\varphi_{\beta,k}(x)} \hat{a}_{\beta,k} - \frac{\varphi_{\beta,k}(x)}{N(k)} \int \overline{\Lambda(k,k')} \hat{a}_{\beta,k'} \mathrm{d}k' + \frac{\varphi_{\beta,k}(x)}{N(k)} \hat{a}^*_{\alpha,k} \bigg) \mathrm{d}k. \tag{2.77}$$

We insert into (1.10) and (1.11) the expression (2.76) as the left field and (2.77) as the right field. Then, moving $\hat{a}^*_{\alpha,k}$ to the left and $\hat{a}_{\beta,k}$ to the right and using $[\hat{a}_{\beta,k}, \hat{a}^*_{\alpha,k'}] = N(k)\delta(k-k')$, we obtain

$$G^{(+)}_{\alpha\beta}(x,y) = \int \frac{1}{N(k)} \overline{\varphi_{\alpha,k}(x)} \varphi_{\beta,k}(y) \mathrm{d}k, \tag{2.78}$$

$$G^{(-)}_{\alpha\beta}(x,y) = \int \frac{1}{N(k)} \overline{\varphi_{\alpha,k}(y)} \varphi_{\beta,k}(x) \mathrm{d}k.$$

2.8 Operator-theoretic (anti-)Feynman propagator

The d'Alembertian $-\Box$ on a Lorentzian manifold M with pseudometric g, in the half-density formalism given by (2.3), is Hermitian (symmetric) on $C_{\mathrm{c}}^\infty(M)$ in the sense of $L^2\big(M\big)$. The same is true for the Klein-Gordon operator $-\Box + Y(x)$ with a real potential Y. Assume that $-\Box + Y(x)$ is *essentially self-adjoint* (if not, we may choose a self-adjoint extension).

Then its resolvent $G(z) := (-\Box + Y(x) - z)^{-1}$ is well-defined for $z \in \mathbb{C} \setminus \mathbb{R}$. It possesses an integral kernel $G(z; x, y)$. Suppose that there exists

$$G^{\mathrm{F}}_{\mathrm{op}}(x,y) := \lim_{\epsilon \searrow 0} G(+\mathrm{i}\epsilon; x, y), \tag{2.79}$$

$$G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,y) := \lim_{\epsilon \searrow 0} G(-\mathrm{i}\epsilon; x, y), \tag{2.80}$$

where we use the distributional limit. The distributions $G^{\mathrm{F}}_{\mathrm{op}}(x,x')$ and $G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,x')$ will be called the *operator-theoretic Feynman and anti-Feynman propagator*.

We expect that the limits (2.79) and (2.80) exist on most physically interesting globally hyperbolic manifolds without boundaries. They will not exist at the point spectrum of $-\Box + Y(x)$ (which is probably quite rare).

We believe that the following argument justifies this definition. Here is an elementary fact about *Fresnel integrals*. Let c be a real symmetric $n \times n$ matrix, u a variable in $\mathbb{R}^n$ and $J \in \mathbb{R}^n$. Then

$$\frac{\int \mathrm{e}^{\pm\mathrm{i}(u^{\mathrm{T}} \frac{c}{2} u + J^{\mathrm{T}} u)} \mathrm{d}u}{\int \mathrm{e}^{\pm\mathrm{i}u^{\mathrm{T}} \frac{c}{2} u} \mathrm{d}u} = \exp\Big(\mp \frac{\mathrm{i}}{2} J^{\mathrm{T}} (c \pm \mathrm{i}0)^{-1} J \Big). \tag{2.81}$$

If we use *path integrals* to construct a quantum field theory, we usually start from defining formally the generating function as

$$Z(J) := \frac{\int \mathrm{e}^{\mathrm{i}S(\phi) + \mathrm{i}\int \phi(x) J(x) \mathrm{d}x} \mathcal{D}\phi}{\int \mathrm{e}^{\mathrm{i}S(\phi)} \mathcal{D}\phi}.$$

If the action is *quadratic*

$$\begin{aligned}S(\phi)=&-\frac{1}{2}\int\big(g^{\mu\nu}(x)\partial_\mu\phi(x)\partial_\nu\phi(x)+m^2\phi(x)^2\big)\sqrt{|g|}(x)\mathrm{d}x\\=&-\frac{1}{2}\big(\phi|(-\Box+m^2)\phi\big),\end{aligned}$$

then the path integral by analogy to (2.81) can be *rigorously defined* as

$$\begin{aligned}Z(J)&=\exp\frac{\mathrm{i}}{2}\big(J|(-\Box+m^2-\mathrm{i}0)^{-1}J\big)\\&=\exp\Big(\frac{\mathrm{i}}{2}\int\int J(x)G_{\mathrm{op}}^{\mathrm{F}}(x,y)J(y)\sqrt{|g|}(x)\sqrt{|g|}(y)\mathrm{d}x\mathrm{d}y\Big).\end{aligned}$$

Spacetimes where the d'Alembertian is essentially self-adjoint include stationary spacetimes, Friedmann-Lemaître-Robertson-Walker (FLRW) spacetimes, $1+0$-dimensional spacetimes, de Sitter and the universal cover of the anti-de Sitter space. Essential self-adjointness was also recently proven on a class of asymptotically Minkowski spacetimes [71, 83]. However, even on well-behaved spacetimes, essential self-adjointness is not always true [63].

Remark 2.2. Essential self-adjointness is typically destroyed if there are boundaries. The problem with boundaries with spacelike normal vectors can sometimes be cured by imposing boundary conditions—we will see this in Section 6 about the universal cover of the anti-de Sitter space. Boundaries with timelike normal vectors are different. In particular, if the time is confined to an interval $]a,b[$ instead of $\mathbb{R}$, then self-adjoint realizations of the Klein-Gordon operators do not lead to physically justified Feynman propagators. Instead, one should consider other types of non-self-adjoint boundary conditions, as explained in [41].

Remark 2.3. There exists a well-developed theory of limits of the resolvents of the Schrödinger operators $H:=-\Delta+V(x)$ on $\mathbb{R}^d$. More precisely, if V is a decaying potential on $\mathbb{R}^d$ satisfying appropriate conditions, $E\neq 0$ is away from the spectrum of H and $s>\frac{1}{2}$, then the following strong operator limit exists:

$$\lim_{\epsilon\searrow 0}(1+|x|)^{-s}\big(H-E\pm\mathrm{i}\epsilon\big)^{-1}(1+|x|)^{-s}. \tag{2.82}$$

The existence of (2.82) goes under the name of Limiting Absorption Principle. The most powerful method to prove this is the so-called Mourre theory, and is treated e.g. in [5, 33]. Obviously, the Limiting Absorption Principle implies the existence of the integral kernel of $\big(H-E\pm\mathrm{i}0\big)^{-1}$.

One can try to apply similar methods to Klein-Gordon operators, as shown in [71, 83].

2.9 Special Klein-Gordon equations

Definition 2.4. Suppose that the Klein-Gordon operator $-\Box+Y(x)$ on a Lorentzian manifold M is essentially self-adjoint. We say that $-\Box+Y(x)$ is *special* if the sum

$$G_{\mathrm{op}}^{\mathrm{F}}(x,x')+G_{\mathrm{op}}^{\overline{\mathrm{F}}}(x,x') \tag{2.83}$$

has causal support.

Definition 2.5. Suppose that the Klein-Gordon operator $-\Box+Y(x)$ is essentially self-adjoint and M is globally hyperbolic. We say that it is *strongly special* if

$$G^{\rm F}_{\rm op}(x,x')+G^{\overline{\rm F}}_{\rm op}(x,x')=G^{\vee}(x,x')+G^{\wedge}(x,x'). \tag{2.84}$$

Clearly, strong specialty implies specialty. We expect that under broad conditions the converse is also true.

Special Klein-Gordon operators are interesting because the associated propagators can be determined in an easy way. Indeed, it is often not very difficult to compute $G^{\rm F}_{\rm op}(x,x')$ and $G^{\overline{\rm F}}_{\rm op}(x,x')$. After all, there are various techniques to compute the kernel of the resolvent of a differential operator. From these, one can determine the retarded and advanced propagators by

$$G^{\vee/\wedge}(x,x')=\theta\big(\pm(x^0-x'^0)\big)\Big(G^{\rm F}_{\rm op}(x,x')+G^{\overline{\rm F}}_{\rm op}(x,x')\Big) \tag{2.85}$$

as well as the Pauli-Jordan function $G^{\rm PJ}=G^{\vee}-G^{\wedge}$.

Strictly speaking, (2.85) is not fully legal, because it involves multiplying a distribution by a discontinuous function $\theta\big(\pm(x^0-x'^0)\big)$. In practice, we expect that this obstacle can be overcome, see [42]. In particular, there is no problem with the multiplication with the theta function when we can apply the method of evolution equations, see Subsect. 3.2.

More interestingly, there is a natural candidate for the Wightman and anti-Wightman two-point function of a distinguished state:

$$G^{(\pm)}:=-{\rm i}\big(G^{\rm F}_{\rm op}-G^{\wedge/\vee}\big)={\rm i}\big(G^{\overline{\rm F}}_{\rm op}-G^{\vee/\wedge}\big). \tag{2.86}$$

Remark 2.6. Actually, we do not know if $G^{(\pm)}$ defined by (2.86) in the case when $-\Box+Y(x)$ is special always satisfy the positivity requirement — in all cases that we worked out they do.

3 Stationary and asymptotically stationary spaces

3.1 Propagators on stationary spacetimes

Assume that $M=\mathbb{R}\times\Sigma$, with the variables typically denoted by $(t,\mathbf{x})$, and sometimes $(s,\mathbf{y})$. Suppose that neither $g_{\alpha\beta}$ nor Y depends on time t, the time slices $\{t\}\times\Sigma$ are spacelike and ∂_t is timelike. Such spacetimes are called *stationary*.

In addition, we will assume that the spacetime is *static*, i.e. there are no time-position cross-terms. This is not a necessary condition for the present analysis, however for static spacetimes many formulas are more explicit. In other words, we assume that the metric is

$$-\alpha^2(\mathbf{x}){\rm d}t^2+h_{ij}(\mathbf{x}){\rm d}\mathbf{x}^i{\rm d}\mathbf{x}^j. \tag{3.1}$$

Here and in the following, Latin indices run over the spatial directions. We write $|h|$ for $\det h$. The Klein-Gordon operator in the half-density formalism is

$$-\Box + Y(\mathbf{x}) = \frac{1}{\alpha^2}\partial_t^2 - \alpha^{-\frac{1}{2}}\, |h|^{-\frac{1}{4}} \partial_i \alpha\, |h|^{\frac{1}{2}} h^{ij} \partial_j\, \alpha^{-\frac{1}{2}}\, |h|^{-\frac{1}{4}} + Y. \tag{3.2}$$

It is convenient to replace (3.2) by

$$-\tilde{\Box} + \tilde{Y} := \alpha\big(-\Box + Y\big)\alpha = \partial_t^2 + L, \tag{3.3}$$

where

$$\begin{aligned} L &:= -\Delta_{\tilde{h}} + \tilde{Y}, \quad \Delta_{\tilde{h}} := \gamma^{-\frac{1}{2}} \partial_i \gamma \tilde{h}^{ij} \partial_j \gamma^{-\frac{1}{2}}, \\ \tilde{h}_{ij} &:= \frac{1}{\alpha^2} h_{ij}, \quad [\tilde{h}^{ij}] = [\tilde{h}_{ij}]^{-1}, \quad \gamma := \frac{|h|^{\frac{1}{2}}}{\alpha}, \quad \tilde{Y} = \alpha^2 Y. \end{aligned} \tag{3.4}$$

Note that

$$\text{if } \tilde{u} \text{ solves } (-\tilde{\Box} + \tilde{Y})\tilde{u} = 0, \text{ then } u := \alpha\tilde{u} \text{ solves } (-\Box + Y)u = 0. \tag{3.5}$$

Let us first describe the approach based on the evolution of Cauchy data, which is particularly simple for static spacetimes. The equation (3.5) for $\tilde{u}(t) = \tilde{u}(t, \mathbf{x})$ can be rewritten as a 1st order equation for the Cauchy data

$$\big(\partial_t + \mathrm{i}B\big)w = 0, \tag{3.6}$$

$$B := \begin{bmatrix} 0 & \mathbb{1} \\ L & 0 \end{bmatrix}, \qquad w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} := \begin{bmatrix} \tilde{u} \\ \mathrm{i}\partial_t \tilde{u} \end{bmatrix}. \tag{3.7}$$

Assume that L is positive and self-adjoint in the sense of $L^2(\Sigma)$. We assume that 0 is not an eigenvalue of L and endow the space of Cauchy data with the (positive) scalar product

$$(w|v)_0 := (w_1|\sqrt{L}v_1) + \big(w_2|\tfrac{1}{\sqrt{L}}v_2\big). \tag{3.8}$$

The completion of $\mathcal{W}_{\mathrm{sc}}$ with respect to this scalar product will be denoted $\mathcal{W}_0$. Note that B can be interpreted as self-adjoint with respect to this scalar product:

$$(Bw|v)_0 = (w|Bv)_0 = (w_2|\sqrt{L}v_1) + (w_1|\sqrt{L}v_2). \tag{3.9}$$

The space $\mathcal{W}_0$ is also endowed with the (indefinite) Klein-Gordon charge form

$$(w|v)_{\mathrm{KG}} = (w|Qv)_0 := (w_1|v_2) + (w_2|v_1), \quad Q = \begin{bmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{bmatrix}. \tag{3.10}$$

Thus $\mathcal{W}_0$ is a Krein space with a distinguished Hilbert space structure.

We can compute the evolution operator and the spectral projection of B onto the positive and negative part of the spectrum:

$$\mathrm{e}^{-\mathrm{i}tB} := \begin{bmatrix} \cos t\sqrt{L} & -\mathrm{i}\frac{\sin t\sqrt{L}}{\sqrt{L}} \\ -\mathrm{i}\sqrt{L}\sin t\sqrt{L} & \cos t\sqrt{L} \end{bmatrix}, \tag{3.11}$$

$$\Pi^{(\pm)} := \mathbb{1}_{\mathbb{R}_+}(\pm B) = \frac{1}{2}\begin{bmatrix} \mathbb{1} & \pm\frac{\mathbb{1}}{\sqrt{L}} \\ \pm\sqrt{L} & \mathbb{1} \end{bmatrix}. \tag{3.12}$$

Note that the evolution $\mathrm{e}^{-\mathrm{i}tB}$ preserves the Klein-Gordon charge form (3.10). $\mathcal{R}(\Pi^{(\pm)})$ are maximal uniformly positive/negative subspaces with respect to the Klein-Gordon charge form. Then we can define the propagators on the level of the Cauchy data as follows:

$$\begin{aligned} E^{\mathrm{PJ}}(t,s) &:= \mathrm{e}^{-\mathrm{i}(t-s)B}, \\ E^{\vee/\wedge}(t,s) &:= \pm\theta\big(\pm(t-s)\big)\mathrm{e}^{-\mathrm{i}(t-s)B}, \\ E^{(\pm)}(t,s) &:= \mathrm{e}^{-\mathrm{i}(t-s)B}\Pi^{(\pm)}, \\ E^{\mathrm{F}/\overline{\mathrm{F}}}(t,s) &:= \mathrm{e}^{-\mathrm{i}(t-s)B}\big(\theta(t-s)\Pi^{(\pm)} - \theta(s-t)\Pi^{(\mp)}\big). \end{aligned}$$

At least formally, $E^{\vee}, E^{\wedge}, E^{\mathrm{F}}, E^{\overline{\mathrm{F}}}$ are inverses and $E^{\mathrm{PJ}}, E^{(+)}, E^{(-)}$ are bisolutions of $\partial_t + \mathrm{i}B$. They are 2×2 matrices:

$$E^{\bullet}(t,s) = \begin{bmatrix} E^{\bullet}_{11}(t,s) & E^{\bullet}_{12}(t,s) \\ E^{\bullet}_{21}(t,s) & E^{\bullet}_{22}(t,s) \end{bmatrix}.$$

We set

$$\begin{aligned} G^{\bullet} &:= \mathrm{i}\alpha E^{\bullet}_{12}\alpha, \quad \bullet = \mathrm{PJ}, \vee, \wedge, \mathrm{F}, \overline{\mathrm{F}}, \\ G^{(\pm)} &:= \pm\alpha E^{(\pm)}_{12}\alpha, \end{aligned} \tag{3.13}$$

obtaining propagators for a general static stable case. Thus

$$G^{\mathrm{PJ}}(t,\mathbf{x};s,\mathbf{y}) = \alpha(\mathbf{x})\frac{\sin(t-s)\sqrt{L}}{\sqrt{L}}(\mathbf{x},\mathbf{y})\alpha(\mathbf{y}), \tag{3.14}$$

$$G^{\vee/\wedge}(t,\mathbf{x};s,\mathbf{y}) = \pm\theta\big(\pm(t-s)\big)\alpha(\mathbf{x})\frac{\sin(t-s)\sqrt{L}}{\sqrt{L}}(\mathbf{x},\mathbf{y})\alpha(\mathbf{y}), \tag{3.15}$$

$$G^{(\pm)}(t,\mathbf{x};s,\mathbf{y}) = \alpha(\mathbf{x})\frac{\mathrm{e}^{\mp\mathrm{i}(t-s)\sqrt{L}}}{2\sqrt{L}}(\mathbf{x},\mathbf{y})\alpha(\mathbf{y}), \tag{3.16}$$

$$G^{\mathrm{F}/\overline{\mathrm{F}}}(t,\mathbf{x};s,\mathbf{y}) = \pm\mathrm{i}\alpha(\mathbf{x})\left(\theta(t-s)\frac{\mathrm{e}^{\mp\mathrm{i}(t-s)\sqrt{L}}}{2\sqrt{L}} + \theta(s-t)\frac{\mathrm{e}^{\pm\mathrm{i}(t-s)\sqrt{L}}}{2\sqrt{L}}\right)(\mathbf{x},\mathbf{y})\alpha(\mathbf{y}). \tag{3.17}$$

Note that all the identities (2.39) hold, where we tacitly assume that $\Omega_\alpha = \Omega_\beta$ corresponds to the natural state given by the fundamental decomposition (3.12). In this setting, the Wightman function is often called the *positive frequency bisolution*, and the anti-Wightman function the *negative frequency bisolution*, since they are obtained from the spectral decomposition of the generator of the dynamics into positive and negative frequencies.

Note also that the specialty condition is true:

$$G^{\mathrm{F}} + G^{\overline{\mathrm{F}}} = G^{\vee} + G^{\wedge}. \tag{3.18}$$

Let us describe now the approach based on the Hilbert space $L^2(M)$. We assume that L is essentially self-adjoint on $C_{\mathrm{c}}^{\infty}(\Sigma)$ in the sense of $L^2(\Sigma)$. Then it is easy to see $\partial_t^2 + L$ is essentially self-adjoint on $C_{\mathrm{c}}^{\infty}(M)$ in the sense of $L^2(M)$. Assume that for some $0 < c, C$ we have $c \leq \alpha(\mathbf{x}) \leq C$. Then $\alpha(\mathbf{x})$ is bounded invertible operator on $L^2(M)$, and using this we can show that $-\Box + Y(\mathbf{x})$ is essentially self-adjoint on $\alpha(\mathbf{x})C_{\mathrm{c}}^{\infty}(M)$. As proven in [39], under some minor additional technical conditions we can then define $G_{\mathrm{op}}^{\mathrm{F}}$ and $G_{\mathrm{op}}^{\overline{\mathrm{F}}}$, and they coincide with G^{F} and $G^{\overline{\mathrm{F}}}$ computed from the evolution equation.

Note that the stability condition $L \geq 0$ was an important ingredient of the analysis based on the evolution equation. Suppose now that L is not positive, but only self-adjoint, which can be called the *tachyonic case*. In the tachyonic case, we do not have the distinguished scalar product (3.8). The formulas (3.14) and (3.15) for the classical propagators $G^{\mathrm{PJ}}, G^{\vee}, G^{\wedge}$ are still true. However, the evolution approach does not allow us to define $G^{(\pm)}$, G^{F} or $G^{\overline{\mathrm{F}}}$. The operator-theoretic $G_{\mathrm{op}}^{\mathrm{F}}$ or $G_{\mathrm{op}}^{\overline{\mathrm{F}}}$, defined as usual by (2.79) and (2.80), will often exist. However, they will not be given by the formula (3.17). The specialty condition (3.18) is no longer true in the tachyonic case.

For instance, in the Minkowski space, with $Y(x) = m^2 < 0$, $G_{\mathrm{op}}^{\mathrm{F}}$ and $G_{\mathrm{op}}^{\overline{\mathrm{F}}}$ are well-behaved tempered distributions while the forward and backward propagators have exponential growth as $t \to \pm\infty$ inside the forward, resp. backward cone. A detailed discussion can for example be found in [42].

3.2 Classical propagators from evolution equations

Let us now consider a generic (not necessarily stationary) globally hyperbolic spacetime M. In order to compute non-classical (actually, also classical) propagators, it is useful to convert the Klein–Gordon equation into a 1st order evolution equation on the phase space describing Cauchy data. To this end, we fix a decomposition $M =]t_-, t_+[\times \Sigma$, where $-\infty \leq t_- < t_+ \leq +\infty$. We assume that $\{t\} \times \Sigma$ is Riemannian for all $t \in]t_-, t_+[$ and ∂_t is always timelike. We will use Latin letters for spatial indices. We introduce

$$\begin{aligned} h = [h_{ij}] = [g_{ij}], &\quad h^{-1} = [h^{ij}], \\ \beta^j := g_{0i}h^{ij}, &\quad \alpha^2 := g_{0i}h^{ij}g_{j0} - g_{00}, \\ |h| = |\det h| = \det h, &\quad |g| = |\det g|. \end{aligned}$$

We assume that $[h_{ij}]$, and hence also $[h^{ij}]$, are positive definite and $\alpha^2 > 0$. In coordinates, the metric can be written as

$$g_{\mu\nu}\mathrm{d}x^\mu\mathrm{d}x^\nu = -\alpha^2\mathrm{d}t^2 + h_{ij}(\mathrm{d}x^i + \beta^i\mathrm{d}t)(\mathrm{d}x^j + \beta^j\mathrm{d}t), \tag{3.19}$$

We have $|g| = \alpha^2|h|$. (3.19) is sometimes called a *metric in the ADM form*, for Arnowitt, Deser and Misner [11].

Y is a real valued function on M. To be on the safe side, let us assume assume that Y is smooth (which actually is not needed for the existence of various propagators). The Klein–Gordon operator in the half-density formalism can now be written

$$\begin{aligned}-\Box + Y(x) = {} & |g|^{-\frac14}(\partial_t - \partial_i\beta^i)\frac{|g|^{\frac12}}{\alpha^2}(\partial_t - \beta^j\partial_j)|g|^{-\frac14} \\ & - |g|^{-\frac14}\partial_i|g|^{\frac12}h^{ij}\partial_j|g|^{-\frac14} + Y.\end{aligned}$$

Instead of the operator $\Box$ on $L^2(M)$, it is more convenient to work with the operator

$$\tilde{\Box} := \alpha\Box\alpha.$$

We have

$$\begin{aligned}-\tilde{\Box} + \alpha^2 Y &= \gamma^{-\frac12}(\partial_t - \partial_i\beta^i)\gamma(\partial_t - \beta^j\partial_j)\gamma^{-\frac12} \\ &\quad - \gamma^{-\frac12}\partial_i\alpha^2\gamma h^{ij}\partial_j\gamma^{-\frac12} + \alpha^2 Y \\ &= (\partial_t + \mathrm{i}W^*)(\partial_t + \mathrm{i}W) + L,\end{aligned}$$

where we introduced

$$\begin{aligned}\gamma &:= \alpha^{-2}|g|^{\frac12} = \alpha^{-1}|h|^{\frac12}, \\ W &:= \frac{\mathrm{i}}{2}\gamma^{-1}\gamma_{,t} + \mathrm{i}\gamma^{\frac12}\beta^i\partial_i\gamma^{-\frac12}, \\ L &:= -\partial_i^{\gamma *}\tilde{h}^{ij}\partial_j^{\gamma} + \tilde{Y},\end{aligned}$$

and we use the shorthands

$$\tilde{h}^{ij} := \alpha^2 h^{ij}, \quad \tilde{Y} := \alpha^2 Y, \quad \partial_i^\gamma := \gamma^{\frac12}\partial_i\gamma^{-\frac12}, \quad \gamma_{,t} := \partial_t\gamma.$$

Clearly, (3.5) is still true, and hence propagators for $\tilde{\Box}$ induce corresponding propagators for $\Box$.

For each $t \in \mathbb{R}$, we define

$$B(t) = \begin{bmatrix} B_{11}(t) & B_{12}(t) \\ B_{21}(t) & B_{22}(t)\end{bmatrix} := \begin{bmatrix} W(t) & \mathbb{1} \\ L(t) & W(t)^*\end{bmatrix}. \tag{3.20}$$

Setting $w_1(t) = \tilde{u}(t)$ and $w_2(t) = (\mathrm{i}\partial_t - W(t))\tilde{u}(t)$, we find that

$$\big(\partial_t + \mathrm{i}B(t)\big)\begin{bmatrix} w_1(t) \\ w_2(t) \end{bmatrix} = 0 \tag{3.21}$$

if and only if $\tilde{u}$ is a solution of the Klein-Gordon equation $\tilde{\Box}\tilde{u} = 0$. Therefore we occasionally call $\partial_t + \mathrm{i}B(t)$ the *first-order Klein–Gordon operator*. The half-densities $w_1(t)$ and $w_2(t)$ may be called the *Cauchy data* for $\tilde{u}$ at time t.

It is natural to introduce the *classical Hamiltonian*

$$H(t) = QB(t) = \begin{bmatrix} L(t) & W^*(t) \\ W(t) & \mathbb{1} \end{bmatrix}, \qquad Q = \begin{bmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{bmatrix}.$$

The operator $L(t)$ is a Hermitian operator on $C_\mathrm{c}^\infty(\Sigma)$ in the sense of the Hilbert space $L^2(\Sigma)$ and $H(t)$ is Hermitian on $C_\mathrm{c}^\infty(\Sigma) \oplus C_\mathrm{c}^\infty(\Sigma)$ in the sense of $L^2(\Sigma) \oplus L^2(\Sigma)$.

We would like to apply the theory of non-autonomous evolution equations due mostly to Kato and described in detail in Appendix C of [40]. The space of Cauchy data $C_\mathrm{c}^\infty(\Sigma) \oplus C_\mathrm{c}^\infty(\Sigma)$ has a natural indefinite Klein-Gordon form

$$(w|v)_{\mathrm{KG}} = (w|Qv) := (w_1|v_2) + (w_2|v_1). \tag{3.22}$$

However, we will need also a positive scalar product. To this end we fix an appropriate positive operator L on $L^2(\Sigma)$ with $\mathcal{N}(L) = 0$ and introduce the scalar product on the Cauchy data

$$(w|v)_L := (w_1|\sqrt{L}v_1) + \big(w_2\big|\tfrac{1}{\sqrt{L}}v_2\big). \tag{3.23}$$

The Krein space given by the completion of $C_\mathrm{c}^\infty(\Sigma) \oplus C_\mathrm{c}^\infty(\Sigma)$ in the scalar product (3.23) will be denoted $\mathcal{W}_{\mathrm{KG}}$.

The choice of the operator L should be adapted to the family of operators $B(t)$. In typical situations, the operator $L(t)$ that appears in (3.20) is positive at least for some $t_0 \in]t_-, t_+[$, and then one could to take $L := L(t_0)$. In any case, as we know, there exists a considerable freedom of choosing L. A detailed discussion of conditions that one should impose on $[g_{ij}]$ and Y is contained in Section 2 and Appendix B of [40], and also in [41]. Under these conditions, the evolution equation leads to a dynamics $R(t,s)$, which is a two-parameter family of bounded operators on $\mathcal{W}_{\mathrm{KG}}$ satisfying

$$\begin{aligned} R(t,t) &= \mathbb{1}, \\ R(t,u) &= R(t,s)R(s,u), \\ \big(\partial_t + \mathrm{i}B(t)\big)R(t,s) &= 0, \\ \partial_s R(t,s) - \mathrm{i}R(t,s)B(t) &= 0. \end{aligned} \tag{3.24}$$

The dynamics is a 2×2 matrix of operators acting on functions on Σ:

$$R(t,s) = \begin{bmatrix} R_{11}(t,s) & R_{12}(t,s) \\ R_{21}(t,s) & R_{22}(t,s) \end{bmatrix} \tag{3.25}$$

with distributional kernels $R_{ij}(t,\mathbf{x};s,\mathbf{y})$. The classical propagators in the Cauchy data formalism are:

$$E^{\mathrm{PJ}}(t,\mathbf{x};s,\mathbf{y}) = \mathrm{i}R(t,\mathbf{x};s,\mathbf{y}), \tag{3.26}$$

$$E^{\vee}(t,\mathbf{x};s,\mathbf{y}) = \mathrm{i}\theta(t-s)R(t,\mathbf{x};s,\mathbf{y}), \tag{3.27}$$

$$E^{\wedge}(t,\mathbf{x};s,\mathbf{y}) = -\mathrm{i}\theta(s-t)R(t,\mathbf{x};s,\mathbf{y}). \tag{3.28}$$

The usual classical propagators well-known from the literature, e.g. constructed in [9], can be obtained by setting

$$G^{\bullet}(t,\mathbf{x};s,\mathbf{y}) = \mathrm{i}\alpha(t,\mathbf{x})E^{\bullet}_{12}(t,\mathbf{x};s,\mathbf{y})\alpha(s,\mathbf{y}), \qquad \bullet = \mathrm{PJ}, \vee, \wedge. \tag{3.29}$$

Note that they are usually constructed by other mehods (e.g. by a local construction involving an expansion in terms of Riesz potentials [9]). The construction presented above has a considerable advantage over other methods: it allows for low regularity of the metric and scalar potential. Its apparent disadvantage is the need to impose assumptions global in the slice Σ. However, using the finite speed of propagation, this problem can be easily bypassed.

Note that the multiplication with step functions in the evolution equation approach in (3.27) and (3.28), and also later in (3.40) and (3.41), is unproblematic. In fact, $R(t,s)$ is an operator-valued function which is *strongly continuous* in t,s. Therefore, $R(t,\mathbf{x};s,\mathbf{y})$ is a *continuous* function with values in distributions. Multiplication of $R(t,\mathbf{x};s,\mathbf{y})$ by $\theta(t-s)$ or $\theta(s-t)$ yields then a distribution.

3.3 Non-classical propagators on asymptotically stationary spacetimes

Assume now that $]t_-,t_+[=\mathbb{R}$, so that the spacetime is $\mathbb{R}\times\Sigma$ and the Klein-Gordon equation is (a) asymptotically stationary and (b) asymptotically stable, i.e.,

$$\text{(a) the strong resolvent limits } \lim_{t\pm\infty} B(t) =: B_\pm \quad \text{exist;} \tag{3.30}$$

$$\text{(b) } H_\pm := QB_\pm \geq 0 \quad \text{in the sense of } L^2(\Sigma)\oplus L^2(\Sigma). \tag{3.31}$$

Assume that 0 is not an eigenvalue of B_+ and B_-. Define the "out/in particle/antiparticle projections":

$$\Pi^{(+)}_{\pm} := \mathbb{1}_{]0,\infty[}(B_\pm), \tag{3.32}$$

$$\Pi^{(-)}_{\pm} := \mathbb{1}_{]0,\infty[}(-B_\pm). \tag{3.33}$$

As in Subsection 3.2, we consider the Klein-Gordon form (3.22). We choose the Krein structure so that both $S_+ := \Pi^{(+)}_{+} - \Pi^{(-)}_{+}$ and $S_- := \Pi^{(+)}_{-} - \Pi^{(-)}_{-}$ are admissible involutions.

We can transport (3.32) and (3.33) by the evolution to any time t:

$$\Pi_{\pm}^{(+)}(t) := \lim_{s\to\pm\infty} R(t,s)\Pi_{\pm}^{(+)}R(s,t), \tag{3.34}$$

$$\Pi_{\pm}^{(-)}(t) := \lim_{s\to\pm\infty} R(t,s)\Pi_{\pm}^{(-)}R(s,t). \tag{3.35}$$

We can now define the "out/in positive/negative frequency bisolutions in the Cauchy data formalism":

$$E_{\pm}^{(+)}(t,s) = \Pi_{\pm}^{(+)}(t)R(t,s), \tag{3.36}$$

$$E_{\pm}^{(-)}(t,s) = \Pi_{\pm}^{(-)}(t)R(t,s). \tag{3.37}$$

Note that $\mathcal{R}(\Pi^{(\pm)})$ and $\mathcal{R}(\Pi^{(\pm)}(t))$ are maximal uniformly positive/negative subspaces of the Krein space $\mathcal{W}_{\mathrm{KG}}$.

We will need also projections $\Pi_{+-}^{(\pm)}(t)$ and $\Pi_{-+}^{(\pm)}(t)$ defined by specifying their range and nullspace:[2]

$$\begin{aligned}
\mathcal{R}\big(\Pi_{+-}^{(+)}(t)\big) &= \mathcal{N}\big(\Pi_{+-}^{(-)}(t)\big) = \mathcal{R}\big(\Pi_{+}^{(+)}(t)\big),\\
\mathcal{R}\big(\Pi_{+-}^{(-)}(t)\big) &= \mathcal{N}\big(\Pi_{+-}^{(+)}(t)\big) = \mathcal{R}\big(\Pi_{-}^{(-)}(t)\big),\\
\mathcal{R}\big(\Pi_{-+}^{(+)}(t)\big) &= \mathcal{N}\big(\Pi_{-+}^{(-)}(t)\big) = \mathcal{R}\big(\Pi_{-}^{(+)}(t)\big),\\
\mathcal{R}\big(\Pi_{-+}^{(-)}(t)\big) &= \mathcal{N}\big(\Pi_{-+}^{(+)}(t)\big) = \mathcal{R}\big(\Pi_{+}^{(-)}(t)\big).
\end{aligned} \tag{3.38}$$

Note that

$$\Pi_{+-}^{(\pm)} + \Pi_{+-}^{(\mp)} = \mathbb{1}. \tag{3.39}$$

Now we can define the in-out Feynman and the out-in anti-Feynman Green functions in the Cauchy data formalism:

$$E_{+-}^{\mathrm{F}}(t,s) = \theta(t-s)\Pi_{+-}^{(+)}(t)R(t,s) - \theta(s-t)\Pi_{+-}^{(-)}(t)R(t,s), \tag{3.40}$$

$$E_{-+}^{\overline{\mathrm{F}}}(t,s) = \theta(t-s)\Pi_{-+}^{(-)}(t)R(t,s) - \theta(s-t)\Pi_{-+}^{(+)}(t)R(t,s). \tag{3.41}$$

Next we set

$$G_{\pm}^{(+)}(t,\mathbf{x};s,\mathbf{y}) = \alpha(t,\mathbf{x})E_{\pm,12}^{(+)}(t,\mathbf{x};s,\mathbf{y})\alpha(s,\mathbf{y}), \tag{3.42}$$

$$G_{\pm}^{(-)}(t,\mathbf{x};s,\mathbf{y}) = -\alpha(t,\mathbf{x})E_{\pm,12}^{(-)}(t,\mathbf{x};s,\mathbf{y})\alpha(s,\mathbf{y}), \tag{3.43}$$

$$G_{+-}^{\mathrm{F}}(t,\mathbf{x};s,\mathbf{y}) = \mathrm{i}\alpha(t,\mathbf{x})E_{+-,12}^{\mathrm{F}}(t,\mathbf{x};s,\mathbf{y})\alpha(s,\mathbf{y}), \tag{3.44}$$

$$G_{-+}^{\overline{\mathrm{F}}}(t,\mathbf{x};s,\mathbf{y}) = \mathrm{i}\alpha(t,\mathbf{x})E_{-+,12}^{\overline{\mathrm{F}}}(t,\mathbf{x};s,\mathbf{y})\alpha(s,\mathbf{y}). \tag{3.45}$$

$G_{-}^{(\pm)}$ are two-point functions of the "in-vacuum" Ω_{-} and $G_{+}^{(\pm)}$ are two-point functions of the "out-vacuum" Ω_{+}. Both are Hadamard states [53].

[2]Note that our notation is different from the convention in [40, 41].

The *in-out Feynman propagator* $G^{\mathrm{F}}_{+-}(x,x')$ and the *out-in anti-Feynman propagator* $G^{\overline{\mathrm{F}}}_{-+}(x,x')$ are the "mixed Feynman propagators" corresponding to those states. In fact it is easy to see that if $(\Omega_+|\Omega_-)\neq 0$ then

$$G^{\mathrm{F}}_{+-}(x,y) = \mathrm{i}\frac{\big(\Omega_+|\,\mathrm{T}\left(\hat\phi(x)\hat\phi(y)\right)\Omega_-\big)}{(\Omega_+|\Omega_-)}, \tag{3.46}$$

$$G^{\overline{\mathrm{F}}}_{-+}(x,y) = -\mathrm{i}\frac{\big(\Omega_-|\overline{\mathrm{T}}\big(\hat\phi(x)\hat\phi(y)\big)\Omega_+\big)}{(\Omega_-|\Omega_+)}. \tag{3.47}$$

Assume in addition that $\alpha(x)$ and $\alpha^{-1}(x)$ are bounded on M. One can then heuristically derive [39, 40], and under some technical assumptions rigorously prove [71, 83], that (3.46) and (3.47) coincide with the operator-theoretic propagators:

$$G^{\mathrm{F}}_{\mathrm{op}}(x,y) = G^{\mathrm{F}}_{+-}(x,y), \tag{3.48}$$

$$G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,y) = G^{\overline{\mathrm{F}}}_{-+}(x,y). \tag{3.49}$$

4 FLRW spacetimes

4.1 1+0-dimensional spacetimes

$1+0$-dimensional spacetimes form an important class of spacetimes for which we can understand various propagators rather completely.

The Klein-Gordon operator on $\mathbb{R}^{1,0}$ can be written as a *one-dimensional Schrödinger operator* (with the wrong sign in front of the second derivative):

$$K := -\Box + Y(t) = \partial_t^2 + Y(t). \tag{4.1}$$

We will assume that

$$Y(t) = -V(t) + m^2, \quad \lim_{t\to\pm\infty} V(t) = 0, \tag{4.2}$$

so that we can write

$$H := -\partial_t^2 + V(t), \quad K = -H + m^2. \tag{4.3}$$

Thus to discuss propagators on $1+0$-dimensional spacetimes one needs to understand the theory of Green functions of the one-dimensional Schrödinger operator H. A standard reference for the subject is [87]. In the following subsection, we present this well-known theory following [38] in a style adjusted to the QFT applications that we have in mind.

4.2 Green functions of one-dimensional Schrödinger operators

Suppose that $k \in \mathbb{C}$ and we are given two solutions ψ_1, ψ_2 of the equation

$$(H + k^2)\psi(t) = 0. \tag{4.4}$$

Their *Wronskian*

$$\mathcal{W}(\psi_1, \psi_2) := \psi_1(t)\psi_2'(t) - \psi_1'(t)\psi_2(t) \tag{4.5}$$

does not depend on t. (4.4) possesses a dinstinguished bisolution defined by

$$G^{\leftrightarrow}(-k^2; t, s) := \frac{\psi_1(t)\psi_2(s) - \psi_2(t)\psi_1(s)}{\mathcal{W}(\psi_1, \psi_2)}. \tag{4.6}$$

Note that

$$G^{\leftrightarrow}(-k^2; t, t) = 0 \quad \text{and} \quad \partial_s G^{\leftrightarrow}(-k^2; t, s)\Big|_{s=t} = -\partial_t G^{\leftrightarrow}(-k^2; t, s)\Big|_{t=s} = 1. \tag{4.7}$$

It is easy to see that $G^{\leftrightarrow}(-k^2; t, s)$ is independent of the choice of ψ_1 and ψ_2. We call $G^{\leftrightarrow}(-k^2; t, s)$ the *canonical bisolution*. It is the analog of the Pauli-Jordan propagator.

We then can define the *forward and backward Green functions* via

$$G^{\rightarrow}(-k^2; t, s) := \theta(t - s)G^{\leftrightarrow}(-k^2; t, s), \tag{4.8}$$

$$G^{\leftarrow}(-k^2; t, s) := -\theta(s - t)G^{\leftrightarrow}(-k^2; t, s). \tag{4.9}$$

Using (4.7), one readily verifies that $G^{\rightarrow}$ and $G^{\leftarrow}$ are indeed Green functions. Needless to say, they are the analogs of the retarded and advanced propagators.

Now let $\mathrm{Re}(k) > 0$. The *Jost solutions* $\psi_\pm(k, t)$ are the unique solutions of (4.4) with the asymptotic behavior

$$\psi_\pm(k, t) \sim \mathrm{e}^{\mp kt} \quad \text{as} \quad t \to \pm\infty. \tag{4.10}$$

The *Jost function* is

$$\omega(k) := \mathcal{W}\big(\psi_+(k, \cdot), \psi_-(k, \cdot)\big). \tag{4.11}$$

Then, it is well-known that the unique fundamental solution with appropriate decay behavior as $|t| \to \infty$, that is, the integral kernel of the resolvent $G(-k^2) := (H + k^2)^{-1}$, is

$$G(-k^2; t, s) := \frac{1}{\omega(k)}\Big(\theta(t - s)\psi_+(k, t)\psi_-(k, s) + \theta(s - t)\psi_-(k, t)\psi_+(k, s)\Big). \tag{4.12}$$

Now let $m > 0$. Setting $k = \pm\mathrm{i}m$ in (4.12) we see that the distributional boundary values of the resolvent on the spectrum are then given by

$$G(m^2 \mp \mathrm{i}0; t, s) = \frac{\theta(t - s)\psi_+(\pm\mathrm{i}m, t)\psi_-(\pm\mathrm{i}m, s) + \theta(s - t)\psi_-(\pm\mathrm{i}m, t)\psi_+(\pm\mathrm{i}m, s)}{\omega(\pm\mathrm{i}m)}. \tag{4.13}$$

Thus we computed all four basic Green functions of the Klein-Gordon equation given by (4.3):

$$\begin{aligned} \text{retarded propagator:} \quad & G^{\rightarrow}(m^2;t,s), && (4.14)\\ \text{advanced propagator:} \quad & G^{\leftarrow}(m^2;t,s), && (4.15)\\ \text{Feynman propagator:} \quad & G(m^2-\mathrm{i}0;t,s), && (4.16)\\ \text{anti-Feynman propagator:} \quad & G(m^2+\mathrm{i}0;t,s). && (4.17)\end{aligned}$$

The Klein-Gordon scalar product essentially coincides with the Wronskian:

$$(\psi_1|\psi_2)_{\mathrm{KG}} = \mathcal{W}(\overline{\psi}_1,\psi_2). \tag{4.18}$$

One can now ask when the Klein-Gordon equation given by the operator (4.3) on a $1+0$-dimensional spacetime is special, i.e., when the following identity holds:

$$G(m^2-\mathrm{i}0)+G(m^2+\mathrm{i}0) = G^{\rightarrow}(m^2)+G^{\leftarrow}(m^2)? \tag{4.19}$$

To answer this question, it is useful to introduce the concept of *reflectionlessness*.

Definition 4.1. Let $A(\pm\mathrm{i}m)$ and $B(\pm\mathrm{i}m)$ denote the coefficients of the scattering matrix, i.e.,

$$\psi_+(\pm\mathrm{i}m,t) = A(\pm\mathrm{i}m)\psi_-(\mp\mathrm{i}m,t)+B(\pm\mathrm{i}m)\psi_+(\mp\mathrm{i}m,t). \tag{4.20}$$

The potential $Y(t)$ is called *reflectionless at energy* m^2 if $B(\pm\mathrm{i}m)=0$.

We have the following theorem.

Theorem 4.2. *The potential $Y(t)$ is reflectionless if and only if the Klein-Gordon equation given by* (4.3) *is special, i.e., if and only if* (4.19) *is true.*

Proof. We have

$$\begin{aligned} & G(m^2-\mathrm{i}0)+G(m^2+\mathrm{i}0)\\ &= \theta(t-s)\left(\frac{\psi_+(\mathrm{i}m,t)\psi_-(\mathrm{i}m,s)}{\omega(\mathrm{i}m)}+\frac{\psi_+(-\mathrm{i}m,t)\psi_-(-\mathrm{i}m,s)}{\omega(-\mathrm{i}m)}\right) && (4.21)\\ &\quad + \theta(s-t)\left(\frac{\psi_-(\mathrm{i}m,t)\psi_+(\mathrm{i}m,s)}{\omega(\mathrm{i}m)}+\frac{\psi_-(-\mathrm{i}m,t)\psi_+(-\mathrm{i}m,s)}{\omega(-\mathrm{i}m)}\right). && (4.22)\end{aligned}$$

Moreover,

$$\omega(\pm\mathrm{i}m) = \pm A(\pm\mathrm{i}m)\mathcal{W}(\psi_-(-\mathrm{i}m),\psi_-(\mathrm{i}m)) + B(\pm\mathrm{i}m)\mathcal{W}(\psi_+(\mp\mathrm{i}m),\psi_-(\pm\mathrm{i}m)). \tag{4.23}$$

Then the part (4.21) becomes

$$\begin{aligned}\theta(t-s)\Bigg(&\frac{A(\mathrm{i}m)\psi_-(-\mathrm{i}m,t)\psi_-(\mathrm{i}m,s)+B(\mathrm{i}m)\psi_+(-\mathrm{i}m,t)\psi_-(\mathrm{i}m,s)}{A(\mathrm{i}m)\mathcal{W}(\psi_-(-\mathrm{i}m),\psi_-(\mathrm{i}m))+B(\mathrm{i}m)\mathcal{W}(\psi_+(-\mathrm{i}m),\psi_-(\mathrm{i}m))} && (4.24)\\ &-\frac{A(-\mathrm{i}m)\psi_-(\mathrm{i}m,t)\psi_-(-\mathrm{i}m,s)+B(-\mathrm{i}m)\psi_+(\mathrm{i}m,t)\psi_-(-\mathrm{i}m,s)}{A(-\mathrm{i}m)\mathcal{W}(\psi_-(-\mathrm{i}m),\psi_-(\mathrm{i}m))-B(-\mathrm{i}m)\mathcal{W}(\psi_+(\mathrm{i}m),\psi_-(-\mathrm{i}m))}\Bigg)\end{aligned}$$

Since $A(\pm\mathrm{i}m)\neq 0$, this is $G^{\rightarrow}$ if and only if $B(\pm\mathrm{i}m)=0$. Similar for (4.22). □

4.3 Mode decomposition of FLRW spacetimes

Consider a *Friedmann-Lemaître-Robertson-Walker (FLRW) spacetime*, that is, a spacetime $M = \mathbb{R} \times \Sigma$ with the line element

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a(t)^2 \mathrm{d}\Sigma^2, \tag{4.25}$$

where $\mathrm{d}\Sigma^2$ is the line element of a fixed $d-1$-dimensional complete Riemannian manifold Σ. The Klein-Gordon operator is

$$-\Box_g + m^2 = \partial_t^2 + (d-1)\frac{\dot{a}(t)}{a(t)}\partial_t - \frac{\Delta_\Sigma}{a(t)^2} + m^2, \tag{4.26}$$

where the dot indicates a derivative with respect to t. Then

$$a^{\frac{d-1}{2}}\big(-\Box_g + m^2\big)a^{-\frac{d-1}{2}} = \partial_t^2 - \frac{d-1}{2}\Big(\frac{\ddot{a}}{a} + \frac{d-3}{2}\Big(\frac{\dot{a}}{a}\Big)^2\Big) - \frac{\Delta_\Sigma}{a(t)^2} + m^2. \tag{4.27}$$

It is well-known that $-\Delta_\Sigma$ is self-adjoint, and by the spectral theorem we can diagonalize $-\Delta_\Sigma$, and then to restrict (4.27) to a (generalized) eigenfunction (a "mode") of $-\Delta_\Sigma$ with eigenvalue λ. Thus, for each such mode, (4.27) becomes $-H_\lambda + m^2$, where

$$H_\lambda := -\partial_t^2 + V_\lambda(t) \tag{4.28}$$

is the one-dimensional Schrödinger operator with potential

$$V_\lambda(t) = \frac{d-1}{2}\Big(\frac{\ddot{a}}{a} + \frac{d-3}{2}\Big(\frac{\dot{a}}{a}\Big)^2\Big) - \frac{\lambda}{a(t)^2}. \tag{4.29}$$

Using Subsection 4.2, we can then write all propagators as the integral over all modes.

As a consequence, the Klein-Gordon equation given by (4.26) is special if and only if (4.28) is reflectionless at energy m^2 for all λ in the spectrum of $-\Delta_\Sigma$.

5 De Sitter space

Our next example is the d-dimensional *de Sitter space* dS_d. De Sitter space is an important example of a non-stationary spacetime and one of the simplest examples to model a universe with an accelerated expansion. It exhibits a particularly rich structure and, being a symmetric space, all its invariant propagators can be given explicitly in terms of special functions.

We will describe four different approaches to investigate propagators on dS_d. The first is based on Wick rotation (analytic continuation) from the sphere $\mathbb{S}^d$. One obtains the so-called Euclidean state, considered to be the most physical invariant state on dS_d. The second approach is the off-shell approach based on the resolvent of the d'Alembertian on $L^2(\mathrm{dS}_d)$. Somewhat surprisingly, it leads to non-physical two-point functions. The third approach is the on-shell approach based on $\mathcal{W}_{\mathrm{KG}}$. It leads to the well-known family of de Sitter invariant two-point functions corresponding to the so-called α-*vacua*. One can then compute invariant correlation functions between *two different* α-vacua. Finally, we may interpret dS_d as a special case of a FLRW spacetime and apply the methods of Section 4.

Note that the first three approaches directly lead to simple expressions for invariant propagators. The last approach breaks manifest de Sitter invariance, and to obtain invariant expressions, one needs to sum over all modes using rather complicated addition formulas for special functions.

There is a very large literature about propagators on de Sitter space. Particularly useful for our considerations were [2, 4, 6, 14, 17, 19, 21, 22, 29, 32, 47, 48, 58–60, 66, 67, 78, 80, 81]. In these references, one finds different approaches to investigate propagators on de Sitter space.

Many of them use mode sums to construct propagators – sometimes explicitly like in [2,17,48, 68], sometimes abstractly like in [4]. The papers [19,21,22] have an axiomatic approach much in the spirit of Gårding and Wightman. Only the reference [78] uses the operator-theoretic approach to define the Feynman propagator in $d = 4$ dimensions.

5.1 Geometry of de Sitter space

The d-dimensional de Sitter space dS_d is defined by an embedding into $d + 1$-dimensional Minkowski space $\mathbb{R}^{1,d}$. Let $[\cdot|\cdot]$ denote the pseudo-scalar product on $\mathbb{R}^{1,d}$ defined by

$$[x|x'] = -x^0 x'^0 + \sum_{i=1}^{d} x^i x'^i. \tag{5.1}$$

Then the d-dimensional de Sitter space is the one-sheeted hyperboloid

$$\mathrm{dS}_d := \{x \in \mathbb{R}^{1,d} \mid [x|x] = 1\}. \tag{5.2}$$

Let us introduce some notation that will frequently appear throughout this section. For $x, x' \in \mathrm{dS}_d \hookrightarrow \mathbb{R}^{1,d}$, we define

$$\begin{aligned}
&\text{the invariant quantity} && Z \equiv Z(x, x') := [x|x'], \\
&\text{the antipodal point to } x\text{:} && x^A := -x, \\
&\text{the time variable} && t \equiv t(x, x') := x^0 - x'^0, \\
&\text{the “antipodal time” variable} && t^A := t(x^A, x') := -(x^0 + x'^0).
\end{aligned} \tag{5.3}$$

While t and t^A are two independent variables, we have $Z(x^A, x') = -Z(x, x') = -Z$.

De Sitter space has various regions:

$$\begin{aligned}
&Z > 1: && x \text{ and } x' \text{ are timelike separated,} \\
&Z = 1: && x \text{ and } x' \text{ are separated by a null-geodesic,} \\
&Z < 1: && x \text{ and } x' \text{ are not connected by a causal curve.}
\end{aligned} \tag{5.4}$$

The last region includes the subregions

$$\begin{aligned} Z &= -1: &\quad x^A \text{ and } x' \text{ are separated by a null-geodesic,} \\ Z &< -1: &\quad x^A \text{ and } x' \text{ are timelike separated.} \end{aligned} \tag{5.5}$$

One may further divide the regions $Z > 1$ and $Z < -1$ into future and past dependent on whether t, resp. t^A are positive or negative. Thus, if we fix a point $x' \in \mathrm{dS}_d$, then we can partition dS_d into 5 regions:

$$\mathrm{dS}_d = V^+ \cup V^- \cup A^+ \cup A^- \cup S \tag{5.6}$$

as depicted in Figure 1.

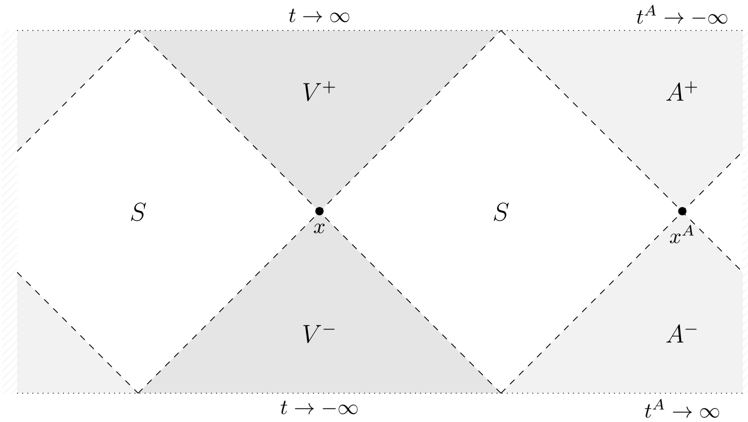

Figure 1: Conformal diagram of de Sitter space with the reference point x and the regions $V^\pm := \{Z(x,x') > 1 \mid t(x,x') \gtrless 0\}$, $A^\pm := \{Z(x,x') < -1 \mid t(x^A,x') \lessgtr 0\}$ and $S := \{|Z(x,x')| < 1\}$. The left and right side of the diagram are glued together and each point represents a $d-2$-sphere.

The de Sitter space possesses a global system of coordinates

$$x^0 = \sinh\tau, \quad x^i = \cosh\tau\, \Omega^i,\ i = 1,\dots,d, \quad \text{where} \quad \tau \in \mathbb{R},\ \Omega \in \mathbb{S}^{d-1} \hookrightarrow \mathbb{R}^d. \tag{5.7}$$

In these coordinates we have $\mathrm{d}s^2 = -\mathrm{d}\tau^2 + \cosh^2(\tau)\mathrm{d}\Omega^2$ and

$$Z = -\sinh\tau\sinh\tau' + \cosh\tau\cosh\tau'\cos\theta, \tag{5.8}$$

where θ is the angle between Ω and Ω'. If $x = (0,1,0\dots)$, then $Z = \cosh\tau'\cos\theta$.

Both the *(full) de Sitter group* $O(1,d)$ and the *restricted de Sitter group* $SO_0(1,d)$, that is, the connected component of the identity in $O(1,d)$, act on dS_d. The Klein-Gordon equation restricted to invariant solutions and written in terms of Z reduces to the Gegenbauer equation, a form of the hypergeometric equation [4, 12, 29, 49, 68, 80] whose properties we discuss in Appendix B.

In the literature one often restricts analysis to subsets of dS_d, such as the *Poincaré patch* or the *static patch*, which allow for coordinate systems with special properties. In our paper we consider only the "*global patch*", that is the full de Sitter space. Otherwise, we would have to consider boundary conditions for the d'Alembertian at the boundary of our patch (which would break the de Sitter invariance and presumably be non-physical).

For more information about de Sitter space, consult the overviews [67, 81] .

5.2 The sphere

The de Sitter space can be viewed as a Wick-rotated sphere. Therefore, in this subsection we recall some facts about the sphere and the Green function of the spherical Laplacian.

Consider the $d+1$ dimensional Euclidean space equipped with the scalar product

$$(x|x') = \sum_{i=1}^{d+1} x^i x'^i. \tag{5.9}$$

The d-dimensional (unit) sphere is defined as

$$\mathbb{S}^d := \{x \in \mathbb{R}^{d+1} \mid (x|x) = 1\}. \tag{5.10}$$

For $\mathrm{Re}(\nu) > 0$ or $\nu \in \mathrm{i}\mathbb{R}_{\geq 0} \setminus \mathrm{i}\big(\frac{d-1}{2} + \mathbb{N}_0\big)$, let us consider the resolvent of the spherical Laplacian $G^{\mathrm{s}}(-\nu^2) := (-\Delta^{\mathrm{s}} + (\frac{d-1}{2})^2 + \nu^2)^{-1}$. Its integral kernel $G^{\mathrm{s}}(-\nu^2; x, x')$ can be expressed in terms of the invariant quantity $(x|x')$ (see e.g. [36, 37], and [31, 82], where Legendre functions are used) as:

$$G^{\mathrm{s}}(-\nu^2; x, x') = C_{d,\nu} \mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}\big(-(x|x')\big), \tag{5.11}$$

where

$$C_{d,\nu} := \frac{\Gamma\big(\frac{d-1}{2} + \mathrm{i}\nu\big)\Gamma\big(\frac{d-1}{2} - \mathrm{i}\nu\big)}{(4\pi)^{\frac{d}{2}}}, \tag{5.12}$$

and $\mathbf{S}_{\alpha,\lambda}(z)$ is the Gegenbauer function described in Appendix B.

5.3 Propagators related to the Euclidean state

We now turn to the d-dimensional de Sitter space for $d \geq 2$. We will analyze bi- and fundamental solutions of the Klein-Gordon equation

$$(-\Box + m^2)\phi(x) = 0 \tag{5.13}$$

in de Sitter space, which are invariant under the full or restricted de Sitter group. Note that m might contain a coupling to the scalar curvature. Hence it is sometimes called *effective mass*. Anyway, we prefer to use the parameter ν defined by

$$\nu := \sqrt{m^2 - \big(\tfrac{d-1}{2}\big)^2} \in \mathbb{C}. \tag{5.14}$$

Thus (5.13) is replaced with

$$\Big(-\Box+\big(\tfrac{d-1}{2}\big)^2+\nu^2\Big)\phi(x)=0. \tag{5.15}$$

We will allow for complex ν^2, choosing the principal sheet of the square root, that is $\nu \in \{\mathrm{Re}(\nu) > 0\}$. The case of positive ν^2 has analogous properties to that of positive m^2 in Minkowski space. In the case $\nu^2 < 0$ we assume that $\nu \in \mathrm{i}\mathbb{R}_{\geq 0}$. It is more intricate than the case $\mathrm{Re}(\nu) > 0$ and contains various subcases with different exotic properties. It is somewhat analogous to the tachyonic case in Minkowski space.

On a generic spacetime the concept of the Wick rotation is not uniquely defined. However, on the de Sitter space embedded in $\mathbb{R}^{1,d}$ there is a natural kind of a Wick rotation, which we will use: the replacement of x^{d+1} with $\pm\mathrm{i}x^0$. We note first that

$$(x|x') = 1 - \frac{(x-x'|x-x')}{2} \quad \text{for} \quad x,x' \in \mathbb{S}^d. \tag{5.16}$$

The replacement of $x^{d+1} - x'^{d+1}$ with $(x^0 - x'^0)\mathrm{e}^{\pm\mathrm{i}\phi}$, $\phi \in [0, \frac{\pi}{2}]$, yields

$$\begin{aligned}&(x^{d+1}-x'^{d+1})^2 \to (x^0-x'^0)^2\mathrm{e}^{\pm 2\mathrm{i}\phi} \xrightarrow{\phi\to\frac{\pi}{2}} -(x^0-x'^0)^2 \pm \mathrm{i}0 \\ \Rightarrow\ &(x|x') \to [x|x'] \mp \mathrm{i}0.\end{aligned} \tag{5.17}$$

Moreover, we need to insert a prefactor $\pm\mathrm{i}$ coming from the change of the integral measure.

Let $\mathrm{Re}(\nu) > 0$ or $\nu \in \mathrm{i}\mathbb{R}_{\geq 0} \setminus \mathrm{i}\big(\frac{d-1}{2} + \mathbb{N}_0\big)$. The Feynman and anti-Feynman propagators in the d-dimensional de Sitter space obtained by Wick rotation of the Green function (5.11) on the sphere are given by

$$G_0^{\mathrm{F}/\overline{\mathrm{F}}}(x,x') = \pm\mathrm{i}C_{d,\nu}\,\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z\pm\mathrm{i}0\big), \tag{5.18}$$

where $C_{d,\nu}$ is given by (5.12) and $Z := [x|x']$. We easily check that (5.18) are Green functions of the Klein-Gordon equation on dS_d.

The sum of the Euclidean Feynman and anti-Feynman propagator has a causal support, for $\mathbf{S}_{\alpha,\lambda}(z)$ is holomorphic on $\mathbb{C}\backslash]-\infty,-1]$, and therefore

$$G_0^{\mathrm{F}} + G_0^{\overline{\mathrm{F}}} = \mathrm{i}C_{d,\nu}\,\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z+\mathrm{i}0\big) - \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z-\mathrm{i}0\big)\Big) \tag{5.19}$$

vanishes for $Z < 1$.

As we will see later, G_0^{F} and $G_0^{\overline{\mathrm{F}}}$ are not the operator-theoretic Feynman and anti-Feynman propagators. However, we can still apply to them the procedure described in Subsection 2.9. This leads to the classical propagators

$$G^{\vee/\wedge}(x,x') = \mathrm{i}\theta\big(\pm(x^0-x'^0)\big)C_{d,\nu}\,\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z+\mathrm{i}0\big) - \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z-\mathrm{i}0\big)\Big), \tag{5.20}$$

$$G^{\mathrm{PJ}}(x,x') = \mathrm{i}\,\mathrm{sgn}\,\big(x^0-x'^0\big)C_{d,\nu}\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z+\mathrm{i}0\big) - \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z-\mathrm{i}0\big)\Big), \tag{5.21}$$

as well as to the positive/negative frequency solutions

$$G_0^{(\pm)}(x,x') = C_{d,\nu}\, \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\Big(-Z \pm \mathrm{i}0 \,\mathrm{sgn}\,\big(x^0 - x'^0\big)\Big). \tag{5.22}$$

$G_0^{(\pm)}$ have the Hadamard property and are two-point functions of a state called the *Euclidean state* Ω_0 (sometimes also called the *Bunch-Davies state*) [4, 25, 29, 49, 68, 80].

Note that the propagators associated to the Euclidean vacuum satisfy all relations (2.39) with $\alpha = \beta = 0$. The classical propagators (5.20) and (5.21) are universal: they do not depend on the Euclidean vacuum, therefore we do not decorate them with the subscript 0.

5.4 Bisolutions and Green functions

The family of invariant propagators on the de Sitter space is quite rich and is not limited to those related to the Euclidean state, discussed in the previous subsection. In order to prepare for their analysis, in this subsection we will descibe invariant solutions of the Klein-Gordon equation on de Sitter space.

From the analysis of previous subsection we easily see that the following functions are bisolutions invariant with respect to the full de Sitter group:

$$\begin{aligned} G_0^{\mathrm{sym}}(x,x') &:= G_0^{(+)}(x,x') + G_0^{(-)}(x,x') \qquad (5.23)\\ &= C_{d,\nu}\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z+\mathrm{i}0\big) + \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z-\mathrm{i}0\big)\Big),\\ G_0^{\mathrm{sym},A}(x,x') &:= G_0^{\mathrm{sym}}(x^A,x') = G_0^{\mathrm{sym}}(x,x'^A) \qquad (5.24)\\ &= C_{d,\nu}\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(Z+\mathrm{i}0\big) + \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(Z-\mathrm{i}0\big)\Big), \end{aligned}$$

The following functions are bisolutions invariant with respect to the restricted de Sitter group:

$$\begin{aligned} G^{\mathrm{PJ}}(x,x') &:= \mathrm{i}\big(G_0^{(+)}(x,x') - G_0^{(-)}(x,x')\big) \qquad (5.25)\\ &= \mathrm{i}\,\mathrm{sgn}\,\big(t\big) C_{d,\nu}\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z+\mathrm{i}0\big) - \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(-Z-\mathrm{i}0\big)\Big),\\ G^{\mathrm{PJ},A}(x,x') &:= G^{\mathrm{PJ}}(x^A,x') = -G^{\mathrm{PJ}}(x,x'^A) \qquad (5.26)\\ &= \mathrm{i}\,\mathrm{sgn}\,\big(t^A\big) C_{d,\nu}\Big(\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(Z+\mathrm{i}0\big) - \mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}\big(Z-\mathrm{i}0\big)\Big). \end{aligned}$$

Indeed, we already know that $G_0^{(\pm)}$ are bisolutions, hence so are (5.23) and (5.25). It is also clear that replacing x with x^A, used in (5.24) and (5.26) leads to invariant bisolutions. We expect that the following is true:

Conjecture 5.1. *For any $\nu \in \mathbb{C}$ such that $\frac{d-1}{2} \pm \mathrm{i}\nu \notin \{0, -1, -2, \dots\}$, $\{G_0^{\mathrm{sym}}, G_0^{\mathrm{sym},A}\}$ is a basis of the space of fully de Sitter invariant bisolutions, and $\{G_0^{\mathrm{sym}}, G_0^{\mathrm{sym},A}, G^{\mathrm{PJ}}, G^{\mathrm{PJ},A}\}$ is a basis of the space of bisolutions invariant under the restricted de Sitter group.*

Note that the Gegenbauer function $\mathbf{S}_{\frac{d}{2}-1,\mathrm{i}\nu}(w)$ is an entire function of ν. If we were only interested in bisolutions, we could drop the restriction $\frac{d-1}{2} \pm \mathrm{i}\nu \notin \{0,-1,-2,\dots\}$ in Thm. 5.1, which is only necessary due to the poles of the prefactor $C_{d,\nu}$ at such ν. However, we eventually want to relate bisolutions to Green functions by time-ordering, and therefore we normalize them properly.

Functions invariant with respect to the full de Sitter group can always be written in terms of the invariant quantity Z alone. The Klein-Gordon equation restricted to invariant solutions and written in terms of Z reduces to the Gegenbauer equation (cf. e.g. [4,17,49])

$$\Big((1-Z^2)\partial_Z^2 - dZ\partial_Z - \nu^2 - \big(\tfrac{d-1}{2}\big)^2\Big) f(Z) = 0. \tag{5.27}$$

Therefore, all bisolutions and Green functions invariant wrt the full de Sitter group can be expressed in terms of Gegenbauer functions.

If we only demand invariance under the restricted de Sitter group, the regions V^+ and V^- as well as A^+ and A^- need to be treated as independent. Hence for $|Z|>1$, propagators invariant under the restricted de Sitter group may depend on $\operatorname{sgn}(t)$ resp. $\operatorname{sgn}(t^A)$.

Assuming the validity of Conjecture 5.1, the general bisolution is

$$\begin{aligned} G^{\mathrm{bisol}}_{\underline{a}} &=:= \mathrm{i}a_1 G_0^{\mathrm{sym}} + a_2 G^{\mathrm{PJ}} + \mathrm{i}a_3 G_0^{\mathrm{sym},A} + a_4 G^{\mathrm{PJ}A} \\ &= \mathrm{i}C_{d,\nu}\Big(\big(a_1 + a_2 \operatorname{sgn}(t)\big)\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z+\mathrm{i}0) \\ &\qquad + \big(a_1 - a_2 \operatorname{sgn}(t)\big)\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z-\mathrm{i}0) \\ &\qquad + \big(a_3 - a_4 \operatorname{sgn}(t^A)\big)\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(Z+\mathrm{i}0) \\ &\qquad + \big(a_3 + a_4 \operatorname{sgn}(t^A)\big)\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(Z-\mathrm{i}0)\Big) \end{aligned} \tag{5.28}$$

and the general fundamental solution is

$$G_{\underline{a}} := G_0^{\mathrm{F}} + G^{\mathrm{bisol}}_{\underline{a}} = \mathrm{i}C_{d,\nu}\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z+\mathrm{i}0) + G^{\mathrm{bisol}}_{\underline{a}}. \tag{5.29}$$

5.5 Resolvent of the d'Alembertian and operator-theoretic propagators

The d'Alembertian $-\Box$ is essentially self-adjoint on $C_c^\infty(\mathrm{dS}_d)$ in the sense of $L^2(\mathrm{dS}_d)$. This follows from a general theory of invariant differential operators on symmetric spaces [10,77] and the fact that de Sitter space can be seen as the quotient of Lie groups $O(1,d)/O(1,d-1)$. In this subsection we will compute its resolvent and operator-theoretic Feynman and anti-Feynman propagators. In the four-dimensional case, this has been studied [78].

Outside of the spectrum of $-\Box + \big(\frac{d-1}{2}\big)^2$, its resolvent (Green operator) will be denoted by

$$G(-\nu^2) := \Big(-\Box + \big(\tfrac{d-1}{2}\big)^2 + \nu^2\Big)^{-1}. \tag{5.30}$$

We will write $G(-\nu^2; x, x')$ for its integral kernel.

In the following statement we will compute $G(-\nu^2; x, x')$. This computation, short and, we believe, quite elegant, is based on Conjecture 5.1, which does not have a complete proof in our paper. Therefore, strictly speaking, all statements in this subsection are not fully proven in our paper, even if we call them "theorems".

One can justify Thm. 5.2 independently, following the (rather complicated) arguments of [48] involving global coordinates and summation formulas for Gegenbauer functions. We will not discuss these arguments in this paper.

Theorem 5.2. *Let* $\operatorname{Re}\nu > 0$.
Odd d**.** *The resolvent is given by*

$$\begin{aligned} &G(-\nu^2; x, x') \\ &= \frac{\pm\Gamma\big(\frac{d-1}{2} \pm \mathrm{i}\nu\big)}{2^{2\pm\mathrm{i}\nu}(2\pi)^{\frac{d-1}{2}} \sinh \pi\nu} \Big(\mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z - \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z + \mathrm{i}0) \Big), \quad \operatorname{Im}\nu \lessgtr 0. \end{aligned} \tag{5.31}$$

Therefore, for $\nu > 0$*, the Feynman and anti-Feynman propagators are*

$$G_{\mathrm{op}}^{\mathrm{F}/\overline{\mathrm{F}}}(x, x') = \frac{\pm\Gamma\big(\frac{d-1}{2} \pm \mathrm{i}\nu\big)}{2^{2\pm\mathrm{i}\nu}(2\pi)^{\frac{d-1}{2}} \sinh \pi\nu} \Big(\mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z - \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z + \mathrm{i}0) \Big). \tag{5.32}$$

Even d**.** *The resolvent is given by*

$$\begin{aligned} &G(-\nu^2; x, x') \\ &= -\frac{\Gamma\big(\frac{d-1}{2} \pm \mathrm{i}\nu\big)}{2^{2\pm\mathrm{i}\nu}(2\pi)^{\frac{d-1}{2}} \cosh \pi\nu} \Big(\mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z + \mathrm{i}0) + \mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z - \mathrm{i}0) \Big), \quad \operatorname{Im}\nu \lessgtr 0. \end{aligned} \tag{5.33}$$

Therefore, for $\nu > 0$*, the operator-theoretic Feynman and anti-Feynman propagators are*

$$\begin{aligned} &G_{\mathrm{op}}^{\mathrm{F}/\overline{\mathrm{F}}}(x, x') \\ &= -\frac{\Gamma\big(\frac{d-1}{2} \pm \mathrm{i}\nu\big)}{2^{2\pm\mathrm{i}\nu}(2\pi)^{\frac{d-1}{2}} \cosh \pi\nu} \Big(\mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z + \mathrm{i}0) + \mathbf{Z}_{\frac{d-2}{2}, \pm\mathrm{i}\nu}(-Z - \mathrm{i}0) \Big). \end{aligned} \tag{5.34}$$

Proof (assuming the validity of Conj. 5.1). Let us first compute the Green operator $G(-\nu^2)$ for $\nu^2 \in \mathbb{C} \setminus \mathbb{R}$. Clearly, its integral kernel is a Green function invariant under the *full* de Sitter group. Its integral kernel (as the integral kernel of a bounded operator) must not grow too fast as $Z \to \pm\infty$. By Conjecture 5.1, the formula (5.29) describes the family of all fully de Sitter invariant Green functions.

To start, we thus use the connection formula (B.11) to write the general fundamental solution (5.29) in terms of the Gegenbauer functions $\mathbf{Z}_{\alpha,\pm\lambda}(-Z \pm \mathrm{i}0)$, which have a determined behavior as $|Z| \to \infty$. Since we require invariance under the full de Sitter group, we must have $a_2 = a_4 = 0$. This yields

$$\frac{\sinh \pi\nu}{2^{\frac{d-3}{2}}\sqrt{\pi}C_{d,\nu}} G_{\underline{a}} = \frac{2^{\mathrm{i}\nu}}{\Gamma\big(\frac{d-1}{2}+\mathrm{i}\nu\big)} \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z+\mathrm{i}0)\Big(1 + a_1 + a_3 \mathrm{e}^{\mathrm{i}\pi\big(\frac{d-1}{2}-\mathrm{i}\nu\big)}\Big) \\ + \frac{2^{\mathrm{i}\nu}}{\Gamma\big(\frac{d-1}{2}+\mathrm{i}\nu\big)} \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z-\mathrm{i}0)\Big(a_1 + a_3 \mathrm{e}^{-\mathrm{i}\pi\big(\frac{d-1}{2}-\mathrm{i}\nu\big)}\Big) - (\nu \leftrightarrow -\nu). \tag{5.35}$$

We have $\mathbf{Z}_{\frac{d-2}{2},\pm\mathrm{i}\nu}(Z) \sim cZ^{-\frac{d-1}{2}\mp\mathrm{i}\nu}$ as $|Z| \to \infty$, while the measure on $L^2(\mathrm{dS}_d, \sqrt{|g|})$ behaves as cZ^{d-2} as $|Z| \to \infty$.[3] Thus, the resolvent should, for $|Z| > 1$, only contain

$$\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(|Z|) \quad \text{if} \quad \mathrm{Im}(\nu) < 0 \quad \text{and} \quad \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(|Z|) \quad \text{if} \quad \mathrm{Im}(\nu) > 0, \tag{5.36}$$

for otherwise it could not be the integral kernel of a bounded operator on $L^2(\mathrm{dS}_d, \sqrt{|g|})$. The parameters that correspond to such a decay behavior are different in even and odd dimensions:

Odd dimensions. In odd dimensions, $\frac{d-1}{2}$ is an integer, and we obtain

$$\text{Solution } \sim \mathbf{Z}_{\frac{d-2}{2},\pm\mathrm{i}\nu}(Z) \text{ for } |Z| > 1: \quad a_1 = \pm\frac{\mathrm{e}^{\mp\pi\nu}}{2\sinh\pi\nu}, \quad a_3 = \pm\frac{(-1)^{\frac{d+1}{2}}}{2\sinh\pi\nu}. \tag{5.37}$$

Even dimensions. In even dimensions, $\frac{d-1}{2}$ is a half-integer but not an integer. We obtain

$$\text{Solution } \sim \mathbf{Z}_{\frac{d-2}{2},\pm\mathrm{i}\nu}(Z) \text{ for } |Z| > 1: \quad a_1 = -\frac{\mathrm{e}^{\mp\pi\nu}}{2\cosh\pi\nu}, \quad a_3 = -\mathrm{i}\frac{(-1)^{\frac{d}{2}}}{2\cosh\pi\nu}. \tag{5.38}$$

These values of a_1 and a_3 yield the formulas for the resolvents. The operator-theoretic Feynman and anti-Feynman propagators are the limits of the resolvents on the spectrum from below resp. above. □

We will give an interpretation of the operator-theoretic (anti-)Feynman propagators in terms of time-ordered two-point functions between two states in Section 5.7. However, from their formulas, we can already see the surprising fact that they are different from the propagators in the Euclidean state Ω_0, which is the only de Sitter-invariant Hadamard state.

One can ask when the Klein-Gordon operator on de Sitter space is special. The situation is quite remarkable:

Theorem 5.3. *Let $\nu > 0$. Then*

$$G^{\mathrm{F}}_{\mathrm{op}} + G^{\overline{\mathrm{F}}}_{\mathrm{op}} = G^{\vee} + G^{\wedge}, \quad \textbf{for odd } d; \tag{5.39}$$

$$\textit{but} \quad G^{\mathrm{F}}_{\mathrm{op}} + G^{\overline{\mathrm{F}}}_{\mathrm{op}} \neq G^{\vee} + G^{\wedge}, \quad \textbf{for even } d. \tag{5.40}$$

[3] This can be verified using the global coordinates (5.7), in which Z is given by (5.8).

Proof. We use the connection formula (B.10) to rewrite $G^{\mathrm{F}}_{\mathrm{op}}$ and $G^{\overline{\mathrm{F}}}_{\mathrm{op}}$ in terms of $\mathbf{S}_{\frac{d-2}{2},\pm\mathrm{i}\nu}(\cdot)$ and compare to the formulas (5.20). Actually, in odd dimensions, the result follows immediately if one uses (B.11) instead of (B.10). □

Let us finally consider the "tachyonic" region of parameters in the de Sitter space. Instead of the parameter ν, it will be convenient to use $\mu := -\mathrm{i}\nu$.

Theorem 5.4. *1.* **Odd** d. *The spectrum of* $-\Box + \left(\frac{d-1}{2}\right)^2$ *equals*

$$]-\infty,0] \cup \{\mu^2 \mid \mu \in \mathbb{N}_0\}, \tag{5.41}$$

and for $\mu \in [0,\infty[\backslash \mathbb{N}_0$*, the resolvent is given by*

$$\begin{aligned} &G(\mu^2;x,x') \\ &= -\mathrm{i}\frac{\Gamma\left(\frac{d-1}{2}+\mu\right)}{2^{2+\mu}(2\pi)^{\frac{d-1}{2}}\sin\pi\mu}\Big(\mathbf{Z}_{\frac{d-2}{2},\mu}(-Z+\mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},\mu}(-Z-\mathrm{i}0)\Big). \end{aligned} \tag{5.42}$$

2. **Even** d. *The spectrum of* $-\Box + \left(\frac{d-1}{2}\right)^2$ *equals*

$$]-\infty,0] \cup \{\mu^2 \mid \mu \in \mathbb{N}_0 + \tfrac{1}{2}\}, \tag{5.43}$$

and for $\mu \in [0,\infty[\backslash\left(\mathbb{N}_0+\frac{1}{2}\right)$*, the resolvent is given by*

$$\begin{aligned} &G(\mu^2;x,x') \\ &= -\frac{\Gamma\left(\frac{d-1}{2}+\mu\right)}{2^{2+\mu}(2\pi)^{\frac{d-1}{2}}\cos\pi\mu}\Big(\mathbf{Z}_{\frac{d-2}{2},\mu}(-Z+\mathrm{i}0) + \mathbf{Z}_{\frac{d-2}{2},\mu}(-Z-\mathrm{i}0)\Big). \end{aligned} \tag{5.44}$$

Proof. Let $\mu > 0$. If the limits of (5.31) as ν approaches the imaginary line exist, they coincide:

$$\lim_{\epsilon\to 0} G((-(\mathrm{i}\mu+\epsilon)^2;x,x') = \lim_{\epsilon\to 0} G((-(-\mathrm{i}\mu+\epsilon)^2;x,x'). \tag{5.45}$$

The results of these limits are the integral kernels of the resolvents in the "tachyonic" case (5.42). Similar for (5.33) and (5.44).

For even d, the limit diverges for $\mu \in \mathbb{N}_0 + \frac{1}{2}$ due to the presence of $\cos\pi\mu$ in the denominator of (5.44). This is not a removable singularity. For $Z < -1$, we have

$$\mathbf{Z}_{\frac{d-2}{2},\mu}(-Z+\mathrm{i}0) = \mathbf{Z}_{\frac{d-2}{2},\mu}(-Z-\mathrm{i}0) = \mathbf{Z}_{\frac{d-2}{2},\mu}(|Z|), \tag{5.46}$$

and this does not vanish identically.

For odd d, the limit diverges for $\mu \in \mathbb{N}_0$ due to the presence of $\sin\pi\mu$ in the denominator of (5.42). Although less obvious than in the even-dimensional case, this is also not a removable singularity. Due to (B.12), we have

$$\mathbf{Z}_{\frac{d-2}{2},\mu}(-Z+\mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},\mu}(-Z-\mathrm{i}0) = 0, \quad |Z|>1,\ \mu\in\mathbb{N}_0. \tag{5.47}$$

But using the connection formula (B.10), we find for $|Z| < 1$ and $\mu \in \mathbb{N}_0$,

$$\mathbf{Z}_{\frac{d-2}{2},\mu}(-Z + \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},\mu}(-Z - \mathrm{i}0) = \frac{-\mathrm{i}\,\mathrm{sgn}(Z) 2^{\mu+\frac{d+1}{2}}}{\Gamma\big(\frac{d-1}{2} + \mu\big)(1 - Z^2)^{\frac{d-2}{2}}} \mathbf{S}_{\frac{d-2}{2},\mu}(-Z). \tag{5.48}$$

This does not vanish identically. □

5.6 Alpha vacua

For the rest of the section on de Sitter space, we restrict ourselves to the case of real and positive $\nu > 0$.

The Euclidean vacuum is not the only de Sitter invariant state on de Sitter space. There exists a whole family of such states, called *alpha vacua* [4, 17, 68]. We describe these states using the Krein space language introduced in Section 2 and then explain the relation to the approach based on mode expansions, which is commonly used in the physics literature [4, 17].

5.6.1 Alpha vacua in the Krein space picture

Let $\mathcal{W}_{\mathrm{KG}}$ be the Krein space of solutions of the Klein-Gordon equation, which has a fundamental decomposition corresponding to positive and negative frequencies with respect to the Euclidean vacuum. That is,

$$\mathcal{W}_{\mathrm{KG}} = \mathcal{Z}_0^{(+)} \oplus \mathcal{Z}_0^{(-)}, \quad \mathcal{Z}_0^{(-)} = \overline{\mathcal{Z}_0^{(+)}}, \tag{5.49}$$

where $\mathcal{Z}_0^{(\pm)} := \mathcal{R}(\Pi_0^{(\pm)})$ are the ranges of the orthogonal projections $\Pi_0^{(\pm)}$, whose Klein-Gordon kernels are the bisolutions $\pm G_0^{(\pm)}$. The fundamental decomposition (5.49) will serve as a reference decomposition of $\mathcal{W}_{\mathrm{KG}}$.

Using the explicit representations (5.22), it is easy to see that

$$G_0^{(+)}(x^A, x'^A) = \overline{G_0^{(+)}(x, x')} = G_0^{(-)}(x, x'). \tag{5.50}$$

Introducing the map $(J^A\varphi)(x) := \varphi(x^A)$, (5.50) implies

$$J^A \Pi_0^{(+)} J^A = \Pi_0^{(-)}, \quad J^A(\mathcal{Z}_0^{(\pm)}) = \mathcal{Z}_0^{(\mp)}. \tag{5.51}$$

Now let $\alpha \in \mathbb{C}$ with $|\alpha| < 1$. We define a Bogoliubov transformation R_α on $\mathcal{W}_{\mathrm{KG}}$ (i.e., a real pseudounitary map) via

$$(R_\alpha\varphi)(x) = \frac{1}{\sqrt{1 - |\alpha|^2}}\varphi(x) + \frac{\overline{\alpha}}{\sqrt{1 - |\alpha|^2}}\varphi(x^A), \quad \varphi \in \mathcal{Z}_0^{(+)}; \tag{5.52}$$

$$(R_\alpha\overline{\varphi})(x) = \frac{1}{\sqrt{1 - |\alpha|^2}}\overline{\varphi(x)} + \frac{\alpha}{\sqrt{1 - |\alpha|^2}}\overline{\varphi(x^A)}, \quad \overline{\varphi} \in \mathcal{Z}_0^{(-)}. \tag{5.53}$$

In other words, as a 2×2 matrix on $\mathcal{Z}_0^{(+)} \oplus \mathcal{Z}_0^{(-)}$,

$$R_\alpha = \begin{bmatrix} \mathbb{1} & \frac{\overline{\alpha}}{\sqrt{1-|\alpha|^2}} J^A \\ \frac{\alpha}{\sqrt{1-|\alpha|^2}} J^A & \frac{1}{\sqrt{1-|\alpha|^2}} \end{bmatrix} \tag{5.54}$$

The projections $R_\alpha \Pi_0^{(\pm)} R_\alpha^{-1}$ define another fundamental decomposition of $\mathcal{W}_{\mathrm{KG}}$, hence another Fock vacuum, called the α-vacuum. Their two-point functions are given by the Klein-Gordon kernels of $\pm R_\alpha \Pi_0^{(\pm)} R_\alpha^{-1}$. Using (5.54) and $G_0^{(\pm)}(x^A, x') = G_0^{(\mp)}(x, x'^A)$ we obtain

$$\begin{aligned} &G_\alpha^{(\pm)}(x, x') \\ &= \frac{1}{1-|\alpha|^2}\Big(\tfrac{1+|\alpha|^2}{2} G_0^{\mathrm{sym}}(x,x') \mp \mathrm{i} \tfrac{1-|\alpha|^2}{2} G^{\mathrm{PJ}}(x,x') + \tfrac{\alpha+\overline{\alpha}}{2} G_0^{\mathrm{sym},A}(x,x') - \mathrm{i} \tfrac{\alpha-\overline{\alpha}}{2} G_0^{\mathrm{PJ},A}(x,x') \Big). \end{aligned} \tag{5.55}$$

From (5.55), we obtain the well-known expressions for the Feynman and anti-Feynman propagator [4, 17]:[4]

$$\begin{aligned} &G_\alpha^{\mathrm{F}/\overline{\mathrm{F}}}(x, x') \\ &= G_0^{\mathrm{F}/\overline{\mathrm{F}}}(x,x') \pm \frac{\mathrm{i}}{1-|\alpha|^2}\Big(|\alpha|^2 G_0^{\mathrm{sym}}(x,x') + \mathrm{i} \tfrac{\alpha+\overline{\alpha}}{2} G_0^{\mathrm{sym},A}(x,x') - \mathrm{i} \tfrac{\alpha-\overline{\alpha}}{2} G_0^{\mathrm{PJ},A}(x,x') \Big). \end{aligned} \tag{5.56}$$

It is known that only the α-vacuum satisfying the Hadamard condition is the Euclidean vacuum, that is, corresponding to $\alpha = 0$ (see [4] and references therein). This can also be read off the expansion of the Gegenbauer function around the singularity.

From the point of view of perturbative QFT, the usefulness of alpha vacua for $\alpha \neq 0$ is therefore questionable. It is not clear how one can renormalize quantities that are local and non-linear in the fields [24]. However, they are reasonable objects in *linear* QFT and possibly also in an effective field-theory. We shall see that the operator-theoretic propagators correspond to field expectation values in specific alpha vacua.

5.6.2 Alpha vacua and mode expansions

In the literature α-vacua are often introduced as follows [4, 17]. First one expands the real scalar Klein-Gordon field $\hat{\phi}(x)$ into modes with respect to the Euclidean vacuum,

$$\hat{\phi}(x) = \sum_n \varphi_n(x) \hat{a}_n^* + \overline{\varphi_n(x)} \hat{a}_n. \tag{5.57}$$

Here, $\hat{a}_n$ and $\hat{a}_n^*$ are annihilation and creation operators and $\varphi_n(x)$ are mode functions that satisfy the orthogonality relations (2.65) with the Dirac delta replaced by the Kronecker delta.

[4] Note that the two references have different conventions for the parameter α, and in addition, both conventions are different from ours. In particular, [4] uses two real labels α, β that are both described by a single $\alpha \in \mathbb{C}$ in our notation.

This is essentially a choice of an orthonormal basis of the space $\mathcal{Z}_0^{(+)}$. The positive frequency solution can then be written as a mode sum,

$$G_0^{(+)}(x,x') = \sum_n \overline{\varphi_n(x)}\varphi_n(x'). \tag{5.58}$$

Next, using the explicit form of the modes, one shows [4, 17] that the modes associated to the Euclidean vacuum can be chosen to satisfy

$$\varphi_n(x) = \overline{\varphi_n(x^A)}. \tag{5.59}$$

Then one defines the Bogoliubov transformation (5.52) by its action on the modes,

$$\varphi_{\alpha,n}(x) := \frac{1}{\sqrt{1-|\alpha|^2}}\varphi_n(x) + \frac{\overline{\alpha}}{\sqrt{1-|\alpha|^2}}\overline{\varphi_n(x)}, \tag{5.60}$$

and the positive frequency solution associated to the alpha vacuum with parameter α is given by

$$G_\alpha^{(+)}(x,x') = \sum_n \overline{\varphi_{\alpha,n}(x)}\varphi_{\alpha,n}(x'). \tag{5.61}$$

Needless to say, the construction using the mode expansion and the construction based on (5.54) are equivalent. In particular, $\varphi_{\alpha,n} = R_\alpha \varphi_n$.

5.6.3 Correlation functions between two different alpha vacua

Suppose now that α, β be two complex parameter with $|\alpha|, |\beta| < 1$ and consider a pair of Bogoliubov transformations R_α, R_β and a pair of Fock vacua Ω_α, Ω_β. Using modes, we can write

$$\begin{aligned}
\varphi_{\beta,n}(x) &:= N_{\alpha,\beta}\varphi_{\alpha,n}(x) + M_{\alpha,\beta}\overline{\varphi_{\alpha,n}(x)}, \\
N_{\alpha,\beta} &= \frac{1-\overline{\beta}\alpha}{\sqrt{(1-|\alpha|^2)(1-|\beta|^2)}}, \\
M_{\alpha,\beta} &= \frac{\overline{\beta}-\overline{\alpha}}{\sqrt{(1-|\alpha|^2)(1-|\beta|^2)}}.
\end{aligned} \tag{5.62}$$

Note that this definition is a special case of the more general form (2.71). It relates to the latter equation via

$$N_{\alpha,\beta} = N_{\alpha,\beta}(n), \quad M_{\alpha,\beta}\delta_{n,m} = \Lambda_{\alpha,\beta}(n,m). \tag{5.63}$$

Therefore, we may use (2.78) to obtain the mixed two-point functions

$$\begin{aligned}
&G_{\alpha,\beta}^{(\pm)}(x,x') \\
&= \frac{1}{1-\overline{\beta}\alpha}\Big(\tfrac{1+\alpha\overline{\beta}}{2}G_0^{\mathrm{sym}}(x,x') \mp \mathrm{i}\tfrac{1-\alpha\overline{\beta}}{2}G^{\mathrm{PJ}}(x,x') + \tfrac{\alpha+\overline{\beta}}{2}G_0^{\mathrm{sym},A}(x,x') - \mathrm{i}\tfrac{\alpha-\overline{\beta}}{2}G_0^{\mathrm{PJ},A}(x,x')\Big).
\end{aligned} \tag{5.64}$$

The corresponding Feynman and anti-Feynman propagator are

$$G^{\mathrm{F}/\overline{\mathrm{F}}}_{\alpha,\beta}(x,x') \tag{5.65}$$
$$= G^{\mathrm{F}/\overline{\mathrm{F}}}_0(x,x') \pm \frac{\mathrm{i}}{1-\overline{\beta}\alpha}\Big(\alpha\overline{\beta}G^{\mathrm{sym}}_0(x,x') + \mathrm{i}\tfrac{\alpha+\overline{\beta}}{2}G^{\mathrm{sym},A}_0(x,x') - \mathrm{i}\tfrac{\alpha-\overline{\beta}}{2}G^{\mathrm{PJ},A}_0(x,x')\Big).$$

5.7 "In" and "out" vacua

The de Sitter space is not asymptotically stationary. Therefore, the usual definition of "in" and "out" vacua is not applicable. Nevertheless, one can define a pair of de Sitter invariant states that deserve to be called the "in" and "out" vacuum. In this subsection we will compute the corresponding propagators.

Every bisolution of the Klein-Gordon equation is a linear combination of appropriately regularized functions $\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(Z)$ and $\mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(Z)$. They behave for large Z proportionally to $Z^{-\frac{d-1}{2}-\mathrm{i}\nu}$, resp. $Z^{-\frac{d-1}{2}+\mathrm{i}\nu}$. We are looking for two-point functions, which in the "causal asymptotic region", that is for $Z\to\infty$ and $t\to\pm\infty$, have a *definite behavior*, that is, they behave either as $cZ^{-\frac{d-1}{2}-\mathrm{i}\nu}$, or as $cZ^{-\frac{d-1}{2}+\mathrm{i}\nu}$.

Note that the propagators have also the "antipodal asymptotic region": $Z\to-\infty, t^A\to\pm\infty$. It will be interesting to determine their behavior in that region as well.

The following theorem describes all de Sitter invariant two-point functions with a definite behavior in the causal asymptotic region.

Theorem 5.5. *1.* **Odd dimensions.** *There exists a unique α-vacuum with the propagators behaving as*

$$G^{(\pm)}_\alpha \sim cZ^{-\frac{d-1}{2}\pm\mathrm{i}\nu},\quad Z\to+\infty,\quad t\to-\infty; \tag{5.66}$$
$$\textit{and}\quad G^{(\pm)}_\alpha \sim cZ^{-\frac{d-1}{2}\mp\mathrm{i}\nu},\quad Z\to+\infty,\quad t\to+\infty. \tag{5.67}$$

These functions vanish for $Z<-1$ and their parameter α is

$$\alpha_- = \alpha_+ = \alpha_{\mathrm{as}} := (-1)^{\frac{d+1}{2}}\mathrm{e}^{-\pi\nu} = \mathrm{e}^{-\pi\nu\pm\mathrm{i}\pi\frac{d+1}{2}}. \tag{5.68}$$

This vacuum could be called the "in" vacuum or the "out" vacuum. We will call it the asymptotic vacuum. *We will write* as *instead of α_{as} in the subscripts of propagators and two-point functions. The two point functions of these states are*

$$\frac{\mathrm{i}\sinh\pi\nu}{2^{\frac{d-3}{2}}\sqrt{\pi}C_{d,\nu}}G^{(\pm)}_{\mathrm{as}}(x,x') \tag{5.69}$$
$$= \frac{2^{-\mathrm{i}\nu}\theta(\pm t)}{\Gamma\big(\frac{d-1}{2}-\mathrm{i}\nu\big)}\Big(\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z-\mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z+\mathrm{i}0)\Big)$$
$$+ \frac{2^{\mathrm{i}\nu}\theta(\mp t)}{\Gamma\big(\frac{d-1}{2}+\mathrm{i}\nu\big)}\Big(\mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z-\mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z+\mathrm{i}0)\Big),$$

and their Feynman and anti-Feynman propagators coincide with the operator-theoretic ones from (5.31)*:*

$$G^{\mathrm{F}}_{\mathrm{as}}(x,x') = G^{\mathrm{F}}_{\mathrm{op}}(x,x'), \quad G^{\overline{\mathrm{F}}}_{\mathrm{as}}(x,x') = G^{\overline{\mathrm{F}}}_{\mathrm{op}}(x,x'). \tag{5.70}$$

2. **Even dimensions.** *There exist two α-vacua that satisfy* (5.66) *and* (5.67)*. One of the two values is*

$$\alpha_- = \mathrm{i}\mathrm{e}^{-\pi\nu}(-1)^{\frac{d}{2}} = \mathrm{e}^{-\pi\nu + \mathrm{i}\pi\frac{d+1}{2}} \tag{5.71}$$

and its positive/negative frequency solutions vanish for $Z < -1$, $t^A < 0$. It will be called the "in" vacuum.

The other value is

$$\alpha_+ = -\mathrm{i}\mathrm{e}^{-\pi\nu}(-1)^{\frac{d}{2}} = \mathrm{e}^{-\pi\nu - \mathrm{i}\pi\frac{d+1}{2}} = -\alpha_- \tag{5.72}$$

and its positive/negative frequency solutions vanish for $Z < -1$, $t^A > 0$. It will be called the "out" vacuum.

We will write $-$, resp. $+$ instead of α_- and α_+ in subscripts. The two-point functions of these states are

$$\begin{aligned}
&\frac{\mathrm{i}\sinh\pi\nu}{2^{\frac{d-3}{2}}\sqrt{\pi}C_{d,\nu}} G^{(\pm)}_{-}(x,x') \\
&= \frac{2^{-\mathrm{i}\nu}\theta(\pm t)}{\Gamma\big(\frac{d-1}{2} - \mathrm{i}\nu\big)}\Big(\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z - \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z + \mathrm{i}0)\Big) \\
&\quad + \frac{2^{\mathrm{i}\nu}\theta(\mp t)}{\Gamma\big(\frac{d-1}{2} + \mathrm{i}\nu\big)}\Big(\mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z - \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z + \mathrm{i}0)\Big) \\
&\quad + \frac{(-1)^{\frac{d}{2}}\theta(t^A)}{2^{\frac{d-3}{2}}\sqrt{\pi}}\Big(\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(Z + \mathrm{i}0) - \mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(Z - \mathrm{i}0)\Big),
\end{aligned} \tag{5.73}$$

and

$$\begin{aligned}
&\frac{\mathrm{i}\sinh\pi\nu}{2^{\frac{d-3}{2}}\sqrt{\pi}C_{d,\nu}} G^{(\pm)}_{+}(x,x') \\
&= \frac{2^{-\mathrm{i}\nu}\theta(\pm t)}{\Gamma\big(\frac{d-1}{2} - \mathrm{i}\nu\big)}\Big(\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z - \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z + \mathrm{i}0)\Big) \\
&\quad + \frac{2^{\mathrm{i}\nu}\theta(\mp t)}{\Gamma\big(\frac{d-1}{2} + \mathrm{i}\nu\big)}\Big(\mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z - \mathrm{i}0) - \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z + \mathrm{i}0)\Big) \\
&\quad + \frac{(-1)^{\frac{d}{2}}\theta(-t^A)}{2^{\frac{d-3}{2}}\sqrt{\pi}}\Big(\mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(Z + \mathrm{i}0) - \mathbf{S}_{\frac{d-2}{2},\mathrm{i}\nu}(Z - \mathrm{i}0)\Big).
\end{aligned} \tag{5.74}$$

The in-out Feynman and the out-in anti-Feynman propagator coincide with the operator-theoretic Feynman and anti-Feynman propagator (5.34)*, resp.:*

$$G^{\mathrm{F}}_{+-} = G^{\mathrm{F}}_{\mathrm{op}}; \quad G^{\overline{\mathrm{F}}}_{-+} = G^{\overline{\mathrm{F}}}_{\mathrm{op}}. \tag{5.75}$$

Remark 5.6. The concrete values for α corresponding to "in" and "out" states are well-known [17, 68] but typically derived by asymptotic properties of the modes. We derive them in the following using a "global picture".

Proof of Thm 5.5. We use (5.55) to express a generic $G^{(\pm)}_\alpha$ in terms of $\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}$ and $\mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}$:

$$\begin{aligned}
&2\mathrm{i}(1-|\alpha|^2)\frac{\sinh\pi\nu}{2^{\frac{d-3}{2}}\sqrt{\pi}C_{d,\nu}}G^{(\pm)}_\alpha \qquad (5.76)\\
&= -\frac{2^{-\mathrm{i}\nu}}{\Gamma\big(\frac{d-1}{2}-\mathrm{i}\nu\big)}\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z+\mathrm{i}0)\Big(\big(1+|\alpha|^2\pm(1-|\alpha|^2)\,\mathrm{sgn}(t)\big)\\
&\qquad\qquad + \big(2\,\mathrm{Re}(\alpha)+2\mathrm{i}\,\mathrm{Im}(\alpha)\,\mathrm{sgn}(t^A)\big)\mathrm{e}^{\mathrm{i}\pi\left(\frac{d-1}{2}+\mathrm{i}\nu\right)}\Big)\\
&\quad -\frac{2^{-\mathrm{i}\nu}}{\Gamma\big(\frac{d-1}{2}-\mathrm{i}\nu\big)}\mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z-\mathrm{i}0)\Big(\big(1+|\alpha|^2\mp(1-|\alpha|^2)\,\mathrm{sgn}(t)\big)\\
&\qquad\qquad + \big(2\,\mathrm{Re}(\alpha)-2\mathrm{i}\,\mathrm{Im}(\alpha)\,\mathrm{sgn}(t^A)\big)\mathrm{e}^{-\mathrm{i}\pi\left(\frac{d-1}{2}+\mathrm{i}\nu\right)}\Big)\\
&\quad -(\nu\leftrightarrow-\nu).
\end{aligned}$$

The analysis of the asymptotic behavior of the latter function differs in odd and even dimensions. We only display the derivation of the more complicated even-dimensional case. The odd-dimensional case can be worked out analogously:

Even dimensions The conditions on the asymptotic behavior read:

$$\text{Solution } G^{(\pm)}_\alpha \sim \mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(Z) \text{ for } Z>1: \tag{5.77a}$$
$$\mp(-1)^{\frac{d-2}{2}}2\mathrm{i}\,\mathrm{sgn}(t)\,\mathrm{Re}(\alpha) = \mathrm{e}^{\mp\,\mathrm{sgn}(t)\pi\nu} - |\alpha|^2\mathrm{e}^{\pm\,\mathrm{sgn}(t)\pi\nu},$$
$$\text{Solution } G^{(\pm)}_\alpha \sim \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(Z) \text{ for } Z>1: \tag{5.77b}$$
$$\mp(-1)^{\frac{d-2}{2}}2\mathrm{i}\,\mathrm{sgn}(t)\,\mathrm{Re}(\alpha) = \mathrm{e}^{\pm\,\mathrm{sgn}(t)\pi\nu} - |\alpha|^2\mathrm{e}^{\mp\,\mathrm{sgn}(t)\pi\nu},$$
$$\text{Solution } G^{(\pm)}_\alpha \sim \mathbf{Z}_{\frac{d-2}{2},\mathrm{i}\nu}(-Z) \text{ for } Z<-1: \tag{5.77c}$$
$$(-1)^{\frac{d-2}{2}}(1+|\alpha|^2) = -2\mathrm{i}\,\mathrm{Re}(\alpha)\sinh\pi\nu + 2\,\mathrm{Im}(\alpha)\,\mathrm{sgn}(t^A)\cosh\pi\nu,$$
$$\text{Solution } G^{(\pm)}_\alpha \sim \mathbf{Z}_{\frac{d-2}{2},-\mathrm{i}\nu}(-Z) \text{ for } Z<-1: \tag{5.77d}$$
$$(-1)^{\frac{d-2}{2}}(1+|\alpha|^2) = 2\mathrm{i}\,\mathrm{Re}(\alpha)\sinh\pi\nu + 2\,\mathrm{Im}(\alpha)\,\mathrm{sgn}(t^A)\cosh\pi\nu.$$

We immediately read off $\mathrm{Re}(\alpha) = 0$. Then, by (5.77a) and (5.77b), the existence of a definite behavior in the region $Z > 1$ implies $|\alpha| = \mathrm{e}^{-\pi\nu}$. Hence $\alpha = \mathrm{e}^{\mathrm{i}\pi(n+\frac{1}{2})-\pi\nu}$ with $n \in \mathbb{Z}$. Then (5.77c) and (5.77d) simplify to

$$(-1)^{\frac{d-2}{2}-n} = \mathrm{sgn}(t^A). \tag{5.78}$$

$n = \frac{d-2}{2}$ yields a solution that vanishes for $Z < -1$ and $t^A > 0$ but has indeterminate behavior as $Z < -1$ and $t^A \to -\infty$, while $n = \frac{d}{2}$ yields a solution that vanishes for $Z < -1$ and $t^A < 0$ but has indeterminate behavior as $Z < -1$ and $t^A \to +\infty$. We obtain the values for α_+ and α_-.

Inserting the obtained values for α into (5.76) yields the explicit formulas for $G_\pm^{(\pm)}$: this rather cumbersome computation involves the connection formula (B.11), the identity (B.12) and repeated use of identities of the type $1 \pm \mathrm{sgn}(\cdot) = 2\theta(\pm\cdot)$. The (anti-)Feynman propagators are obtained from (5.65) and also using the connection formulas. □

5.8 Symmetric Scarf Hamiltonian

We will discuss in the next subsection another approach to the Klein-Gordon equation on the de Sitter space. In this approach we will use the one-dimensional Schrödinger Hamiltonian on $L^2(\mathbb{R})$ of the form

$$H_\alpha^{\mathrm{S}} := -\partial_\tau^2 - \frac{\alpha^2 - \frac{1}{4}}{\cosh(\tau)^2}. \tag{5.79}$$

It is sometimes called *symmetric Scarf Hamiltonian* [43]. It is well-known that this Hamiltonian for some values of parameters is reflectionless. For completeness, let us verify this.

First we check that $H_\alpha^{\mathrm{S}} + \lambda^2$ is equivalent to the Gegenbauer equation after the consecutive change of variables $\sinh\tau = w$, $\mathrm{i}w = v$:

$$\begin{aligned} &\cosh(\tau)^{-\alpha-\frac{1}{2}}\big(H_\alpha^{\mathrm{S}} + \lambda^2\big)\cosh(\tau)^{\alpha+\frac{1}{2}} \\ &= -\partial_\tau^2 - (2\alpha+1)\tanh(\tau)\partial_\tau - \big(\alpha + \tfrac{1}{2}\big)^2 + \lambda^2 \\ &= -(1+w^2)\partial_w^2 - 2(\alpha+1)w\partial_w - \big(\alpha + \tfrac{1}{2}\big)^2 + \lambda^2 \\ &= (1-v^2)\partial_v^2 - 2(\alpha+1)v\partial_v - \big(\alpha + \tfrac{1}{2}\big)^2 + \lambda^2. \end{aligned} \tag{5.80}$$

For $\mathrm{Re}(\lambda) > 0$, the Jost solutions can thus be expressed in terms of the Gegenbauer Z-function:

$$\psi_\pm(\lambda,\tau) = 2^{\mp\lambda}\Gamma(1\pm\lambda)\mathrm{e}^{\mathrm{i}\frac{\pi}{2}(\frac{1}{2}+\alpha\pm\lambda)}\cosh(\tau)^{\alpha+\frac{1}{2}} Z_{\alpha,\pm\lambda}(\pm\mathrm{i}\sinh\tau), \tag{5.81}$$

such that

$$\psi_\pm(\lambda,\tau) \sim \mathrm{e}^{\mp\lambda\tau}, \quad \pm\tau \to \infty. \tag{5.82}$$

The Gegenbauer functions on the righthand-side of (5.81) have purely imaginary arguments. They are to be interpreted as living on the cut plane $\mathbb{C} \setminus \big(]-\infty,-1] \cup [1,\infty[\big)$ instead of the usual $\mathbb{C}\backslash]-\infty,1]$. $\psi_+(\lambda,\cdot)$ is expressed in terms of the analytic continuation of $Z_{\alpha,\lambda}(w)$ defined on the standard sheet $\mathbb{C}\backslash]-\infty,1]$ *to the upper half-plane*, while $\psi_-(\lambda,\cdot)$ is expressed in terms of the analytic continuation of $Z_{\alpha,-\lambda}(w)$ defined on the standard sheet $\mathbb{C}\backslash]-\infty,1]$ *to the lower half plane*. Using the connection formulas (B.10) and (B.11), and the fact that $\mathbf{S}_{\alpha,\lambda}$ is holomorphic on $]-1,1[$, one can derive a connection formula for the two holomorphic continuations:

$$\begin{aligned}&\mathbf{Z}_{\alpha,\lambda}(w+\mathrm{i}0) \\ =&\ \frac{\mathrm{i}\cos\pi\alpha\,\mathrm{e}^{-\mathrm{i}\pi(\alpha+\lambda)}\mathbf{Z}_{\alpha,\lambda}(w-\mathrm{i}0)}{\sin\pi\lambda}-\frac{\mathrm{i}2^{2\lambda}\mathrm{e}^{-\mathrm{i}\pi\alpha}\pi\mathbf{Z}_{\alpha,-\lambda}(w-\mathrm{i}0)}{\Gamma\big(\frac{1}{2}+\alpha+\lambda\big)\Gamma\big(\frac{1}{2}-\alpha+\lambda\big)\sin\pi\lambda},\quad w\in]-1,1[.\end{aligned}\tag{5.83}$$

In particular, $\mathbf{Z}_{\alpha,\lambda}(w+\mathrm{i}0)$ is proportional to $\mathbf{Z}_{\alpha,-\lambda}(w-\mathrm{i}0)$ if and only if $\cos\pi\alpha=0$, i.e., if and only if $\alpha\in\mathbb{Z}+\frac{1}{2}$.

Consequently, the symmetric Scarf Hamiltonian is reflectionless for all energies ν^2 iff $\alpha\in\mathbb{Z}+\frac{1}{2}$.

5.9 Partial wave decomposition

Using the global system of coordinates (5.7), the de Sitter space can be viewed as a FLRW space, and can be identified with $\mathbb{R}\times\mathbb{S}^{d-1}$. In these coordinates, the (gauged) Klein-Gordon operator takes the form

$$\begin{aligned}&\cosh(\tau)^{\frac{d-1}{2}}\big(-\square_g+m^2\big)\cosh(\tau)^{-\frac{d-1}{2}}\\ =&\ \partial_\tau^2-\frac{d-1}{2}\Big(1+\frac{(d-3)\sinh(\tau)^2}{2\cosh(\tau)^2}\Big)-\frac{\Delta_{\mathbb{S}^{d-1}}}{\cosh(\tau)^2}+m^2\\ =&\ \partial_\tau^2+\frac{\big(\frac{d-2}{2}\big)^2-\frac{1}{4}-\Delta_{\mathbb{S}^{d-1}}}{\cosh(\tau)^2}+\nu^2\end{aligned}\tag{5.84}$$

The spectrum of $-\Delta_{\mathbb{S}^{d-1}}$ is $\{l(l+d-2)\mid l\in\mathbb{N}_0\}$. Hence, restricted to eigenfunctions with eigenvalue $l(l+d-2)$, the above operator becomes $-H_\alpha^{\mathrm{S}}+\nu^2$, where H_α^{S} is the *symmetric Scarf Hamiltonian* with $\alpha=l+\frac{d-2}{2}$. The symmetric Scarf potential is reflectionless for all energies $\nu^2\in\mathbb{R}$ and $\alpha\in\frac{1}{2}+\mathbb{Z}$. This corresponds to odd dimensions. Thus for each mode the in-state coincides with the out-state. In even dimensions $\alpha\in\mathbb{Z}$, and then for each mode the in-state is different from the out-state.

6 Anti-de Sitter space and its universal cover

Our final examples of Lorentzian manifolds are the d-dimensional anti-de Sitter space AdS_d and its universal covering $\widetilde{\mathrm{AdS}}_d$.

AdS_d is pathological from several points of view. First of all, it has time loops, which makes it unsuitable as a model of a spacetime. It does not make much sense to speak about propagators on AdS_d.

The cyclicity of time can be cured by replacing the proper anti-de Sitter space by its universal cover $\widetilde{\mathrm{AdS}}_d$. It is still not globally hyperbolic, because of a boundary with a spacelike normal at spacelike infinity. However the latter problem is not very serious, and various propagators can be defined on $\widetilde{\mathrm{AdS}}_d$.

Therefore, most of this section will be devoted to $\widetilde{\mathrm{AdS}}_d$. We will apply two methods to define propagators: through the resolvent of the d'Alembertian on $L^2(\widetilde{\mathrm{AdS}}_d)$, and by considering the evolution of the Cauchy data. The latter approach is facilitated by the fact that $\widetilde{\mathrm{AdS}}_d$ is static. The absence of global hyperbolicity is not a problem for the first approach. For the second approach it manifests itself by the need to set boundary conditions at the spatial infinity for m^2 below a certain value.

Various propagators of massive scalar fields on $\widetilde{\mathrm{AdS}}_d$ have been intensively studied. Among the vast literature, we mention the references [1, 3, 6, 18, 20, 26, 34, 35, 45, 62, 78], which are particularly useful for understanding the analytic structure. Similar to the de Sitter example, the only of these references using the operator-theoretic view on the Feynman propagator is [78] (here in two dimensions). The references [18, 20] have an axiomatic approach. Appendix A of [3] is particularly helpful to understand the analytic structure of propagators on the universal cover. Subsection 6.3.4, where we present the approach based on the evolution of Cauchy data, is based on the seminal work [62].

6.1 Geometry of anti-de Sitter space

The d-dimensional anti-de Sitter space AdS_d can be defined as an embedded submanifold of $\mathbb{R}^{2,d-1}$:

$$\mathrm{AdS}_d = \{x \in \mathbb{R}^{2,d-1} \mid \langle x|x\rangle = -1\}, \tag{6.1}$$

where

$$\langle x|x'\rangle := -x^0x'^0 - x^dx'^d + \sum_{i=1}^{d-1} x^ix'^i =: Z(x,x') \equiv Z. \tag{6.2}$$

A coordinate system covering all of AdS_d is given by

$$\begin{gathered} x^0 = \cosh\rho\cos\tau, \quad x^i = \sinh\rho\,\Omega^i, \quad x^d = \cosh\rho\sin\tau, \\ \text{where} \quad \tau\in[-\pi,\pi[,\ \rho\in\mathbb{R}_{\geq 0},\ \Omega\in\mathbb{S}_{d-2}\hookrightarrow\mathbb{R}^{d-1} \quad \text{and} \quad i=1,\dots,d-1. \end{gathered} \tag{6.3}$$

In these coordinates, the line element reads

$$\mathrm{d}s^2 = -\cosh(\rho)^2\mathrm{d}\tau^2 + \mathrm{d}\rho^2 + \sinh(\rho)^2\mathrm{d}\Omega^2. \tag{6.4}$$

Note the famous cyclicity of time, $x(\tau + 2\pi k, \rho, \Omega) = x(\tau, \rho, \Omega)$ for all $k \in \mathbb{Z}$. Therefore, AdS_d has closed timelike curves and is not globally hyperbolic.

AdS_d is equipped with an involution $x \mapsto -x$. This involution maps the coordinates (τ, ρ, Ω) to $(\tau + \pi, \rho, -\Omega)$.

Another system of coordinates is obtained by replacing ρ with $u \in [0, \frac{\pi}{2}[$, where $\sinh \rho = \tan u$. In these coordinates, the line element (6.4) becomes

$$\mathrm{d}s^2 = \frac{-\mathrm{d}\tau^2 + \mathrm{d}u^2 + \sin(u)^2\,\mathrm{d}\Omega^2}{\cos(u)^2}. \tag{6.5}$$

In the coordinates (6.3) and (6.5), we find

$$Z = -\cosh\rho\cosh\rho'\cos(\tau - \tau') + \sinh\rho\sinh\rho'\cos\theta \tag{6.6}$$

$$= -\frac{\cos(\tau - \tau')}{\cos u \cos u'} + \frac{\sin u \sin u' \cos\theta}{\cos u \cos u'}. \tag{6.7}$$

where θ is the angle between Ω and Ω'.

Let us fix the vector $x' = (1, 0 \ldots, 0)$. Then $-\langle x|x'\rangle = \frac{\cos\tau}{\cos u}$ and we can partition AdS_d into the following regions:

$$V_0 := \{|\tau| < u\}, \tag{6.8a}$$

$$V_2 := \{\pi - \tau < u\} \cup \{\pi + \tau < u\}, \tag{6.8b}$$

$$V_1 := \{\min(\tau, \pi - \tau) > u\}, \tag{6.8c}$$

$$V_{-1} := \{\min(-\tau, \pi + \tau) > u\}. \tag{6.8d}$$

Note that

$$-Z > 1, \quad \tau \in [-\tfrac{\pi}{2}, \tfrac{\pi}{2}] \qquad \text{on } V_0, \tag{6.9a}$$

$$Z > 1, \quad \tau \in [-\pi, -\tfrac{\pi}{2}] \cup [\tfrac{\pi}{2}, \pi] \qquad \text{on } V_2, \tag{6.9b}$$

$$|Z| < 1, \quad \tau \in [0, \pi] \qquad \text{on } V_1, \tag{6.9c}$$

$$|Z| < 1, \quad \tau \in [-\pi, 0] \qquad \text{on } V_{-1}. \tag{6.9d}$$

The Klein-Gordon equation on anti de Sitter space reads

$$(-\Box + m^2)\phi(x) = 0. \tag{6.10}$$

Instead of m we will use the parameter ν

$$\nu := \sqrt{m^2 + \left(\tfrac{d-1}{2}\right)^2}, \tag{6.11}$$

where as usual we use the principal branch of the square root. Thus (6.10) is replaced with

$$\Big(-\Box - \left(\tfrac{d-1}{2}\right)^2 + \nu^2\Big)\phi(x) = 0. \tag{6.12}$$

The Klein-Gordon equation on anti de Sitter space restricted to invariant solutions and written in terms of Z reduces to the Gegenbauer equation, where the sign in front of ν^2 is opposite from de Sitter space:

$$\Big((1-Z^2)\partial_Z^2 - dZ\partial_Z + \nu^2 - \big(\tfrac{d-1}{2}\big)^2\Big)f(Z) = 0. \tag{6.13}$$

6.2 Universal cover of anti de Sitter space

AdS_d has the topology of $\mathbb{S}_1 \times \mathbb{R}^{d-1}$. Therefore it has a universal covering space

$$\widetilde{\mathrm{AdS}}_d \to \mathrm{AdS}_d. \tag{6.14}$$

In the literature, this universal cover is sometimes called anti-de Sitter space instead [57]. We will, however, use the name anti-de Sitter space for the embedded submanifold (6.1), adding the adjective "proper" whenever we think it is necessary to avoid confusion.

It is easy to describe $\widetilde{\mathrm{AdS}}_d$ in coordinates: we just assume that $\tau \in \mathbb{R}$, and keep the line element (6.4) or (6.5). $\widetilde{\mathrm{AdS}}_d$ is a static Lorentzian manifold. It is still not globally hyperbolic, since there are geodesics, which in finite time escape to its boundary.

Let us fix the vector $x' = (1, 0 \dots, 0)$. Then we can partition $\widetilde{\mathrm{AdS}}_d$ into the following regions:

$$V_{2n} := \{|\tau - n\pi| < u\}, \tag{6.15}$$
$$V_{2n+1} := \{\min(\tau - n\pi, (n+1)\pi - \tau) > u\}. \tag{6.16}$$

Note that

$$-(-1)^n Z > 1, \quad \tau \in [(n-\tfrac{1}{2})\pi, (n+\tfrac{1}{2})\pi] \qquad \text{on } V_{2n} \tag{6.17}$$
$$|Z| < 1, \quad \tau \in [n\pi, (n+1)\pi] \qquad \text{on } V_{2n+1}. \tag{6.18}$$

The spaces AdS_d and $\widetilde{\mathrm{AdS}}_d$ with their various regions are depicted in Figure 2.

6.3 Wick rotation

Anti-de Sitter space is closely related to the hyperbolic space

$$\mathbb{H}^d := \{x \in \mathbb{R}^{1,d} \mid [x|x] = -1\}, \tag{6.19}$$

where

$$[x|x'] = -x^0 x'^0 + \sum_{i=1}^{d} x^i x'^i, \tag{6.20}$$

as in (5.1). Let Δ^{h} be the Laplace-Beltrami operator on $\mathbb{H}^d$. Set

$$G^{\mathrm{h}}(-\nu^2) := \Big(-\Delta^{\mathrm{h}} - (\tfrac{d-1}{2})^2 + \nu^2\Big)^{-1}. \tag{6.21}$$

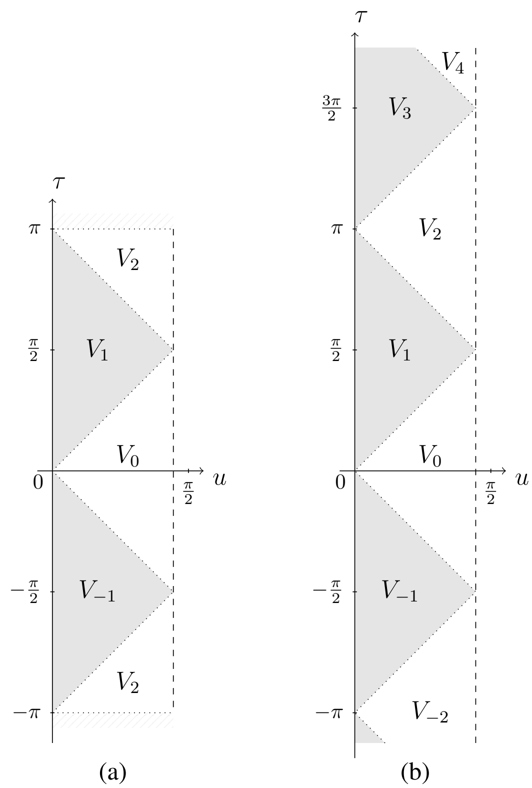

Figure 2: (a) Anti-de Sitter space in the coordinates $u \in [0, \frac{\pi}{2}[$ and $\tau \in]-\pi, \pi]$ from (6.5) and its partition into the regions V_0, V_2, V_1 and V_{-1}. Each point represents a $d-2$-sphere of the coordinates Ω. The lines $\tau = \pi$ and $\tau = -\pi$ are glued together, reflecting the cyclicity of time. An observer can reach spatial infinity ($u = \frac{\pi}{2}$, indicated by the dashed line) in finite time, which makes it necessary to impose boundary conditions when solving the Cauchy problem for certain masses, see Section 6.3.4. (b) The universal cover of anti-de Sitter space in the same coordinates, where however τ ranges over all of $\mathbb{R}$, removing the cylicity of time. The boundary at $u = \frac{\pi}{2}$ is still present.

For $\mathrm{Re}(\nu) > 0$, the integral kernel of $G^{\mathrm{h}}(-\nu^2)$ can be expressed in terms of the invariant quantity $[x|x']$ and the Gegenbauer function $\mathbf{Z}_{\alpha,\lambda}(w)$ as (see e.g. [36,37], and for an equivalent expression in terms of associated Legendre functions [31])

$$G^{\mathrm{h}}\big(-\nu^2; x, x'\big) = \frac{\sqrt{\pi}\Gamma(\frac{d-1}{2} + \nu)}{\sqrt{2}(2\pi)^{\frac{d}{2}} 2^{\nu}} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-[x|x']\big). \tag{6.22}$$

Let us try to introduce a kind of a Wick rotation from $\mathbb{H}^d$ to anti-de Sitter space by replacing x^d with $\pm \mathrm{i} x^d$. We have

$$[x|x'] = -1 - \frac{[x - x'|x - x']}{2}, \quad x, x' \in \mathbb{H}^d, \tag{6.23}$$
$$Z := \langle x|x'\rangle = -1 - \frac{\langle x - x'|x - x'\rangle}{2}, \quad x, x' \in \mathrm{AdS}_d.$$

Thus, similar to the case of de Sitter space, we have to replace $-[x|x']$ in the argument of the Gegenbauer function in (6.22) by $-\big(\langle x|x'\rangle \mp \mathrm{i}0\big) = -\langle x|x'\rangle \pm \mathrm{i}0$ and insert a prefactor $\pm\mathrm{i}$ coming from the change of the integral measure. In this way, we obtain

$$\pm\mathrm{i}\frac{\sqrt{\pi}\Gamma(\frac{d-1}{2} + \nu)}{\sqrt{2}(2\pi)^{\frac{d}{2}} 2^{\nu}} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-Z \pm \mathrm{i}0\big) \tag{6.24}$$

as candidates for (anti-)Feynman propagators on AdS_d.

On the proper anti-de Sitter space AdS_d the latter expression cannot be a Green function. In fact, due to the identity (B.12), the application of the Klein-Gordon operator to (6.24) yields a nonzero distribution supported at $\{Z = -1\} \cup \{Z = 1\}$ (the diagonal and the antipode of the diagonal).

This problem dissapears on the universal cover $\widetilde{\mathrm{AdS}}_d$ of anti-de Sitter space. The expression (6.24), properly continued to further regions, yields a Green function of the Klein-Gordon operator, as we shall see in the next subsection.

The following four functions are bisolutions of the Klein-Gordon equation:

$$\sim \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-Z \pm \mathrm{i}0\,\mathrm{sgn}(\tau)\big) \quad \text{and} \quad \sim \mathbf{Z}_{\frac{d}{2}-1,-\nu}\big(-Z \pm \mathrm{i}0\,\mathrm{sgn}(\tau)\big). \tag{6.25}$$

We expect that the following is true:

Conjecture 6.1. *On W_0, the functions (6.25) form a basis of bisolutions of the Klein-Gordon equation invariant wrt the restricted anti de Sitter group.*

6.3.1 Resolvent of the d'Alembertian

The essential self-adjointness of the d'Alembertian $-\Box$ on $C_{\mathrm{c}}^\infty(\widetilde{\mathrm{AdS}}_d)$ is not covered by the references [10,77]. However, we expect that the methods of above references can be extended to $\widetilde{\mathrm{AdS}}_d$, so that one can show that the d'Alembertian is indeed essentially self-adjoint on $C_{\mathrm{c}}^\infty(\widetilde{\mathrm{AdS}}_d)$.

The main aim of this subsection is a computation of the integral kernel of the resolvent of the d'Alembertian on $\widetilde{\mathrm{AdS}}_d$. As before, it is convenient to set

$$G(-\nu^2) := \Big(-\Box - \big(\tfrac{d-1}{2}\big)^2 + \nu^2\Big)^{-1}, \tag{6.26}$$

and denote the integral kernel of $G(-\nu^2)$ by $G(-\nu^2; x, x')$. Below we will compute $G(-\nu^2; x, x')$. We state this computation as a theorem. However, the arguments that we present, quite simple and convincing, use Conjecture 6.1, which we have not proved. A natural strategy for a complete proof would involve global coordinates and summation formulas for Gegenbauer functions, and is much more complicated. It will not be given in this paper.

To describe $G(-\nu^2; x, x')$ explicitly, it is convenient for $n \in \mathbb{Z}$ to introduce open regions

$$W_n := \Big(V_{2n-1} \cup V_{2n} \cup V_{2n+1}\Big)^{\mathrm{cl}}\Big)^{\circ}, \quad n \in \mathbb{Z}, \tag{6.27}$$

with V_n as defined in Subsection 6.1 and with cl denoting the closure and $\circ$ the interior. We have $W_n \cap W_{n+1} = V_{2n+1}$ and

$$\widetilde{\mathrm{AdS}}_d = \bigcup_{n\in\mathbb{Z}} W_n. \tag{6.28}$$

Theorem 6.2. *For $\nu^2 \in \mathbb{C} \setminus \mathbb{R}$ and $\mathrm{Re}(\nu) > 0$, the integral kernel of the resolvent (6.26) is given on W_n by the formula*

$$G(-\nu^2; x, x') = \frac{\sqrt{\pi}\Gamma(\frac{d-1}{2} + \nu)}{\sqrt{2}(2\pi)^{\frac{d}{2}} 2^\nu} \tag{6.29}$$
$$\times \begin{cases} \mathrm{i}\mathrm{e}^{-\mathrm{i}|n|(\frac{d-1}{2}+\nu)\pi} \mathbf{Z}_{\frac{d}{2}-1,\nu}\Big(- (-1)^n Z + (-1)^n \mathrm{i}0 s\Big), & \mathrm{Im}\,\nu < 0; \\ -\mathrm{i}\mathrm{e}^{\mathrm{i}|n|(\frac{d-1}{2}+\nu)\pi} \mathbf{Z}_{\frac{d}{2}-1,\nu}\Big(- (-1)^n Z - (-1)^n \mathrm{i}0 s\Big), & \mathrm{Im}\,\nu > 0, \end{cases}$$

Here s can be represented by $s = \mathrm{sgn}(\sin(|\tau - \tau'|))$, or

$$\begin{aligned} (x, x') \in V_{2n-1} &\Rightarrow s = (-1)^n \,\mathrm{sgn}(2n - 1), \\ (x, x') \in V_{2n} &\Rightarrow s = 0, \\ (x, x') \in V_{2n+1} &\Rightarrow s = (-1)^{n+1} \,\mathrm{sgn}(2n + 1). \end{aligned} \tag{6.30}$$

(Note that in V_{2n} we may set $s = -1$ or $s = 1$ because the function is univalent).

Proof (assuming the validity of Conj. 6.1). We split the proof of (6.29) in two steps. First, we show that (6.29) is a fundamental solution with appropriate decay behavior as $|Z| \to \infty$ *and* $|\tau| \to \infty$. Second, we argue that adding any bisolution, which is a (non-zero) linear combination of (6.25) has exponential growth as $\tau \to +\infty$ or $\tau \to -\infty$.

On W_0, consider (6.24). On the overlap $V_1 = W_0 \cap W_2$, we have

$$\mathbf{Z}_{\frac{d}{2}-1,\nu}\big(- Z \pm \mathrm{i}0\big) = \mathrm{e}^{\mp \mathrm{i}\pi\left(\frac{d-1}{2}+\nu\right)} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(- (-Z) \pm (-1)\mathrm{i}0\big). \tag{6.31}$$

On the chart W_2, the integral kernel of the resolvent must be a bisolution and it must on V_1 agree with (6.31). Therefore, the i0 should switch the sign from V_1 to V_3. On V_1, we have $\tau \in]0, \pi[$. Hence

$$(6.31) = \mathrm{e}^{\mp \mathrm{i}\pi\left(\frac{d-1}{2}+\nu\right)} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(- (-Z) \pm (-1)\mathrm{i}0 \,\mathrm{sgn}(\sin(|\tau - \tau'|))\big) \quad \text{on} \quad V_1 \tag{6.32}$$

and (6.32) is the appropriate continuation of (6.31) to W_2.

Now notice that $\mathrm{sgn}(\sin(|\tau - \tau'|)) = -1$ on V_3. Therefore, in this region,

$$\begin{aligned} &\mathrm{e}^{\mp \mathrm{i}\pi\left(\frac{d-1}{2}+\nu\right)} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(- (-Z) \pm (-1)\mathrm{i}0 \,\mathrm{sgn}(\sin(|\tau - \tau'|))\big) \\ &= \mathrm{e}^{\mp \mathrm{i}\pi\left(\frac{d-1}{2}+\nu\right)} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(- (-Z) \pm \mathrm{i}0\big) \\ &= \mathrm{e}^{\mp 2\pi \mathrm{i}\left(\frac{d-1}{2}+\nu\right)} \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(- (-1)^2 Z \pm (-1)^2 \mathrm{i}0 \,\mathrm{sgn}(\sin(|\tau - \tau'|))\big). \end{aligned} \tag{6.33}$$

Inductively, we obtain (6.29) for $n \geq 0$. The continuation to negative n works analogously. Since only $\mathbf{Z}_{\frac{d}{2}-1,\nu}$ appears, both formulas have an appropriate decay behavior as $|Z| \to \infty$ for any sign of $\mathrm{Im}(\nu)$. However, the exponential prefactor

$$\mathrm{e}^{\mp |n| \pi \mathrm{i}\left(\frac{d-1}{2}+\nu\right)} \tag{6.34}$$

decays only for $\mathrm{Im}(\nu) \lessgtr 0$ as $|n| \to \infty$ (or equivalently, as $|\tau| \to \infty$).

Assuming Conjecture 6.1 we see that these are the only fundamental solutions with appropriate decay behavior. Thus a basis of bisolutions that decay as $|Z| \to \infty$ is on W_0 given by

$$\begin{aligned} &\mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-Z+\mathrm{i}0)\big) + \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-Z-\mathrm{i}0\big) \\ \text{and}\quad &\mathrm{sgn}(\tau)\Big(\mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-Z+\mathrm{i}0)\big) - \mathbf{Z}_{\frac{d}{2}-1,\nu}\big(-Z-\mathrm{i}0\big)\Big). \end{aligned} \tag{6.35}$$

Both choices contain $+\mathrm{i}0$ and $-\mathrm{i}0$, and it is easy to see that their continuation to the higher W_n contains terms that exponentially increase with time at least in one of the directions $\tau > 0$ resp. $\tau < 0$. □

6.3.2 Propagators from the resolvent

From the formula for the resolvent we can immediately determine the operator-theoretic Feynman and anti-Feynman propagators for for $n \in \mathbb{Z}$ in the regions W_n. We have

$$G_{\mathrm{op}}^{\mathrm{F}/\overline{\mathrm{F}}}(x,x') = \pm\,\mathrm{i}\frac{\sqrt{\pi}\Gamma(\frac{d-1}{2}+\nu)}{\sqrt{2}(2\pi)^{\frac{d}{2}}2^{\nu}}\mathrm{e}^{\mp\mathrm{i}|n|(\frac{d-1}{2}+\nu)\pi}\mathbf{Z}_{\frac{d}{2}-1,\nu}\Big(-(-1)^n Z \pm (-1)^n\mathrm{i}0s\Big), \tag{6.36}$$

where s is as in Theorem 6.2.

The sum $G_{\mathrm{op}}^{\mathrm{F}} + G_{\mathrm{op}}^{\overline{\mathrm{F}}}$ has a causal support (or in the terminology of Def. 2.4 the specialty condition holds):

$$\begin{aligned} G_{\mathrm{op}}^{\mathrm{F}}(x,x') + G_{\mathrm{op}}^{\overline{\mathrm{F}}}(x,x') = \mathrm{i}\frac{\sqrt{\pi}\Gamma(\frac{d-1}{2}+\nu)}{\sqrt{2}(2\pi)^{\frac{d}{2}}2^{\nu}}\Bigg(&\mathrm{e}^{-\mathrm{i}|n|(\frac{d-1}{2}+\nu)\pi}\mathbf{Z}_{\frac{d}{2}-1,\nu}\Big(-(-1)^n Z + (-1)^n\mathrm{i}0s\Big) \\ -\,\mathrm{e}^{\mathrm{i}|n|(\frac{d-1}{2}+\nu)\pi}\mathbf{Z}_{\frac{d}{2}-1,\nu}\Big(-(-1)^n Z - (-1)^n\mathrm{i}0s\Big)\Bigg)&. \end{aligned} \tag{6.37}$$

In fact, (6.37) vanishes for $x \in V_0$. We obtain the retarded and advanced propagator by multiplying it with $\theta\big(\pm(\tau-\tau')\big)$. The Pauli-Jordan propagator is then the difference of the retarded and advanced propagator. We use (2.39c) to define $G^{(\pm)}$ obtaining on the chart W_n:

$$\begin{aligned} G^{(\pm)}(x,x') =& \frac{\sqrt{\pi}\Gamma(\frac{d-1}{2}+\nu)}{\sqrt{2}(2\pi)^{\frac{d}{2}}2^{\nu}}\mathrm{e}^{\mp\mathrm{i}n(\frac{d-1}{2}+\nu)\pi} \\ &\times \mathbf{Z}_{\frac{d}{2}-1,\nu}\Big(-(-1)^n Z \pm (-1)^n\mathrm{i}0\tilde{s}\Big). \end{aligned} \tag{6.38}$$

Here $\tilde{s}$ can be represented by $\tilde{s} = \mathrm{sgn}(\sin(\tau-\tau'))$, or

$$(x,x') \in V_{2n-1} \Rightarrow \tilde{s} = (-1)^n, \tag{6.39}$$

$$(x,x') \in V_{2n} \Rightarrow \tilde{s} = 0, \tag{6.40}$$

$$(x,x') \in V_{2n+1} \Rightarrow \tilde{s} = (-1)^{n+1}. \tag{6.41}$$

Note that for $\nu^2 < 0$ the specialty condition is no longer true. Therefore, although we can define $G_{\mathrm{op}}^{\mathrm{F}}$ and $G_{\mathrm{op}}^{\overline{\mathrm{F}}}$, we are not able to obtain other propagators from them.

6.3.3 Trigonometric Pöschl-Teller Hamiltonian

In our further analysis of the anti-de Sitter space we will need properties of the following 1-dimensional Schrödinger operator on $L^2[0, \frac{\pi}{2}]$:

$$H_{\alpha,\nu}^{\mathrm{PT}} := -\partial_u^2 + \frac{\alpha^2 - \frac{1}{4}}{\sin(u)^2} + \frac{\nu^2 - \frac{1}{4}}{\cos(u)^2}. \tag{6.42}$$

It is called the *trigonometric Pöschl-Teller Hamiltonian* [75] and is one of the 1-dimensional Schrödinger operators exactly solvable in terms of hypergeometric functions.

By an extension of standard arguments (cf. [76, Chapter X]), one finds that $H_{\alpha,\nu}^{\mathrm{PT}}$, viewed as an operator on $L^2[0, \frac{\pi}{2}]$, is essentially self-adjoint if both $\nu^2 \geq 1$ and $\alpha^2 \geq 1$, it has a positive Friedrichs extension if $\nu^2 \geq 0$ and $\alpha^2 \geq 0$, and all self-adjoint extensions are unbounded from below if $\nu^2 < 0$ or $\alpha^2 < 0$.

6.3.4 Propagators from the evolution of Cauchy data

In this subsection we present an approach to propagators on $\widetilde{\mathrm{AdS}}_d$ different from that of Subsection 6.3.2. It is based on the evolution of the Cauchy data. We will use the stationarity of $\widetilde{\mathrm{AdS}}_d$.

The Klein-Gordon operator with effective mass m in the coordinates (6.5) is given by

$$\begin{aligned} -\Box_g + m^2 &= -\frac{1}{\sqrt{|\det g|}}\partial_\mu g^{\mu\nu}\sqrt{|\det g|}\partial_\nu + m^2 \\ &= \cos(u)^2\Big(\partial_\tau^2 - \frac{\Delta_{\mathbb{S}^{d-2}}}{\sin(u)^2} - \tan(u)^{2-d}\partial_u \tan(u)^{d-2}\partial_u + \frac{m^2}{\cos(u)^2}\Big) \end{aligned} \tag{6.43}$$

with $\Delta_{\mathbb{S}^{d-2}}$ being the Laplace-Beltrami operator on the $d-2$-dimensional sphere parametrized by the coordinates Ω. Gauging (6.43) we obtain

$$\tan(u)^{\frac{d-2}{2}}\big(-\Box_g + m^2\big)\tan(u)^{\frac{2-d}{2}} \tag{6.44}$$

$$= \cos(u)^2\left(\partial_\tau^2 - \partial_u^2 + \frac{-\Delta_{\mathbb{S}^{d-2}} + \left(\frac{d-3}{2}\right)^2 - \frac{1}{4}}{\sin(u)^2} + \frac{\nu^2 - \frac{1}{4}}{\cos(u)^2}\right) \tag{6.45}$$

with ν^2 as in (6.11). For $d \geq 3$, the spectrum of $-\Delta_{\mathbb{S}^{d-2}}$ is $\{l(l+d-3) \mid l \in \mathbb{N}_0\}$. For $d = 2$, the term proportional to $\sin(u)^{-2}$ vanishes.

Hence, restricted to eigenfunctions of $-\Delta_{\mathbb{S}^{d-2}}$, (6.44) becomes, up to the prefactor $\cos(u)^2$, the trigonometric Pöschl-Teller Hamiltonian (6.42) with $\alpha := l + \frac{d-3}{2}$ if $d \geq 3$ and $\alpha^2 = \frac{1}{4}$ if $d = 2$.

To define dynamics in $\widetilde{\mathrm{AdS}}^d$, one needs to fix a self-adjoint extension of $H_{\alpha,\nu}^{\mathrm{PT}}$, i.e., boundary conditions at spacelike infinity. A comprehensive analysis of boundary conditions for H_{PT} and their application to anti-de Sitter QFT has been carried out by Ishibashi and Wald [62].

Notice first that $\alpha^2 < 1$ if and only if $d = 2$ or $d \in \{3, 4\}$ and $l = 0$. Hence, one might expect that boundary conditions at the origin need to be fixed in these cases. But one can show that this is merely an artifact of the choice of coordinates and that no boundary conditions at $u = 0$ are required [62]. The important part is fixing the boundary conditions (i.e., a self-adjoint extension of $H^{\mathrm{PT}}_{\alpha,\nu}$) at spatial infinity $u = \frac{\pi}{2}$.

Now for $\nu^2 \geq 1$ the operator $H^{\mathrm{PT}}_{\alpha,\nu}$ is essentially self-adjoint, so the dynamics is uniquely determined. We can compute all propagators—they agree with those obtained from the operator-theoretic Feynman propagator. In particular, the specialty condition is true.

For $0 \leq \nu^2 < 1$ we have a one-parameter family of self-adjoint extensions, depending on the boundary condition at spatial infinity. All of them can be used to define the propagators. Among them there is a distinguished boundary condition given by the Friedrichs extension, or equivalently, by the analytic continuation in the parameter ν. By the uniqueness of analytic continuation, this leads to propagators that agree with those obtained from the operator-theoretic Feynman propagator.

Finally, for $\nu^2 < 0$ there is a one-parameter family of realizations of $H^{\mathrm{PT}}_{\alpha,\nu}$, and all are unbounded from below. Each of them can be used to define an evolution of Cauchy data, and hence the retarded and advanced propagator. However, in contrast to the case $0 \leq \nu^2 < 1$, none of them is distinguished.

A Projections and Krein spaces

The main goal of this appendix is a short presentation of basic facts about Krein spaces, which provide a natural functional-analytic setting for the Klein-Gordon equation. There exist comprehensive textbook treatments of spaces with indefinite inner products [7, 15]. Our treatment is perhaps more concise, concentrating on the concepts directly needed in our paper. To a large extent we follow [41], with some simplifications and improvements.

We start with some useful but not well-known lemmas about projections, involutions and complementary subspaces, presenting constructions related to pairs of complementary subspaces, which go back to Kato [64]. Then we describe elements of the theory of Krein spaces. The main result that we prove is the proposition saying that every pair consisting of a maximal uniformly positive and maximal uniformly negative subspace is complementary, which is crucial in the construction of the in-out Feynman propagator.

A.1 Involutions

Let $\mathcal{W}$ be a vector space. We do not need topology on $\mathcal{W}$ for the moment. We use the term “invertible” as a synonym of “bijective”.

Definition A.1. We say that a pair $(\mathcal{Z}_\bullet^{(+)}, \mathcal{Z}_\bullet^{(-)})$ of subspaces of $\mathcal{W}$ is *complementary* if

$$\mathcal{Z}_\bullet^{(+)} \cap \mathcal{Z}_\bullet^{(-)} = \{0\}, \quad \mathcal{Z}_\bullet^{(+)} + \mathcal{Z}_\bullet^{(-)} = \mathcal{W}.$$

Definition A.2. We say that a pair of operators $(\Pi_\bullet^{(+)}, \Pi_\bullet^{(-)})$ on $\mathcal{W}$ is a pair of complementary projections if

$$(\Pi_\bullet^{(\pm)})^2 = \Pi_\bullet^{(\pm)}, \quad \Pi_\bullet^{(+)} + \Pi_\bullet^{(-)} = \mathbb{1}.$$

Definition A.3. An operator $S_\bullet$ on $\mathcal{W}$ is called an *involution*, if $S_\bullet^2 = \mathbb{1}$.

Note that there is a 1-1 correspondence between involutions, pairs of complementary projections and pairs of complementary subspaces:

$$\Pi_\bullet^{(\pm)} := \frac{1}{2}(\mathbb{1} \pm S_\bullet), \quad \mathcal{Z}_\bullet^{(\pm)} := \mathcal{R}(\Pi_\bullet^{(\pm)}). \tag{A.1}$$

A.2 Pair of involutions I

In this subsection we give a criterion for complementarity of two subspaces, and then we construct the corresponding projections following Kato [64].

Suppose that S_1 and S_2 are two involutions on $\mathcal{W}$. Let

$$\Pi_i^{(\pm)} := \frac{1}{2}(\mathbb{1} \pm S_i), \quad \mathcal{Z}_i^{(\pm)} := \mathcal{R}(\Pi_i^{(\pm)}), \quad i = 1, 2,$$

be the corresponding pairs of complementary projections and subspaces. Define

$$\Upsilon = \frac{1}{4}(S_1 + S_2)^2. \tag{A.2}$$

Observe that Υ commutes with $\Pi_1^{(+)}$, $\Pi_1^{(-)}$, $\Pi_2^{(+)}$ and $\Pi_2^{(-)}$.

Proposition A.4. *The following conditions are equivalent:*

(i) Υ *is invertible.*

(ii) $\Pi_1^{(+)} + \Pi_2^{(-)}$ *and* $\Pi_2^{(+)} + \Pi_1^{(-)}$ *are invertible.*

Moreover, if one of the above holds, then the pairs $(\mathcal{Z}_1^{(+)}, \mathcal{Z}_2^{(-)})$ *as well as* $(\mathcal{Z}_2^{(+)}, \mathcal{Z}_1^{(-)})$ *are complementary.*

Proof. The equivalence of (i) and (ii) follows from

$$\Upsilon = (\Pi_1^{(+)} + \Pi_2^{(-)})(\Pi_2^{(+)} + \Pi_1^{(-)}) \tag{A.3}$$

by the following easy fact: If R, S, T are maps such that $R = ST = TS$, then R is bijective if and only if both T and S are bijective.

The last implication follows from the next proposition. □

In the setting of the above proposition we can use Υ to construct two pairs of complementary projections:

Proposition A.5. *Suppose that Υ is invertible. Then*

$$\begin{aligned}
\Lambda_{12}^{(+)} &:= \Pi_1^{(+)}\Upsilon^{-1}\Pi_2^{(+)} && \textit{is the projection onto } \mathcal{Z}_1^{(+)} \textit{ along } \mathcal{Z}_2^{(-)},\\
\Lambda_{12}^{(-)} &:= \Pi_2^{(-)}\Upsilon^{-1}\Pi_1^{(-)} && \textit{is the projection onto } \mathcal{Z}_2^{(-)} \textit{ along } \mathcal{Z}_1^{(+)},\\
\Lambda_{21}^{(+)} &:= \Pi_2^{(+)}\Upsilon^{-1}\Pi_1^{(+)} && \textit{is the projection onto } \mathcal{Z}_2^{(+)} \textit{ along } \mathcal{Z}_1^{(-)},\\
\Lambda_{21}^{(-)} &:= \Pi_1^{(-)}\Upsilon^{-1}\Pi_2^{(-)} && \textit{is the projection onto } \mathcal{Z}_1^{(-)} \textit{ along } \mathcal{Z}_2^{(+)}.
\end{aligned}$$

In particular,

$$\Lambda_{12}^{(+)} + \Lambda_{12}^{(-)} = \mathbb{1}, \quad \Lambda_{21}^{(+)} + \Lambda_{21}^{(-)} = \mathbb{1}.$$

Proof. First we check that $\Lambda_{12}^{(+)}$ is a projection:

$$\begin{aligned}
\big(\Lambda_{12}^{(+)}\big)^2 &= \Pi_1^{(+)}\Upsilon^{-1}\Pi_2^{(+)}\Pi_1^{(+)}\Upsilon^{-1}\Pi_2^{(+)}\\
&= \Pi_1^{(+)}\Upsilon^{-1}(\Pi_2^{(+)}\Pi_1^{(+)} + \Pi_1^{(-)}\Pi_2^{(-)})\Upsilon^{-1}\Pi_2^{(+)} = \Lambda_{12}^{(+)}.
\end{aligned}$$

Moreover,

$$\Lambda_{12}^{(+)} = \Pi_1^{(+)}(\Pi_2^{(+)} + \Pi_1^{(-)})\Upsilon^{-1} = \Upsilon^{-1}(\Pi_1^{(+)} + \Pi_2^{(-)})\Pi_2^{(+)}.$$

But $(\Pi_2^{(+)} + \Pi_1^{(-)})\Upsilon^{-1}$ and $\Upsilon^{-1}(\Pi_1^{(+)} + \Pi_2^{(-)})$ are invertible. Hence $\mathcal{R}(\Lambda_{12}^{(+)}) = \mathcal{R}(\Pi_1^{(+)})$ and $\mathcal{N}(\Lambda_{12}^{(+)}) = \mathcal{N}(\Pi_2^{(+)}) = \mathcal{R}(\Pi_2^{(-)})$. This proves the statement of the proposition about $\Lambda_{12}^{(+)}$. The remaining statements are proven analogously. □

Remark A.6. Note that the notation for projections $\Lambda_{12}^{(\pm)}$ and $\Lambda_{21}^{(\pm)}$ is different than in [41].

A.3 Pair of involutions II

Let S_i, $(\Pi_i^{(+)}, \Pi_i^{(-)})$, $(\mathcal{Z}_i^{(+)}, \mathcal{Z}_i^{(-)})$, $i = 1, 2$, be as in the previous subsection. Set

$$K := S_2 S_1. \tag{A.4}$$

Proposition A.7. *K is invertible and*

$$S_1 K S_1 = S_2 K S_2 = K^{-1}. \tag{A.5}$$

In what follows we will use the decomposition $\mathcal{W} = \mathcal{Z}_1^{(+)} \oplus \mathcal{Z}_1^{(-)}$. Under the assumption that $\mathbb{1} + K$ is invertible, we define

$$c := \Pi_1^{(+)} \frac{\mathbb{1} - K}{\mathbb{1} + K} \Pi_1^{(-)}, \quad d := \Pi_1^{(-)} \frac{\mathbb{1} - K}{\mathbb{1} + K} \Pi_1^{(+)}. \tag{A.6}$$

where c, resp. d are interpreted as operators from $\mathcal{Z}_1^{(-)}$ to $\mathcal{Z}_1^{(+)}$, resp. from $\mathcal{Z}_1^{(+)}$ to $\mathcal{Z}_1^{(-)}$.

Proposition A.8. *The following conditions are equivalent:*

(i) Υ *is invertible (or Condition (ii) of Proposition A.4 is true).*

(ii) $\mathbb{1}+K$ *is invertible.*

Suppose that the above conditions are true. As we know from Prop. A.4, the pairs of subspaces $(\mathcal{Z}_1^{(+)}, \mathcal{Z}_2^{(-)})$ *and* $(\mathcal{Z}_2^{(+)}, \mathcal{Z}_1^{(-)})$ *are then complementary. Here are new formulas for the corresponding projections:*

$$\Lambda_{12}^{(+)} = \begin{bmatrix} \mathbb{1} & c \\ 0 & 0 \end{bmatrix} \qquad \textit{projects onto } \mathcal{Z}_1^{(+)} \textit{ along } \mathcal{Z}_2^{(-)},$$

$$\Lambda_{12}^{(-)} = \begin{bmatrix} 0 & -c \\ 0 & \mathbb{1} \end{bmatrix} \qquad \textit{projects onto } \mathcal{Z}_2^{(-)} \textit{ along } \mathcal{Z}_1^{(+)},$$

$$\Lambda_{21}^{(+)} = \begin{bmatrix} \mathbb{1} & 0 \\ -d & 0 \end{bmatrix} \qquad \textit{projects onto } \mathcal{Z}_2^{(+)} \textit{ along } \mathcal{Z}_1^{(-)},$$

$$\Lambda_{21}^{(-)} = \begin{bmatrix} 0 & 0 \\ d & \mathbb{1} \end{bmatrix} \qquad \textit{projects onto } \mathcal{Z}_1^{(-)} \textit{ along } \mathcal{Z}_2^{(+)}.$$

Besides, $\mathbb{1}-dc$ *and* $\mathbb{1}-cd$ *are invertible, and we have the following formulas:*

$$\Upsilon = \frac{1}{4}(\mathbb{1}+K)(\mathbb{1}+K^{-1}) = \begin{bmatrix} (\mathbb{1}-cd)^{-1} & 0 \\ 0 & (\mathbb{1}-dc)^{-1} \end{bmatrix}, \tag{A.7a}$$

$$K = \begin{bmatrix} (\mathbb{1}+cd)(\mathbb{1}-cd)^{-1} & -2c(\mathbb{1}-dc)^{-1} \\ -2d(\mathbb{1}-cd)^{-1} & (\mathbb{1}+dc)(\mathbb{1}-dc)^{-1} \end{bmatrix}, \tag{A.7b}$$

$$\Pi_1^{(+)} = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{bmatrix}, \quad \Pi_2^{(+)} = \begin{bmatrix} (\mathbb{1}-cd)^{-1} & c(\mathbb{1}-dc)^{-1} \\ -d(\mathbb{1}-cd)^{-1} & -dc(\mathbb{1}-dc)^{-1} \end{bmatrix}, \tag{A.7c}$$

$$\Pi_1^{(-)} = \begin{bmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{bmatrix}, \quad \Pi_2^{(-)} = \begin{bmatrix} -cd(\mathbb{1}-cd)^{-1} & -c(\mathbb{1}-dc)^{-1} \\ d(\mathbb{1}-cd)^{-1} & (\mathbb{1}-dc)^{-1} \end{bmatrix}, \tag{A.7d}$$

$$S_1 = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix}, \quad S_2 = \begin{bmatrix} (\mathbb{1}+cd)(\mathbb{1}-cd)^{-1} & 2c(\mathbb{1}-dc)^{-1} \\ -2d(\mathbb{1}-cd)^{-1} & -(\mathbb{1}+dc)(\mathbb{1}-dc)^{-1} \end{bmatrix}. \tag{A.7e}$$

Proof. We have

$$\Upsilon = \frac{1}{4}(S_1+S_2)^2 = \frac{1}{4}(\mathbb{1}+K)(\mathbb{1}+K^{-1}). \tag{A.8}$$

But $(\mathbb{1}+K^{-1}) = K^{-1}(\mathbb{1}+K)$. Hence $\mathbb{1}+K$ is invertible iff $\mathbb{1}+K^{-1}$ is. Therefore, (i)⇔(ii).

For the remainder of the proof we assume that $\mathbb{1}+K$ is invertible. We have

$$S_1 \frac{\mathbb{1}-K}{\mathbb{1}+K} S_1 = -\frac{\mathbb{1}-K}{\mathbb{1}+K}. \tag{A.9}$$

Therefore

$$\Pi_1^{(+)} \frac{\mathbb{1}-K}{\mathbb{1}+K} \Pi_1^{(+)} = \Pi_1^{(-)} \frac{\mathbb{1}-K}{\mathbb{1}+K} \Pi_1^{(-)} = 0. \tag{A.10}$$

Hence,

$$\frac{\mathbb{1}-K}{\mathbb{1}+K}=\begin{bmatrix}0&c\\d&0\end{bmatrix}. \tag{A.11}$$

This implies

$$\frac{1}{\mathbb{1}+K}=\frac{1}{2}\begin{bmatrix}\mathbb{1}&c\\d&\mathbb{1}\end{bmatrix},\qquad \frac{1}{\mathbb{1}+K^{-1}}=\frac{1}{2}\begin{bmatrix}\mathbb{1}&-c\\-d&\mathbb{1}\end{bmatrix}. \tag{A.12}$$

Multiplying the two expressions of (A.12) yields

$$\Upsilon^{-1}=\begin{bmatrix}\mathbb{1}-cd&0\\0&\mathbb{1}-dc\end{bmatrix}. \tag{A.13}$$

Hence we proved both identities of (A.7a), as well as invertibility of $\mathbb{1}-cd$ and $\mathbb{1}-dc$.

We check that

$$\begin{bmatrix}\mathbb{1}&c\\d&\mathbb{1}\end{bmatrix}^{-1}=\begin{bmatrix}(\mathbb{1}-cd)^{-1}&-c(\mathbb{1}-dc)^{-1}\\-d(\mathbb{1}-cd)^{-1}&(\mathbb{1}-dc)^{-1}\end{bmatrix}. \tag{A.14}$$

Now

$$K=2\begin{bmatrix}\mathbb{1}&c\\d&\mathbb{1}\end{bmatrix}^{-1}-\begin{bmatrix}\mathbb{1}&0\\0&\mathbb{1}\end{bmatrix} \tag{A.15}$$

yields (A.7b).

The formulas for $\Pi_1^{(\pm)}$ and S_1 are obvious. We obtain S_2 from $S_2=KS_1$. From S_2 we get $\Pi_2^{(\pm)}$.

Now $\Lambda_{12}^{(+)}=\Pi_1^{(+)}\Upsilon^{-1}\Pi_2^{(+)}$ yields (A.7c), etc. □

The operators c, d are sometimes called *angular operators*.

A.4 Pair of self-adjoint involutions in a Hilbert space

Suppose now that $\mathcal{W}$ is a Hilbert space and S_i, $i=1,2$, is a pair of self-adjoint involutions. Obviously, the corresponding projections $\Pi_i^{(+)}$, $\Pi_i^{(-)}$ are then orthogonal.

We will use the orthogonal decomposition $\mathcal{W}=\mathcal{Z}_1^{(+)}\oplus\mathcal{Z}_1^{(-)}$. In this decomposition we can write

$$\Pi_2^{(+)}=\begin{bmatrix}A&B\\B^*&C\end{bmatrix},\qquad \text{where}\quad 0\leq A\leq\mathbb{1},\quad 0\leq C\leq\mathbb{1}. \tag{A.16}$$

Using $(\Pi_2^{(+)})^2=\Pi_2^{(+)}$ we obtain

$$\left(A-\tfrac{1}{2}\right)^2=\tfrac{1}{4}-BB^*,\qquad \left(C-\tfrac{1}{2}\right)^2=\tfrac{1}{4}-B^*B. \tag{A.17}$$

For an operator K, $\sigma(K)$ will denote its spectrum. If K is self-adjoint we will write

$$\inf K = \inf \sigma(K), \quad \sup K = \sup \sigma(K). \tag{A.18}$$

It follows from (A.17) that $\frac{1}{4} \geq \sup BB^* = \sup B^*B = \|B\|^2$, and hence

$$0 \leq \inf \left(\tfrac{1}{4} - BB^*\right) = \inf \left(\tfrac{1}{4} - B^*B\right). \tag{A.19}$$

The following proposition describes the situation where the angle between the projections $\Pi_1^{(+)}$ and $\Pi_2^{(+)}$ is not more than $\frac{\pi}{4}$:

Proposition A.9. *The following conditions are equivalent:*

1. $A \geq \frac{1}{2}$ *and* $C \leq \frac{1}{2}$.
2. $A = \frac{1}{2} + \sqrt{\frac{1}{4} - BB^*}$ *and* $C = \frac{1}{2} - \sqrt{\frac{1}{4} - B^*B}$.

Proof. 1.$\Leftarrow$ 2. is obvious.

1.$\Rightarrow$ 2. follows from (A.17), where by 1. we need to take the positive square root. □

The following consequence of Prop. A.9 will be useful in the theory of Krein spaces:

Lemma A.10. *Let P be an orthogonal projection and S a self-adjoint involution. Let $1 \geq \alpha > 0$ and*

$$PSP \geq \alpha P, \tag{A.20}$$

$$(\mathbb{1} - P)S(\mathbb{1} - P) \leq 0. \tag{A.21}$$

Then

$$(\mathbb{1} - P)S(\mathbb{1} - P) \leq -\alpha(\mathbb{1} - P). \tag{A.22}$$

and $T := S(1 - P) + PS$ is invertible with

$$\|T^{-1}\| \leq \frac{1}{1 - \sqrt{1 - \alpha^2}}. \tag{A.23}$$

Proof. We set $S_1 := 2P - \mathbb{1}$, so that $P = \Pi_1^{(+)}$, and $S_2 := S$. Thus we are in the setting of this subsection. We write $\Pi_2^{(+)} = \frac{S_2 + \mathbb{1}}{2}$ as in (A.16), so that

$$S = \begin{bmatrix} 2A - \mathbb{1} & 2B \\ 2B^* & 2C - \mathbb{1} \end{bmatrix}. \tag{A.24}$$

Thus,

$$PSP \geq 0 \;\Leftrightarrow\; A \geq \frac{1}{2}, \tag{A.25}$$

$$(\mathbb{1} - P)S(\mathbb{1} - P) \leq 0 \Leftrightarrow\; C \leq \frac{1}{2}. \tag{A.26}$$

Hence (A.20) and (A.21) imply the conditions of Proposition A.9, which allows us to rewrite (A.25) as

$$S = \begin{bmatrix} \sqrt{\mathbb{1} - 4BB^*} & 2B \\ 2B^* & -\sqrt{\mathbb{1} - 4B^*B} \end{bmatrix}. \tag{A.27}$$

By (A.20), $\sqrt{\mathbb{1} - 4BB^*} \geq \alpha$. So $1 - \alpha^2 \geq 4BB^*$. This implies $1 - \alpha^2 \geq 4B^*B$, and hence $-\sqrt{\mathbb{1} - 4B^*B} \leq -\alpha$, which proves (A.22).

Now

$$TT^* = \mathbb{1} + 3P - SPS - SPSP - PSPS. \tag{A.28}$$

Written as a 2×2 matrix, it is

$$\begin{aligned} TT^* &= \begin{bmatrix} \mathbb{1} + 12BB^* & -4\sqrt{\mathbb{1} - 4BB^*}B \\ -4B^*\sqrt{\mathbb{1} - 4BB^*} & \mathbb{1} - 4B^*B \end{bmatrix} \\ &= \begin{bmatrix} (\mathbb{1} - 2\sqrt{BB^*})^2 & 0 \\ 0 & (\mathbb{1} - 2\sqrt{B^*B})^2 \end{bmatrix} + WW^*, \end{aligned} \tag{A.29}$$

where

$$W := \begin{bmatrix} 2B(B^*B)^{-\frac{1}{4}}\sqrt{\mathbb{1} + 2\sqrt{B^*B}} \\ -2(B^*B)^{\frac{1}{4}}\sqrt{\mathbb{1} - 2\sqrt{B^*B}} \end{bmatrix},$$

$$\text{so that} \quad W^* = \begin{bmatrix} 2\sqrt{\mathbb{1} + 2\sqrt{B^*B}}(B^*B)^{-\frac{1}{4}}B^* & -2\sqrt{\mathbb{1} - 2\sqrt{B^*B}}(B^*B)^{\frac{1}{4}} \end{bmatrix}. \tag{A.30}$$

Now $WW^* \geq 0$ and

$$\inf(\mathbb{1} - 2\sqrt{BB^*})^2 = \inf(\mathbb{1} - 2\sqrt{B^*B})^2 \geq (1 - \sqrt{1 - \alpha^2})^2. \tag{A.31}$$

Thus $TT^* \geq (1 - \sqrt{1 - \alpha^2})^2$. An analogous argument (where P is replaced with $\mathbb{1} - P$) shows $T^*T \geq (1 - \sqrt{1 - \alpha^2})^2$. This proves (A.23). □

A.5 Hilbertizable spaces

Definition A.11. Let $\mathcal{W}$ be a complex[5] topological vector space. We say that it is *Hilbertizable* if it has the topology of a Hilbert space for some scalar product $(\cdot|\cdot)_\bullet$ on $\mathcal{W}$. We will then say that $(\cdot|\cdot)_\bullet$ is *compatible with (the Hilbertizable structure of)* $\mathcal{W}$. The Hilbert space $\big(\mathcal{W}, (\cdot|\cdot)_\bullet\big)$ will be occasionally denoted $\mathcal{W}_\bullet$. We denote the corresponding norm by $\|\cdot\|_\bullet$, the orthogonal complement of $\mathcal{Z} \subset \mathcal{W}$ by $\mathcal{Z}^{\perp\bullet}$ and the Hermitian adjoint of an operator A by $A^{*\bullet}$.

[5] Analogous definitions and results are valid for *real* Hilbertizable spaces.

In what follows $\mathcal{W}$ is a Hilbertizable space. Let $(\cdot|\cdot)_1$, $(\cdot|\cdot)_2$ be two scalar products compatible with $\mathcal{W}$. Then there exist constants $0 < c \leq C$ such that

$$c(w\,|\,w)_1 \leq (w\,|\,w)_2 \leq C(w\,|\,w)_1.$$

Let R be a linear operator on $\mathcal{W}$. We say that it is *bounded* if for some (hence for all) compatible scalar products $(\cdot|\cdot)_\bullet$ there exists a constant $C_\bullet$ such that

$$\|Rw\|_\bullet \leq C_\bullet \|w\|_\bullet.$$

Let Q be a sesquilinear form on $\mathcal{W}$. We say that it is *bounded* if for some (hence for all) compatible scalar products $(\cdot|\cdot)_\bullet$ there exists $C_\bullet$ such that

$$|(v\,|\,Qw)| \leq C_\bullet \|v\|_\bullet \|w\|_\bullet, \quad v, w \in \mathcal{W}.$$

A.6 Pseudounitary spaces

Let $(\mathcal{W}, Q)$ be a Hilbertizable space equipped with a bounded Hermitian form,

$$(v|Qw) = \overline{(w|Qv)}, \quad v, w \in \mathcal{W}. \tag{A.32}$$

Definition A.12. Let $\mathcal{Z} \subset \mathcal{W}$. We define its *Q-orthogonal companion* as follows:

$$\mathcal{Z}^{\perp Q} := \{w \in \mathcal{W} \mid (w\,|\,Qv) = 0,\ v \in \mathcal{Z}\}.$$

Clearly, $\mathcal{Z}^{\perp Q}$ is a closed subspace of $\mathcal{W}$.

Definition A.13. Let $w \in \mathcal{W}$. We say that w is *positive, negative, resp. neutral* if

$$(w|Qw) \geq 0, \quad (w|Qw) \leq 0, \quad \text{resp.} \quad (w|Qw) = 0. \tag{A.33}$$

We say that a subspace $\mathcal{Z} \subset \mathcal{W}$ is *positive, negative, resp. neutral* if all its elements are positive, negative, resp. neutral elements.

Definition A.14. We say that $(\mathcal{W}, Q)$ is a *pseudounitary space* if $\mathcal{W}^{\perp Q} = \{0\}$.

A.7 Krein spaces

Let $(\mathcal{W}, Q)$ be a Hilbertizable space equipped with a bounded Hermitian form.

Definition A.15. A bounded involution $S_\bullet$ on $\mathcal{W}$ will be called *admissible* if it preserves Q, that is,

$$(S_\bullet v\,|\,QS_\bullet w) = (v\,|\,Qw), \tag{A.34}$$

and

$$(v\,|\,w)_\bullet := (v\,|\,QS_\bullet w) = (S_\bullet v\,|\,Qw) \tag{A.35}$$

is a scalar product compatible with the Hilbertizable structure of $\mathcal{W}$.

Definition A.16. A space $(\mathcal{W}, Q)$ is called a *Krein space* if it possesses an admissible involution.

Clearly, a Krein space is a pseudounitary space.

Remark A.17. In the literature sometimes instead of the term "admissible involution" one finds "fundamental symmetry".

For any admissible involution $S_\bullet$, we define the corresponding *particle projection* $\Pi_\bullet^{(+)}$ and *particle space* $\mathcal{Z}_\bullet^{(+)}$, as well as the *antiparticle projection* $\Pi_\bullet^{(-)}$ and *antiparticle space* $\mathcal{Z}_\bullet^{(-)}$, as in (A.1). The decomposition $\mathcal{W} \simeq \mathcal{Z}_\bullet^{(+)} \oplus \mathcal{Z}_\bullet^{(-)}$ is often called a *fundamental decomposition*. Note the following relations:

$$\begin{aligned}(v\,|\,w)_\bullet &= (\Pi_\bullet^{(+)}v\,|\,\Pi_\bullet^{(+)}w)_\bullet + (\Pi_\bullet^{(-)}v\,|\,\Pi_\bullet^{(-)}w)_\bullet,\\ (v\,|\,Qw) &= (\Pi_\bullet^{(+)}v\,|\,\Pi_\bullet^{(+)}w)_\bullet - (\Pi_\bullet^{(-)}v\,|\,\Pi_\bullet^{(-)}w)_\bullet.\end{aligned}$$

Definition A.18. Let A be a bounded operator on $\mathcal{W}$. Then there exists a unique operator A^{*Q} called the *Q-adjoint of* A such that

$$(A^{*Q}v\,|\,Qw) = (v\,|\,QAw), \quad v, w \in \mathcal{W}. \tag{A.36}$$

Let $\mathcal{Z} \subset \mathcal{W}$ and let A be an operator on $\mathcal{W}$. We have the identities:

$$\mathcal{Z}^{\perp Q} = S_\bullet \mathcal{Z}^{\perp\bullet}, \tag{A.37}$$

$$A^{*Q} = S_\bullet A^{*\bullet} S_\bullet. \tag{A.38}$$

With the help of these identities it is easy to show various properties of $\perp Q$ and $*\bullet$:

Proposition A.19.

1. *If $\mathcal{Z}$ is a closed subspace, then $(\mathcal{Z}^{\perp Q})^{\perp Q} = \mathcal{Z}$.*
2. *If $\mathcal{Z}_1, \mathcal{Z}_2$ are complementary subspaces in $\mathcal{W}$, then so are $\mathcal{Z}_1^{\perp Q}, \mathcal{Z}_2^{\perp Q}$.*
3. *Suppose that $(\Pi^{(+)}, \Pi^{(-)})$ is a pair of complementary projections. Then $(\Pi^{(+)*Q}, \Pi^{(-)*Q})$ is also a pair of complementary projections and*

$$\mathcal{R}(\Pi^{(\pm)*Q}) = \mathcal{N}(\Pi^{(\mp)*Q}) = \mathcal{R}(\Pi^{(\mp)})^{\perp Q} = \mathcal{N}(\Pi^{(\pm)})^{\perp Q}. \tag{A.39}$$

Definition A.20. Let R be a bounded invertible operator on $(\mathcal{W}, Q)$. We say that R is *pseudo-unitary* if

$$(Rv\,|\,QRw) = (v\,|\,Qw). \tag{A.40}$$

A.8 Krein spaces with conjugation

Definition A.21. An antilinear involution $v \mapsto \varepsilon v$ on a Krein space $(\mathcal{W}, Q)$ will be called a *conjugation* if it antipreserves Q, that is

$$(v|Qw) = -\overline{(\varepsilon v|Q\varepsilon w)} \tag{A.41}$$

and there exists an admissible involution $S_\bullet$ such that $\varepsilon S_\bullet \varepsilon = -S_\bullet$.

Note that then

$$(\varepsilon v\,|\,\varepsilon w)_\bullet = \overline{(v\,|\,w)_\bullet}.$$

Definition A.22. We say that an operator R is *real* if $\overline{R} := \varepsilon R \varepsilon = R$. We say that R is *anti-real* if $\overline{R} = -R$, that is, if $\mathrm{i}R$ is real.

Krein spaces with conjugations are especially important: Suppose that $(\mathcal{W}, Q)$ is a Krein space with conjugation. Clearly, if $S_\bullet$ is an admissible anti-real involution, then

$$\overline{\Pi_\bullet^{(+)}} = \Pi_\bullet^{(-)}, \quad \overline{\mathcal{Z}_\bullet^{(+)}} = \mathcal{Z}_\bullet^{(-)},$$

so that $\mathcal{W} = \mathcal{Z}_\bullet^{(+)} \oplus \overline{\mathcal{Z}_\bullet^{(+)}}$.

A.9 Maximal uniformly positive/negative subspaces

Let $(\mathcal{W}, Q)$ be a Krein space. We want to characterize definite subspaces with good properties. Following [15] we make the following definition.

Definition A.23. Let $\mathcal{Z}$ be a subspace of $\mathcal{W}$.

1. We say that it is *uniformly positive/negative* if for some scalar product $(\cdot|\cdot)_\bullet$ compatible with the Hilbertizable structure of $\mathcal{W}$ there exists $\alpha_\bullet > 0$ such that

$$v \in \mathcal{Z} \Rightarrow (v\,|\,Qv) \geq \alpha_\bullet (v|v)_\bullet, \quad \text{resp.} \quad v \in \mathcal{Z} \Rightarrow (v\,|\,Qv) \leq -\alpha_\bullet (v|v)_\bullet. \tag{A.42}$$

2. We say that $\mathcal{Z}$ is *maximal uniformly positive/negative* if it is a maximal subspace with the property of uniform positivity/negativity.

The following proposition, whose statement partially overlaps with Thm. V.5.2. and Cor. V. 7.4. in [15], relates maximal uniformly positive/negative spaces to fundamental decompositions and admissible involutions.

Proposition A.24. *Let $\mathcal{Z}_\bullet^{(+)}$ be a subspace of $\mathcal{W}$. Set $\mathcal{Z}_\bullet^{(-)} := \mathcal{Z}_\bullet^{(+)\perp Q}$. The following conditions are equivalent:*

1. *$\mathcal{Z}_\bullet^{(+)}$ is maximal uniformly positive.*

2. *$\mathcal{Z}_\bullet^{(+)}$ is maximal uniformly positive and $\mathcal{Z}_\bullet^{(-)}$ is maximal uniformly negative.*

3. *The spaces $\mathcal{Z}_\bullet^{(+)}$ and $\mathcal{Z}_\bullet^{(-)}$ are complementary, and if $(\Pi_\bullet^{(+)}, \Pi_\bullet^{(-)})$ is the corresponding pair of projections, then $S_\bullet := \Pi_\bullet^{(+)} - \Pi_\bullet^{(-)}$ is an admissible involution.*

Proof of Prop. A.24. Assume 3). Then $(\cdot|\cdot)_\bullet := (\cdot|QS_\bullet\cdot)$ is compatible and

$$(v|Qv)_\bullet = \pm(v|v)_\bullet, \quad v \in \mathcal{Z}_\bullet^{(\pm)}. \tag{A.43}$$

Hence $\mathcal{Z}_\bullet^{(\pm)}$ are maximal uniformly positive/negative. This proves 3)⇒2).

2)⇒1) is obvious.

Now assume 1). Let S_0 be an arbitrary admissible involution with the corresponding scalar product $(\cdot|\cdot)_0$. First note that $\mathcal{Z}_\bullet^{(-)}$ is negative. Indeed, suppose that $v_1 \in \mathcal{Z}_\bullet^{(-)}$ is strictly positive. Then for some α_1

$$(v_1|Qv_1) \geq \alpha_1(v_1|v_1)_0. \tag{A.44}$$

Hence $\mathrm{Span}(\mathcal{Z}_\bullet^{(+)}, v_1)$ is uniformly positive, which contradicts the maximality of $\mathcal{Z}_\bullet^{(+)}$.

Let P by the orthogonal projection (in the sense of $(\cdot|\cdot)_0$) onto $\mathcal{Z}_\bullet^{(+)}$. Then an arbitrary element of $\mathcal{Z}_\bullet^{(+)}$ has the form Pv and of $\mathcal{Z}_\bullet^{(-)}$ the form $S_0(\mathbb{1} - P)v$ for some $v \in \mathcal{W}$.

By the uniform positivity of $\mathcal{Z}_\bullet^{(+)}$, resp. by negativity of $\mathcal{Z}_\bullet^{(-)}$, we have

$$(v|PS_0Pv)_0 = (Pv|S_0Pv)_0 = (Pv|QPv) \geq \alpha(Pv|Pv)_0 \tag{A.45}$$

and

$$\begin{aligned}(v|(\mathbb{1} - P)S_0(\mathbb{1} - P)v)_0 &= (S_0(\mathbb{1} - P)v|(\mathbb{1} - P)v)_0 \\ &= (S_0(\mathbb{1} - P)v|QS_0(\mathbb{1} - P)v) \leq 0.\end{aligned} \tag{A.46}$$

Lemma A.10 then implies the uniform negativity of $\mathcal{Z}_\bullet^{(-)}$:

$$\begin{aligned}(v|(\mathbb{1} - P)S_0(\mathbb{1} - P)v)_0 &\leq -\alpha(v|(\mathbb{1} - P)v)_0 \\ &= -\alpha(S_0(\mathbb{1} - P)v|S_0(\mathbb{1} - P)v)_0.\end{aligned} \tag{A.47}$$

Clearly, $0 \neq w \in \mathcal{Z}_\bullet^{(+)} \cap \mathcal{Z}_\bullet^{(-)}$ has to be simultaneously positive and negative. Hence $\mathcal{Z}_\bullet^{(+)} \cap \mathcal{Z}_\bullet^{(-)} = \{0\}$.

As maximal positive/negative subspaces, $\mathcal{Z}_\bullet^{(+)}$ and $\mathcal{Z}_\bullet^{(-)}$ are automatically closed.

Set

$$T := S_0(\mathbb{1} - P) + PS_0. \tag{A.48}$$

For any $w \in \mathcal{W}$, $PS_0 w \in \mathcal{Z}_\bullet^{(+)}$ and $S_0(\mathbb{1} - P)w \in \mathcal{Z}_\bullet^{(-)}$. Hence the range of T is contained in $\mathcal{Z}_\bullet^{(+)} + \mathcal{Z}_\bullet^{(-)}$. By Lemma A.10, T is invertible, hence the range of T is $\mathcal{W}$. Therefore, $\mathcal{W} = \mathcal{Z}_\bullet^{(+)} + \mathcal{Z}_\bullet^{(-)}$.

We have proved that $\mathcal{Z}_\bullet^{(+)}$ and $\mathcal{Z}_\bullet^{(-)}$ are complementary. Let $S_\bullet$ be the corresponding involution. It is obviously bounded. Besides,

$$(v|v)_\bullet := (v|QS_\bullet v) \geq \alpha(v|v)_0. \tag{A.49}$$

Hence $(\cdot|\cdot)_\bullet$ is compatible. This ends the proof of 1)⇒3). □

Here is another proposition about fundamental decompositions. Note that it does not involve a reference to the topology of $\mathcal{W}$, but only to the form Q.

Proposition A.25. *Let $\mathcal{Z}_\bullet^{(+)}$ and $\mathcal{Z}_\bullet^{(-)}$ be complementary subspaces of a Krein space $(\mathcal{W}, Q)$, Q-orthogonal to one another. Assume that $\mathcal{Z}_\bullet^{(\pm)}$ are positive resp. negative, contain no neutral elements apart from 0 and are complete in the norm $\|v\|_{(\pm)} := \sqrt{\pm(v|Qv)}$. Then $\mathcal{Z}_\bullet^{(\pm)}$ is maximal uniformly positive/negative and $\mathcal{Z}_\bullet^{(-)} := \mathcal{Z}_\bullet^{(+)\perp Q}$, so that we are precisely in the setting described by Prop. A.24.*

Proof. Let $S_\bullet$ be the involution defined by $\mathcal{W} = \mathcal{Z}_\bullet^{(+)} \oplus \mathcal{Z}_\bullet^{(-)}$. As usual, we introduce the corresponding scalar product $(v|w)_\bullet := (v|QS_\bullet w)$ and the norm $\|\cdot\|_\bullet$. Note that $\|v\|_\bullet = \|v\|_{(\pm)}$ if $v \in \mathcal{Z}_\bullet^{(\pm)}$.

Let $\|\cdot\|_1$ be any compatible norm. Clearly, by the boundedness of Q, we have

$$\|v\|_\bullet \leq C\|v\|_1. \tag{A.50}$$

Consider the identity operator from $\mathcal{W}$ with $\|\cdot\|_\bullet$ to $\mathcal{W}$ with $\|\cdot\|_1$. In both norms $\mathcal{W}$ is complete. Then the identity is bounded. Hence it is closed. The operator is bijective. Hence by Banach's theorem its inverse is bounded. Therefore we have

$$\|v\|_1 \leq c\|v\|_\bullet. \tag{A.51}$$

Thus, $\mathcal{Z}_\bullet^{(\pm)}$ are uniformly positive resp. negative. □

Proposition A.26. *Let S_1, S_2 be a pair of admissible involutions. Define K, c, d as in (A.4) and (A.6). Then K is pseudo-unitary on $(\mathcal{W}, Q)$ and K is positive with respect to both $(\cdot|\cdot)_1$ and $(\cdot|\cdot)_2$. Besides, $\|c\| < 1$ and $c^* = d$ with respect to $(\cdot|\cdot)_1$.*

Proof. K is pseudo-unitary as the product of two pseudo-unitary transformations. The inequality

$$(v|Kv)_1 = (S_1 v|QS_2 S_1 v) = (S_1 v|S_1 v)_2 \geq a(S_1 v|S_1 v)_1 = a(v|v)_1$$

with $a > 0$ shows the positivity of K with respect to $(\cdot|\cdot)_1$. Therefore, $\mathbb{1} + K$ is invertible and $\|\frac{\mathbb{1}-K}{\mathbb{1}+K}\| < 1$. Hence $\|c\| < 1$. □

We finally show that any pair consisting of a maximal uniformly positive and a maximal uniformly negative subspace is complementary. (See also Lem. V.7.6. in [15]).

Proposition A.27. *Suppose that $\mathcal{Z}_1^{(+)}$ is a maximal uniformly positive space and $\mathcal{Z}_2^{(-)}$ is a maximal uniformly negative space. Then they are complementary.*

Proof. Set $\mathcal{Z}_1^{(-)} := \mathcal{Z}_1^{(+)\perp Q}$ and $\mathcal{Z}_2^{(+)} := \mathcal{Z}_2^{(-)\perp Q}$. Let S_1 resp. S_2 be the involutions corresponding to the pairs of complementary subspaces $(\mathcal{Z}_1^{(+)}, \mathcal{Z}_1^{(-)})$, resp. $(\mathcal{Z}_2^{(+)}, \mathcal{Z}_2^{(-)})$. They are admissible. By Prop. A.26, $K = S_2 S_1$ is positive. Hence $\mathbb{1} + K$ is invertible. Thus the result follows from Prop. A.8. □

B Gegenbauer equation

For the convenience of the reader, we present in this appendix basic statements about Gegenbauer functions needed in Sections 5 and 6. More details on Gegenbauer functions can be found e.g. in [36], on which this section is based.

Here is the *Gegenbauer equation*:

$$\left((1-w^2)\partial_w^2 - 2(1+\alpha)w\partial_w + \lambda^2 - \left(\alpha + \frac{1}{2}\right)^2\right) f(w) = 0. \tag{B.1}$$

We will express its solutions in terms of the *Olver normalized Gauss hypergeometric function*:

$$\mathbf{F}(a,b;c;z) := \frac{F(a,b;c;z)}{\Gamma(c)} = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n z^n}{\Gamma(c+n) n!}. \tag{B.2}$$

The defining series converges only in the unit disc, but $\mathbf{F}(a,b;c;z)$ extends to a holomorphic function on $\mathbb{C}\backslash[1,\infty[$ as well as on a universal cover of $\mathbb{C}\backslash\{0,1\}$.

In what follows complex power functions should be interpreted as their principal branches (holomorphic on $\mathbb{C}\backslash]-\infty,0]$). For example $w \mapsto (1-w)^\alpha$ is holomorphic away from $[1,\infty[$. In addition, we will frequently use the notation

$$(w^2-1)_\bullet^\alpha := (w-1)^\alpha (w+1)^\alpha. \tag{B.3}$$

The function $(w^2-1)_\bullet^\alpha$ is holomorphic on $\mathbb{C}\backslash]-\infty,1]$, whereas $(w^2-1)^\alpha$ is holomorphic on $\mathbb{C}\backslash\big([-1,1]\cup \mathrm{i}\mathbb{R}\big)$. One has $(w^2-1)_\bullet^\alpha = (w^2-1)^\alpha$ only for $\mathrm{Re}(w) > 0$. However, $(1-w^2)^\alpha = (1-w)^\alpha(1+w)^\alpha$ for all $w \notin]-\infty,-1]\cup[1,\infty[$.

Standard solutions of the Gegenbauer equations are characterized by simple behavior at one of the three singular points $1, -1, \infty$. Due to the $w \mapsto -w$ symmetry of the equation (B.1), solutions of the second type are obtained from solutions of the first type by negating the argument. Therefore we consider 4 functions, corresponding to 2 behaviors at 1 and 2 behaviors at ∞. All of them are holomorphic on $\mathbb{C}\backslash]-\infty,1]$.

- The solution characterized by asymptotics ~ 1 at 1:

$$S_{\alpha,\pm\lambda}(w) := F\Big(\frac{1}{2}+\alpha+\lambda, \frac{1}{2}+\alpha-\lambda; \alpha+1; \frac{1-w}{2}\Big) \tag{B.4}$$

$$= \Big(\frac{2}{w+1}\Big)^{\alpha} F\Big(\frac{1}{2}+\lambda, \frac{1}{2}-\lambda; \alpha+1; \frac{1-w}{2}\Big). \tag{B.5}$$

  $S_{\alpha,\lambda}$ is distinguished among the four solutions introduced here by the fact that it is holomorphic on $\mathbb{C}\backslash]-\infty,-1]$ rather than only on $\mathbb{C}\backslash]-\infty,1]$.

- The solution $\frac{2^{2\alpha}}{(w^2-1)_\bullet^{\alpha}} S_{-\alpha,\lambda}(w)$ is characterized by asymptotics $\sim \frac{2^{\alpha}}{(w-1)^{\alpha}}$ at 1.

- The solution characterized by asymptotics $\sim w^{-\frac{1}{2}-\alpha-\lambda}$ at $+\infty$:

$$Z_{\alpha,\lambda}(w) = (w\pm 1)^{-\frac{1}{2}-\alpha-\lambda} F\Big(\frac{1}{2}+\lambda, \frac{1}{2}+\lambda+\alpha; 1+2\lambda; \frac{2}{1\pm w}\Big) \tag{B.6}$$

$$= w^{-\frac{1}{2}-\alpha-\lambda} F\Big(\frac{1}{4}+\frac{\alpha}{2}+\frac{\lambda}{2}, \frac{3}{4}+\frac{\alpha}{2}+\frac{\lambda}{2}; 1+\lambda; \frac{1}{w^2}\Big).$$

- The solution $Z_{\alpha,-\lambda}(w)$ is characterized by asymptotics $\sim w^{-\frac{1}{2}-\alpha+\lambda}$ at $+\infty$.

All these 4 functions can be expressed in terms of $S_{\alpha,\lambda}$, but for typographical reasons it is convenient to introduce also $Z_{\alpha,\lambda}$. We will use Olver's normalization:

$$\mathbf{S}_{\alpha,\lambda}(w) := \frac{1}{\Gamma(\alpha+1)} S_{\alpha,\lambda}(w), \qquad \mathbf{Z}_{\alpha,\lambda}(w) := \frac{1}{\Gamma(\lambda+1)} Z_{\alpha,\lambda}(w). \tag{B.7}$$

We note the identities

$$\mathbf{S}_{\alpha,\lambda}(w) = \mathbf{S}_{\alpha,-\lambda}(w), \quad \mathbf{Z}_{\alpha,\lambda}(w) = \frac{\mathbf{Z}_{-\alpha,\lambda}(w)}{(w^2-1)_\bullet^{\alpha}}. \tag{B.8}$$

Here are the connection formulas:

$$\mathbf{S}_{\alpha,\lambda}(-w) = -\frac{\cos(\pi\lambda)}{\sin(\pi\alpha)} \mathbf{S}_{\alpha,\lambda}(w) + \frac{2^{2\alpha}\pi \mathbf{S}_{-\alpha,-\lambda}(w)}{\sin(\pi\alpha)\Gamma(\frac{1}{2}+\alpha+\lambda)\Gamma(\frac{1}{2}+\alpha-\lambda)(1-w^2)^{\alpha}}, \tag{B.9}$$

$$\mathbf{Z}_{\alpha,\lambda}(w) = -\frac{2^{\lambda-\alpha-\frac{1}{2}}\sqrt{\pi}\mathbf{S}_{\alpha,\lambda}(w)}{\sin(\pi\alpha)\Gamma(\frac{1}{2}-\alpha+\lambda)} + \frac{2^{\lambda+\alpha-\frac{1}{2}}\sqrt{\pi}}{\sin(\pi\alpha)\Gamma(\frac{1}{2}+\alpha+\lambda)} \frac{\mathbf{S}_{-\alpha,-\lambda}(w)}{(w^2-1)_\bullet^{\alpha}}, \tag{B.10}$$

$$\mathbf{S}_{\alpha,\lambda}(w) = \frac{2^{-\lambda+\alpha-\frac{1}{2}}\sqrt{\pi}}{\sin\pi\lambda}\bigg(-\frac{\mathbf{Z}_{\alpha,\lambda}(w)}{\Gamma\big(\frac{1}{2}+\alpha-\lambda\big)} + \frac{2^{2\lambda}\mathbf{Z}_{\alpha,-\lambda}(w)}{\Gamma\big(\frac{1}{2}+\alpha+\lambda\big)}\bigg). \tag{B.11}$$

From its definition, it is clear that $\mathbf{Z}_{\alpha,\lambda}$ satisfies

$$\mathbf{Z}_{\alpha,\lambda}(-w\mp \mathrm{i}0) = \mathrm{e}^{\pm\mathrm{i}\pi\left(\frac{1}{2}+\alpha+\lambda\right)} \mathbf{Z}_{\alpha,\lambda}(w\pm \mathrm{i}0), \quad w\in\mathbb{R}. \tag{B.12}$$

For further information on Gegenbauer functions (in various conventions), consult for example [36, 46, 55, 73, 86].

Acknowledgement. The work of J.D. and C.G. was supported by National Science Center of Poland under the grant UMO-2019/35/B/ST1/01651. We would like to thank Markus Fröb, Christian Gérard, Wojciech Kamiński, Nicola Pinamonti and Karl-Henning Rehren for enlightening discussions.

Data availability statement. All relevant data is contained in the manuscript.

Conflicts of interest. The authors declare no conflict of interest.

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