# An Evolution Equation Approach to the Klein–Gordon Operator on Curved Spacetime

Jan Dereziński, Daniel Siemssen

Department of Mathematical Methods in Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093, Warszawa, Poland. E-mail: jan.derezinski@fuw.edu.pl; daniel.siemssen@fuw.edu.pl.

**Abstract.** We develop a theory of the Klein–Gordon equation on curved spacetimes. Our main tool is the method of (non-autonomous) evolution equations on Hilbert spaces. This approach allows us to treat low regularity of the metric, of the electromagnetic potential and of the scalar potential. Our main goal is a construction of various kinds of propagators needed in quantum field theory.

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# 1 Introduction

We consider the Klein–Gordon operator on a Lorentzian manifold (M, g) minimally coupled to an electromagnetic potential A and with a scalar potential Y. In local coordiantes it can be written as

$$K := \Box_A + Y = |g|^{-\frac{1}{2}} (D_\mu - A_\mu) |g|^{\frac{1}{2}} g^{\mu\nu} (D_\nu - A_\nu) + Y, \qquad (1.1)$$

where  $|g| = |\det[g_{\mu\nu}]|$  and  $D_{\mu} = -i\partial_{\mu}$ . As in our recent work [9], we are interested in inverses and bisolutions of the Klein–Gordon operator *K*.

Heuristically, an inverse or bisolution of *K* is an operator which satisfies one of the following conditions:

(i) *G* is a *bisolution* of *K* if it satisfies

$$KG = 0$$
 and  $GK = 0$ .

(ii) G is an inverse of K if it satisfies

$$KG = 1$$
 and  $GK = 1$ .

Of course one must be careful to make rigorous sense of these statements by specifying the spaces between which these operators act. In particular one must make sure that the composition of *K* and *G* between appropriate spaces is well-defined. Often, *G* can be understood as an operator from  $C_c^{\infty}(M)$  to  $C^{\infty}(M)$ .

The Klein–Gordon operator has many inverses and bisolutions. They are known by many names in the literature, *e.g.*, "propagator" or "two-point function". Inverses are often also called "Green's functions".

The most well-known propagators are probably the *forward (retarded) propagator*  $G^{\vee}$  and the *backward (advanced) propagator*  $G^{\wedge}$ . Their difference  $G^{PJ} = G^{\vee} - G^{\wedge}$  will be called *Pauli–Jordan propagator* here, but is also known as "commutator function" or "causal propagator". These three propagators are important in the Cauchy problem of the classical theory, thus we will call them *classical propagators*. It is well-known that the classical propagators are uniquely defined on globally hyperbolic spacetimes.

The construction of the classical propagators is well-understood and described in numerous sources, for example, using the Hadamard parametrix method, in [2, 12]. Often only compactly supported smooth Cauchy data are considered and the propagators are understood from  $C_c^{\infty}(M)$  to  $C^{\infty}(M)$ . Of course, once well-posedness of the Cauchy problem is shown, the existence of the (Cauchy) evolution (*viz.*, the map which propagates Cauchy data) is immediate. Then the existence of the classical propagators and their properties is easily derived, see *e.g.* [10, 26] and also the more recent works [11, 16, 17].

In quantum field theory, one needs to consider also other propagators: the *Feynman* propagator  $G^{F}$  (and the *anti-Feynman* propagator  $G^{\overline{F}}$ ), as well as the positive and negative frequency bisolutions  $G^{(\pm)}$ . We will call them *non-classical* propagators. A positive frequency bisolution yields the two-point function of a vacuum state – a pure quasi-free state whose GNS representation yields a Hilbert space for the quantum field theory. The Feynman propagator appears when taking the expectation value of time-ordered products of quantum fields, and is used to evaluate Feynman diagrams.

It is clear how to define the non-classical propagators on static spacetimes. The positive and negative frequency bisolutions, as well as the Feynman and anti-Feynman propagators are constructed from the spectral projections of the generator of the dynamics. These constructions, at least implicitly, can be found in various works devoted to quantum field theory on curved spacetimes. In a systematic way they were described recently in [9], see also Chap. 18 of [6]. Note that in the static case there exists a natural Hilbert space structure for the Cauchy data. The most obvious choice is the so-called energy Hilbert space. It is also natural to consider a whole scale of Hilbert spaces, which includes the energy space. The generator of the dynamics is self-adjoint on all of these spaces. Thus the functional analytic setting in the static case is rather clean and simple.

It is not obvious how to define non-classical propagators on non-static spacetimes. The most popular view on this subject says that instead of a single positive frequency bisolution one should consider a whole class of bisolutions locally similar to the Minkowski two-point function, known as *Hadamard states*. There exists a considerable literature about them; in particular we would like to mention [27, 30]. Properties of Hadamard states play a central role in most formulations of perturbation theory and renormalization on curved spacetimes, see *e.g.* [20, 21].

To every Hadamard state one can naturally associate a Green's function which describes the expectation values of time-ordered fields. These Green's functions can be viewed as possible generalizations of the usual Feynman propagator to the non-static case.

This paper is devoted to the study of the Klein–Gordon equation on a rather general (non-static) spacetime. We develop a global approach based on functional analytic methods from the theory of *non-autonomous evolution equations*, as developed by Kato in [24]. We suppose that the spacetime is equipped with a time variable, and the coefficients of the Klein–Gordon operator satisfy certain certain continuity conditions with respect to time. For simplicity, we also assume that the metric does not have any spatio-temporal cross terms. (In every globally hyperbolic spacetime one can find such a time variable.)

Unlike in the static spacetime, we do not have a unique distinguished energy space. Instead, we have a whole time dependent family of instantaneous energy Hilbert spaces describing the Cauchy data at each time. Under the assumptions we impose, these spaces can be identified with one another. They have a variable scalar product, but a common topology – thus the Cauchy data at each time belong to a single *Hilbertizable space*.

The classical propagators are easily constructed from the evolution operator. Of course, as we mentioned earlier, they can also be constructed without a global functional analytic setting. Because of the finite speed of propagation they can be constructed locally, as it is done in many sources in the literature. In particular, one essentially does not need global assumptions, except for the global hyperbolicity.

The main motivation of our paper are however non-classical propagators, which are inherently global objects. They require global assumptions and more tools from functional analysis.

Throughout our paper we impose rather weak assumptions on the regularity of various

objects (the metric, electromagnetic potential and the scalar potential). We think that low regularity may be present in some physical applications. For us this is however not the main motivation to assume low regularity. We are convinced that such assumptions play an important theoretical role because they impose a certain discipline on a mathematical theory, forcing us to find better arguments and a more natural setting for the problem.

One of possibilities to define non-classical propagators in the non-static case is to use spectral projections of the generator of the evolution at a fixed instance of time, as we describe in Sect. 8. This allows us to define instantaneous positive and negative frequency bisolutions, and also the corresponding Feynman inverses. These yield the so-called instantaneous vacua. It is however known that instantaneous vacua suffer from some problems. Not only they depend on an arbitrary and unphysical choice of a preferred time, but it is a folklore knowledge that they are generally not Hadamard states. In a forthcoming article [8] we will show, using methods from our formalism, that an instantaneous positive frequency bisolution yields a Hadamard state if the Klein–Gordon operator *K* is infinitesimally static at the Cauchy surface where the positive/negative frequency splitting was performed.

Spacetimes that become asymptotically static in the past and the future form a class that in our opinion is especially natural from the point of view of quantum field theory. For such spacetimes one can define positive/negative frequency bisolutions corresponding to the asymptotic past and future, see Sect. 9. We can call them *in-* and *out-positive/negative frequency bisolutions*. One can argue that the corresponding *in-vacuum* yields the representation of incoming states (prepared in the experiment) and the corresponding *out-vacuum* gives the representation of final observables (measured in the experiment). Therefore, the in- and out states are not only distinguished, they also have a clear and important physical meaning. If the spacetime becomes static sufficiently fast, it can be shown that the states thus defined are Hadamard [18], see also [8].

As we described above, and is well-known, spacetimes with asymptotically static past and future posses two pairs of distinguished and physically well-motivated propagators: the in- and out- positive and negative frequency bisolution. It is perhaps less known that a large class of spacetimes possesses another pair of natural and physically motivated propagators: the so-called *canonical Feynman* and *anti-Feynman propagator*. The canonical Feynman propagator appears naturally when we evaluate Feynman diagrams. On the mathematical side, it is related to an intriguing and poorly understood question about the self-adjointness of the Klein–Gordon operator. A study of these propagators will be presented in our following paper [7]. The formalism and results of the present paper will play an important role in [7].

The limitation of the method of evolution equation is the need to impose global assumptions on the spacetime. Note, however, that some kind of such assumptions is indispensable if we want to define and study non-classical propagators.

It is clear to us that the methods used in our paper are natural, powerful and well-suited to the Klein–Gordon equation on curved spacetimes, especially concerning the questions relevant to quantum field theory. Therefore, we were greatly surprised that in the literature it is difficult to find a similar treatment of this problem. We are only aware of one more publication where the methods of evolution equations have been applied to the problem at hand: In [15], Furlani constructs the evolution under quite restrictive assumptions, namely, assuming that Cauchy surfaces are compact and have a decreasing volume along a finite time-interval. The treatment of Dimock, Kay, and Gerard–Wrochna may also resemble our method. However, in almost all papers the existence of the evolution is taken for granted, given by the local theory, and not constructed within the formalism of evolution equations on some Banach space.

For simplicity and improved clarity, we have restricted our attention to the scalar field in this work. The generalization to a vector bundle *F* with a fibre equipped with a positive definite scalar product can be performed. Then the scalar potential *Y* can be replaced by an element of Hom(*F*, *F*) and the electromagnetic potential *A* by an element of Hom(*F*,  $T^*M \otimes F$ ).

#### 1.1 Notation and conventions

Throughout this paper we adopt essentially the same notations and conventions as in [9] but for the convenience of the reader we repeat the relevant conventions. We also introduce some new notation.

Suppose that *T* is an operator on a Banach space  $\mathcal{X}$ . We denote by Dom *T* its domain and by Ran *T* its range. For its spectrum we write sp *T* and for the resolvent set rs *T*.

Suppose that *T* is a operator on a Hilbert space  $\mathcal{H}$  with inner product  $(\cdot | \cdot)$ . If *T* is positive, *i.e.*,  $(u | Tu) \ge 0$ , we write  $T \ge 0$ . If also Ker  $T = \{0\}$ , then we write T > 0.

A useful function is the so-called 'Japanese bracket', defined as  $\langle T \rangle := (1 + |T|^2)^{1/2}$ .

A topological vector space  $\mathcal{X}$  is called *Hilbertizable* if there exists a scalar product on  $\mathcal{X}$  that determines its topology and makes it into a Hilbert space. Clearly, two scalar products determine the topology of  $\mathcal{X}$  iff they are equivalent.

The *p*-times continuously differentiable  $\mathcal{X}$ -valued functions on a manifold *M* are denoted  $C^p(M; \mathcal{X})$ ; if  $\mathcal{X} = \mathbb{C}$ , we simply write  $C^p(M)$ . Sets of compactly supported or bounded functions are indicated by a subscript 'c' or 'b'.

 $AC(\mathbb{R})$  denotes the set of absolutely continuous functions, *i.e.*, functions whose distributional derivative belongs to  $L^1_{loc}(\mathbb{R})$ .  $AC^1(\mathbb{R})$  denotes the set of functions whose distributional derivative belongs to  $AC(\mathbb{R})$ .

When calculating integrals, we denote by  $\int'$  the 'Cauchy principal value' at infinity, *e.g.*,

$$\int_{i\mathbb{R}}' f(t) dt = \lim_{R \to \infty} \int_{-iR}^{iR} f(t) dt.$$

Observe that we pass to infinity symmetrically in the lower and upper integration limits.

Suppose we fix a positive density  $\gamma$  on M. The space  $L^2(M, \gamma)$  of square-integrable functions on M is then defined as the completion of  $C_c^{\infty}(M)$  with respect to the scalar product

$$(u | v)_g \coloneqq \int_M \overline{u} v \gamma, \quad u, v \in C_c^\infty(M).$$

If *g* is the metric tensor *g* on *M* (of any signature), then we set  $|g| := |\det[g_{\mu\nu}]|$ . *M* is then equipped with a canonical density  $|g|^{\frac{1}{2}}$ . Sometimes it is however convenient to fix a density  $\gamma$  independent of the metric tensor.

Often it is convenient to use the formalism of (complexified) half-densities on *M*. If  $\gamma$  is a positive density on *M*, then  $\gamma^{\frac{1}{2}}$  is a half-density. The canonical example for a half-density on a pseudo-Riemannian manifold is  $|g|^{\frac{1}{4}}$ . Since the integral over a density on a manifold is well-defined, half-densities come equipped with a natural  $L^2$ -structure

$$(\tilde{u} | \tilde{v}) = \int_{M} \overline{\tilde{u}} \, \tilde{v}, \quad \tilde{u}, \tilde{v} \in C_{c}^{\infty}(\Omega^{\frac{1}{2}}M)$$

We denote by  $L^2(\Omega^{\frac{1}{2}}M)$  the completion of  $C_c^{\infty}(\Omega^{\frac{1}{2}}M)$  with respect to the corresponding norm. Note that if we fix an everywhere positive density  $\gamma$ , then

$$L^2(M,\gamma) \ni u \mapsto \tilde{u} := u\gamma^{\frac{1}{2}} \in L^2(\Omega^{\frac{1}{2}}M)$$

is the natural unitary identification of the  $L^2$ -space in the scalar formalism and in the halfdensity formalism.

The operator  $D = -i\partial$  acts naturally on scalars, and  $D^{\gamma} = \gamma^{\frac{1}{2}} D \gamma^{-\frac{1}{2}}$  acts naturally on half-densities.

In our paper we generally prefer to use the half-density formalism rather than the scalar formalism. The Klein–Gordon operator K is presented in (1.1) in the scalar formalism. Transformed to the half-density formalism it is

$$K_{\frac{1}{2}} := |g|^{\frac{1}{4}} K|g|^{-\frac{1}{4}} = |g|^{-\frac{1}{4}} (D_{\mu} - A_{\mu})|g|^{\frac{1}{2}} g^{\mu\nu} (D_{\nu} - A_{\nu})|g|^{-\frac{1}{4}} + Y.$$
(1.2)

In what follows we drop the subscript  $\frac{1}{2}$  from  $K_{\frac{1}{2}}$  and by *K* we will mean (E.1).

# 2 Assumptions and setting

#### 2.1 Basic assumption

In this work we consider spacetimes of the form  $M = \mathbb{R} \times \Sigma$ . The generic notation for a point of M will be  $(t, \vec{x})$ , with t having the interpretation of time.  $\Sigma$  are spatial hypersurfaces of constant time. We often suppress the spatial dependence of objects defined on M, *e.g.*, we identify  $f(t) = f(t, \cdot)$  for some function f on M. Sometimes we also suppress the time-dependence, but it should be kept in mind that the central quantities considered here, the metric g, the electromagnetic potential A and the scalar potential Y, generically are non-static, *i.e.*, time-dependent. Sometimes we denote derivatives with respect to time by a dot.

We assume that M is equipped with a (continuous) metric

$$g(t,\vec{x}) = -\beta(t,\vec{x})dt \otimes dt + g_{\Sigma}(t,\vec{x}), \qquad (2.1)$$

where  $\beta > 0$  and  $g_{\Sigma}$  restricts to a Riemannian metric on  $\Sigma$ . Note that every globally hyperbolic spacetime is isometric to a spacetime of this class [4].

We will write

$$V(t) = -A_0(t)$$

for the electric potential.

#### 2.2 Klein–Gordon operator

The main object of our paper is the Klein–Gordon operator (E.1), denoted by K.

Using the fact that the metric g splits into a temporal and a spatial part (without any cross-terms), which is expressed in (2.1), K can be written as

$$K = -\beta^{-\frac{1}{2}} \gamma^{-\frac{1}{2}} (D_t + V) \gamma (D_t + V) \gamma^{-\frac{1}{2}} \beta^{-\frac{1}{2}} + \beta^{-\frac{1}{2}} \gamma^{-\frac{1}{2}} (D_i - A_i) \beta \gamma g^{ij} (D_j - A_j) \gamma^{-\frac{1}{2}} \beta^{-\frac{1}{2}} + Y,$$

where we introduced

$$\gamma := \beta^{-1} |g|^{\frac{1}{2}} = \beta^{-\frac{1}{2}} |g_{\Sigma}|^{\frac{1}{2}}.$$

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

$$\begin{split} \tilde{K} &:= \beta^{\frac{1}{2}} K \beta^{\frac{1}{2}} = -\gamma^{-\frac{1}{2}} (D_t + V) \gamma (D_t + V) \gamma^{-\frac{1}{2}} \\ &+ \gamma^{-\frac{1}{2}} (D_i - A_i) \beta \gamma g^{ij} (D_j - A_j) \gamma^{-\frac{1}{2}} + \beta Y \\ &= - (D_t + \overline{W}) (D_t + W) + L, \end{split}$$

where we introduced

$$W(t) \coloneqq V(t) + \frac{i}{2} (\gamma(t)^{-1} \dot{\gamma}(t)),$$
  
$$L(t) \coloneqq D_i^{A,\gamma*}(t) \tilde{g}^{ij}(t) D_j^{A,\gamma}(t) + \tilde{Y}(t)$$

and we use the shorthands

$$\begin{split} \tilde{g}^{ij}(t) &\coloneqq \beta(t) g^{ij}(t), \\ \tilde{Y}(t) &\coloneqq \beta(t) Y(t), \\ D^{A,\gamma}(t) &\coloneqq \gamma(t)^{\frac{1}{2}} (D - A(t)) \gamma(t)^{-\frac{1}{2}}. \end{split}$$

Clearly, propagators for  $\tilde{K}$  induce corresponding propagators for K.

Note that by passing from *K* to  $\tilde{K}$  we removed conformally the factor  $\beta$  from the metric, so that now the coefficient at  $\partial_t^2 = -D_t^2$  is 1.

#### 2.3 First-order formalism

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

$$B(t) := \begin{pmatrix} W(t) & \mathbb{1} \\ L(t) & \overline{W}(t) \end{pmatrix}.$$

Setting  $u_1(t) = u(t)$  and  $u_2(t) = -(D_t + W(t))u(t)$ , we find that

$$\left(\partial_t + \mathbf{i}B(t)\right) \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = 0$$

if and only if u is a (weak) solution of the Klein–Gordon equation  $\tilde{K}u = 0$ . Therefore we occasionally call  $\partial_t + iB(t)$  the *first-order Klein–Gordon operator*. The half-densities  $u_1(t)$  and  $u_2(t)$  may be called the *Cauchy data* for u at time t.

#### 2.4 Assumptions local in time

**Assumption 1.** We suppose that the following assumptions hold:

- 1.a. For all  $t \in \mathbb{R}$ , L(t) extends to a positive invertible self-adjoint operator on  $L^2(\Omega^{\frac{1}{2}}\Sigma)$  (denoted by the same symbol).
- 1.b. There exists  $a \in C(\mathbb{R})$  such that a(t) < 1 and  $||W(t)L(t)^{-\frac{1}{2}}|| \le a(t)$ .
- 1.c. There exists a positive  $C \in L^1_{loc}(\mathbb{R})$  such that for all  $|t s| \leq 1$

$$\left\|L(t)^{-\frac{1}{2}} \left(L(t) - L(s)\right) L(t)^{-\frac{1}{2}} \right\| + 2 \left\| \left(W(t) - W(s)\right) L(t)^{-\frac{1}{2}} \right\| \le \left\| \int_{s}^{t} C(r) dr \right\|, \quad (2.2)$$

where we place the absolute value on the right-hand side to account for the arbitrary order of *t* and *s*.

1.d.  $t \mapsto \beta(t)^{\pm \frac{1}{2}}$  are norm-continuous on  $L(s)^{-\frac{1}{2}}L^2(\Omega^{\frac{1}{2}}\Sigma)$  for any  $s \in \mathbb{R}$ , and  $t \mapsto \dot{\beta}(t)$  is norm-continuous on  $L^2(\Omega^{\frac{1}{2}}\Sigma)$ .

A few remarks about these assumptions are in order:

First, Assumption 1.a can always be realized if  $\gamma(t)^{-1}\partial_i\gamma(t)$ ,  $A_i(t) \in L^2_{loc}(\Sigma)$ ,  $\tilde{g}_{ij}(t) \in L^\infty_{loc}(\Sigma)$  and  $\tilde{Y}(t) \in L^1_{loc}(\Sigma)$  such that  $\tilde{Y}(t)$  is bounded from below by a positive constant. In that case L(t) can be understood as the form

$$(u|L(t)v) = \int_{\Sigma} \left( \left( \overline{D_i^{A,\gamma}(t)u} \right) \tilde{g}^{ij}(t) \left( D_j^{A,\gamma}(t)v \right) + \overline{u} \, \tilde{Y}(t)v \right),$$

on its (natural) maximal form domain  $\text{Dom } L(t)^{\frac{1}{2}} \supset C_c^{\infty}(\Omega^{\frac{1}{2}}\Sigma)$  (but it is not generally clear if  $C_c^{\infty}(\Omega^{\frac{1}{2}}\Sigma)$  is a form core). This form then defines a self-adjoint operator in the usual way. The details of this construction are given in Appx. A; its main aspects can be found in Thm. VI.2.6 of [25].

Assumptions 1.a and 1.b among other things guarantee positivity of the Hamiltonian. We thus avoid the so-called Klein "paradox" (see the appendix of [14] for a description), which appears if the Hamiltonian is not positive, and leads to various difficulties in the construction of the non-classical propagators. However, as far as the derivation of the evolution and the classical propagators is concerned, these assumptions can be weakened to allow for a non-positive Hamiltonian, see also Rem. 5.5.

Among other things, Assumption 1.c guarantees that for any t, s there exists c(t, s) > 0 such that

$$L(t) \le c(t,s)L(s). \tag{2.3}$$

Therefore, for  $\delta \in [-1, 1]$  we can define the Hilbertizable spaces

$$\mathcal{K}^{\delta} \coloneqq L(t)^{-\delta/2} L^2(\Omega^{\frac{1}{2}} \Sigma)$$

where the Hilbertian structures on the right-hand side are equivalent for different t because of (2.3).

Finally, Assumption 1.d implies the norm-continuity of  $t \mapsto \beta(t)^{\pm \frac{1}{2}}$  on  $\mathcal{K}^{\delta}$  for  $\delta \in [-1, 1]$ . Indeed,  $t \mapsto \beta(t)^{\pm \frac{1}{2}}$  are norm-continuous on  $\mathcal{K}^{-\frac{1}{2}}$  by duality, and then we can interpolate using, *e.g.*, the Heinz–Kato inequality (Thm. D.1).

While it should be obvious how Assumption 1.a, 1.b and 1.d can be realized in an example, Assumption 1.c is slightly less obvious. Therefore in Appx. B we briefly explain how Assumption 1.c can follow from more concrete assumptions on the metric, the vector potential and the scalar potential.

# 2.5 Assumptions global in time

While we always require that Assumption 1 holds, the following additional assumptions are only imposed when we derive asymptotic properties of propagators.

#### Assumption 2.

- 2.a. L(t) is uniformly bounded away from zero.
- 2.b. There exists a < 1 such that  $||W(t)L(t)^{-\frac{1}{2}}|| \le a$  for all t.
- 2.c. There exists a positive  $C \in L^1(\mathbb{R})$  such that for all  $t, s \in \mathbb{R}$

$$\left\|L(t)^{-\frac{1}{2}}(L(t)-L(s))L(t)^{-\frac{1}{2}}\right\|+2\left\|(W(t)-W(s))L(t)^{-\frac{1}{2}}\right\|\leq \left|\int_{s}^{t}C(r)\,\mathrm{d}r\right|,$$

where we place the absolute value on the right-hand side to account for the arbitrary order of *t* and *s*.

2.d.  $t \mapsto \beta(t)^{\pm \frac{1}{2}}$  are uniformly bounded on  $\mathcal{K}^1$  and  $t \mapsto \dot{\beta}$  is uniformly bounded on  $\mathcal{K}^0$ .

Note that, by the same argument as for Assumption 1.d, one can show that Assumption 2.d implies the uniform boundedness of  $t \mapsto \beta(t)^{\pm \frac{1}{2}}$  on  $\mathcal{K}^{\delta}$  for  $\delta \in [-1, 1]$ .

# 3 The energy space and the dynamical space

We will occasionally use the Hilbert space

$$\mathcal{H} := L^2(\Omega^{\frac{1}{2}}\Sigma) \oplus L^2(\Omega^{\frac{1}{2}}\Sigma) = \mathcal{K}^0 \oplus \mathcal{K}^0$$

with the canonical inner product also denoted by  $(\cdot | \cdot)$  and the corresponding norm  $||\cdot||$ .

The Hilbert space  $\mathcal{H}$  plays only an auxiliary role in our work. More important are the Hilbertizable spaces  $\mathcal{H}_a$ ,  $\alpha \in [-1, 1]$ , defined as

$$\mathcal{H}_{\alpha} := \mathcal{K}^{(\alpha+1)/2} \oplus \mathcal{K}^{(\alpha-1)/2}. \tag{3.1}$$

Note that for any t

$$\mathcal{H}_{\alpha} = \left( L(t) \oplus L(t) \right)^{-\alpha/4} \mathcal{H}_{0}, \quad \alpha \in [-1, 1].$$
(3.2)

We will treat the space  $\mathcal{H}_0$  as the central element of the family (3.2), identifying  $\mathcal{H}_0$  with  $\mathcal{H}_0^*$ , the *antidual* of  $\mathcal{H}_0$  (the space of bounded antilinear functionals on  $\mathcal{H}_0$ ). Then we have a natural identification of  $\mathcal{H}_{-\alpha}$  with  $\mathcal{H}_{\alpha}^*$ .

The central role in this work is played by the *energy space*, the *dynamical space* and the antidual of the energy space:

$$\mathcal{H}_{\mathrm{en}} \coloneqq \mathcal{H}_{1} = \left( L(t)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \mathcal{H} = H_{0}(t)^{-\frac{1}{2}} \mathcal{H}, \tag{3.3a}$$

$$\mathcal{H}_{\rm dyn} := \mathcal{H}_0 = \left( L(t)^{-\frac{1}{4}} \oplus L(t)^{\frac{1}{4}} \right) \mathcal{H}, \tag{3.3b}$$

$$\mathcal{H}_{\mathrm{en}}^* \coloneqq \mathcal{H}_{-1} = \left(\mathbb{1} \oplus L(t)^{\frac{1}{2}}\right) \mathcal{H} = \left(QH_0(t)Q\right)^{\frac{1}{2}} \mathcal{H},\tag{3.3c}$$

where we set

$$H_0(t) := L(t) \oplus \mathbb{1} = \begin{pmatrix} L(t) & 0 \\ 0 & \mathbb{1} \end{pmatrix},$$

and we also used the charge form

$$(u | Qv) := (u_1 | v_2) + (u_2 | v_1), \quad Q := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

It is evident that the charge form is bounded on  $\mathcal{H}$ . More importantly, it is also bounded on  $\mathcal{H}_{dyn}$  (but, *e.g.*, not on  $\mathcal{H}_{en}$ ).

Note that

$$\operatorname{Im}(u | Qv) = \frac{1}{2i} ((u | Qv) - (v | Qu))$$

is a symplectic form on  $\mathcal{H}_{dyn}$ . Therefore, the formalism based on the charge form is equivalent to the symplectic formalism, commonly used in the literature.

# 4 Instantaneous energy spaces and instantaneous dynamical spaces

An important role in our paper is played by the instantaneous Hamiltonian, defined formally for each t as

$$H(t) = QB(t) = B(t)^*Q.$$

One can define rigorously H(t) as a form bounded perturbation of  $H_0(t)$ :

Proposition 4.1. The operator

$$H(t) \coloneqq \begin{pmatrix} L(t) & \overline{W}(t) \\ W(t) & \mathbb{1} \end{pmatrix}$$

is self-adjoint on  ${\mathcal H}$  with the form domain  ${\mathcal H}_{en}\!.$  We have

$$(1-a(t))H_0(t) \le H(t) \le (1+a(t))H_0(t), \tag{4.1}$$

where  $0 \le a(t) < 1$  was introduced in Assumption 1.b.

**Proof.** We show only the right-hand side of the inequality (4.1). Set  $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ . Using the Cauchy–Schwarz inequality and Assumption 1.b, we find

$$\begin{aligned} (u|H(t)u) &\leq \|L(t)^{\frac{1}{2}}u_{1}\|^{2} + \|u_{2}\|^{2} + 2\|W(t)u_{1}\|\|u_{2}\| \\ &\leq \|L(t)^{\frac{1}{2}}u_{1}\|^{2} + \|u_{2}\|^{2} + 2a(t)\|L(t)^{\frac{1}{2}}u_{1}\|\|u_{2}\| \\ &\leq (1+a(t))(\|L(t)^{\frac{1}{2}}u_{1}\|^{2} + \|u_{2}\|^{2}) \\ &= (1+a(t))(u|H_{0}(t)u). \end{aligned}$$

We define for each time  $t \in \mathbb{R}$  the (*instantaneous*) energy scalar products given by

$$(u | v)_{\mathrm{en},t} := (u | H(t)v)$$

on  $\mathcal{H}_{en}$ . By (4.1) the scalar product  $(\cdot | \cdot)_{en,t}$  is compatible with the topology of  $\mathcal{H}_{en}$ . We call the resulting Hilbert space *instantaneous energy space at t* and denote it by  $\mathcal{H}_{en,t}$ .

Similarly, we can also define the operator  $QH(t)^{-1}Q$ . We find that its form domain is  $\mathcal{H}_{en}^*$ . Indeed,

$$(1+a(t))^{-1}QH_0(t)^{-1}Q \le QH(t)^{-1}Q \le (1-a(t))^{-1}QH_0(t)^{-1}Q.$$
(4.2)

Then we define for each t the scalar product

$$(u \mid v)_{\mathrm{en}^*, t} := (u \mid QH(t)^{-1}Qv)$$

and note that it is compatible with the topology of  $\mathcal{H}_{en}^*$ ; we denote the resulting Hilbert space by  $\mathcal{H}_{en,t}^*$ .

The central operator in this work is B(t). In the next section we construct the evolution of B(t) solving the first-order Klein–Gordon equation.

**Proposition 4.2.** Considered as an operator on  $\mathcal{H}_{en,t}^*$  with domain  $\mathcal{H}_{en}$ ,

$$B(t) \coloneqq \begin{pmatrix} W(t) & \mathbb{1} \\ L(t) & \overline{W}(t) \end{pmatrix}$$

is self-adjoint and 0 is in its resolvent set.

**Proof.** For notational simplicity, we drop the time dependence of B(t) and the other objects. We first check that B(t) is well-defined:

$$\begin{pmatrix} \mathbb{1} & 0 \\ 0 & L^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} W & \frac{1}{W} \end{pmatrix} \begin{pmatrix} L^{-\frac{1}{2}} & 0 \\ 0 & \mathbb{1} \end{pmatrix} = \begin{pmatrix} WL^{-\frac{1}{2}} & \mathbb{1} \\ \mathbb{1} & L^{-\frac{1}{2}}\overline{W} \end{pmatrix},$$

which is bounded by Assumption 1.b.

Next, we show that  $0 \in \operatorname{rs} B$ , and consequently also that B is closed. We rewrite B as

$$B = \begin{pmatrix} \mathbb{1} & 0 \\ \overline{W} & \mathbb{1} \end{pmatrix} \begin{pmatrix} 0 & \mathbb{1} \\ L - |W|^2 & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ W & \mathbb{1} \end{pmatrix}$$

and check that  $B^{-1}$  is bounded from  $\mathcal{H}_{en}^*$  to  $\mathcal{H}_{en}$ :

$$\begin{pmatrix} L^{\frac{1}{2}} & 0 \\ 0 & 1 \end{pmatrix} B^{-1} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & L^{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ -L^{-\frac{1}{2}} \overline{W} & 1 \end{pmatrix} \begin{pmatrix} 0 & (\mathbb{1} - L^{-\frac{1}{2}} |W|^2 L^{-\frac{1}{2}})^{-1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -W L^{-\frac{1}{2}} & 1 \end{pmatrix},$$

where the first and last factor on the right-hand side are bounded by Assumption 1.b, and

 $1 - L^{-\frac{1}{2}} |W|^2 L^{-\frac{1}{2}}$ 

is invertible because  $\|L^{-\frac{1}{2}}|W|^2L^{-\frac{1}{2}}\| < 1$ , also by Assumption 1.b.

Finally, we check that *B* is Hermitian on  $\mathcal{H}_{en}^*$ . We calculate

$$(QHQ)^{-1}B^{-1} = (BQHQ)^{-1} = (QHQHQ)^{-1} = (QHQB^*)^{-1} = B^{*-1}(QHQ)^{-1}.$$

We can now define for each time  $t \in \mathbb{R}$  a whole scale of Hilbert spaces

$$\mathcal{H}_{\alpha,t} := |B(t)|^{-(1+\alpha)/2} \mathcal{H}_{\mathrm{en},t}^*, \quad \alpha \in \mathbb{R},$$

with scalar products

$$(u \mid v)_{\alpha,t} := \left( u \mid |B(t)|^{1+\alpha} v \right)_{\mathrm{en}^*,t}, \quad u, v \in \mathcal{H}_{\alpha,t}.$$

Above we performed the polar decomposition with respect to the Hilbert space  $\mathcal{H}_{en,t}^*$ , where we have

$$|B(t)| = \sqrt{B(t)^2} = \sqrt{QH(t)QH(t)}.$$

It follows from its definition, that B(t) extends/restricts to a self-adjoint operator on each of the spaces  $\mathcal{H}_{a,t}$ . When B(t) is interpreted as an operator on  $\mathcal{H}_{a,t}$ , its domain is  $\mathcal{H}_{a+2,t}$ .

Clearly the scales  $\mathcal{H}_{\alpha,t}$  contain  $\mathcal{H}_{en,t}^* = \mathcal{H}_{-1,t}$ . They also contain the (instantaneous) energy spaces  $\mathcal{H}_{en,t} = \mathcal{H}_{1,t}$ , because a short calculation shows  $H(t) = QH(t)^{-1}Q|B(t)|^2$ . Furthermore, we define the (instantaneous) dynamical spaces

$$\mathcal{H}_{\mathrm{dyn},t} \coloneqq \mathcal{H}_{0,t}$$

which are treated as the central spaces in these scales. Note that  $\mathcal{H}_{dyn,t}$  is the form domain of B(t). We identify  $\mathcal{H}_{0,t}^*$ , with  $\mathcal{H}_{0,t}$ , and hence  $\mathcal{H}_{\alpha,t}^*$  is identified with  $\mathcal{H}_{-\alpha,t}$ . Thus we obtain the rigged Hilbert space setting

$$\mathcal{H}_{\text{en},t} \subset \mathcal{H}_{\text{dyn},t} \subset \mathcal{H}_{\text{en},t}^*$$
.

Proposition 4.3. In the sense of Hilbertizable spaces, we have

$$\mathcal{H}_{\alpha,t} = \mathcal{H}_{\alpha}, \quad \alpha \in [-1,1], \tag{4.3}$$

thus justifying our notation. In particular,

$$\mathcal{H}_{\mathrm{en},t} = \mathcal{H}_{\mathrm{en}}, \quad \mathcal{H}_{\mathrm{dyn},t} = \mathcal{H}_{\mathrm{dyn}}, \quad \mathcal{H}_{\mathrm{en},t}^* = \mathcal{H}_{\mathrm{en}}^*.$$

**Proof.** It follows from (4.1) and (4.2) that  $\mathcal{H}_{en,t} = \mathcal{H}_{en}$  and  $\mathcal{H}^*_{en,t} = \mathcal{H}^*_{en}$ . Since both  $L(t)^{\frac{1}{2}} \oplus L(t)^{\frac{1}{2}}$  and |B| can be understood as invertible bounded operators from  $\mathcal{H}_{en}$  to  $\mathcal{H}^*_{en}$ , there exists c > 1 such that

$$c^{-1} \left\| \left( L(t) \oplus L(t) \right)^{\frac{1}{2}} u \right\|_{\mathrm{en}^*} \le \left\| |B(t)| u \right\|_{\mathrm{en}^*} \le c \left\| \left( L(t) \oplus L(t) \right)^{\frac{1}{2}} u \right\|_{\mathrm{en}^*}$$

By interpolation (e.g., using the Heinz–Kato inequality, Thm. D.1),

$$c^{-\delta} \left\| \left( L(t) \oplus L(t) \right)^{\delta/2} u \right\|_{\mathrm{en}^*} \le \left\| |B(t)|^{\delta} u \right\|_{\mathrm{en}^*} \le c^{\delta} \left\| \left( L(t) \oplus L(t) \right)^{\delta/2} u \right\|_{\mathrm{en}^*} \right\|_{\mathrm{en}^*}$$

for  $\delta \in [0, 1]$ . It follows that the norms for  $\mathcal{H}_{\alpha}$  and  $\mathcal{H}_{\alpha,t}$  with  $\alpha \in [-1, 1]$  are equivalent and thus (4.3) follows.

Note that for  $|\alpha| > 1$  the spaces  $\mathcal{H}_{\alpha,t}$  may depend on *t* and do not have to coincide with  $\mathcal{H}_{\alpha}$ .

#### 5 Evolution

In the last section we laid the foundations for an application of the theory of non-autonomous evolution equations to the situation at hand, *i.e.*, the first-order Klein–Gordon equation

$$\partial_t u(t) + \mathbf{i}B(t)u(t) = 0.$$

Autonomous evolution equations (*viz.*, with a time-independent generator) posses a wellunderstood theory in terms of the theory of strongly continuous semigroups and groups. The theory for non-autonomous evolution equations is significantly more complicated and subtle. In Appx. C we discuss the relevant results based on the work of Kato [24].

Here we apply Thm. C.10 to the operator B(t) on the spaces

$$\mathcal{X}_t = \mathcal{H}_{\mathrm{en},t}^* \quad \text{and} \quad \mathcal{Y}_t = \mathcal{H}_{\mathrm{en},t}.$$
 (5.1)

For this purpose, we need to check whether the conditions (a)–(c) of Thm. C.10 hold. The self-adjointness condition (c) is clearly true, see Sect. 3. The next proposition implies that condition (b), a continuity condition on the norms of the Hilbert spaces  $\mathcal{H}_{en,t}$  and  $\mathcal{H}_{en,t}^*$ , holds:

**Proposition 5.1.** Let  $C \in L^1_{loc}(\mathbb{R})$  as in Assumption 1.c,  $a(t) \in C(\mathbb{R})$  as in Assumption 1.b and  $|t-s| \leq 1$  with  $t \geq s$ . Set  $c(t) := (1-a(t))^{-1}$ . Then

$$\|u\|_{a,t} \exp\left(-c(t)\int_{s}^{t} C(r) dr\right) \le \|u\|_{a,s} \le \|u\|_{a,t} \exp\left(c(t)\int_{s}^{t} C(r) dr\right)$$
(5.2)

for  $\alpha \in [-1, 1]$ .

**Proof.** First we show (5.2) for  $\alpha = 1$ , *i.e.*, for the energy space.

By Assumption 1.c, we have

$$\begin{split} \left\| \left( L(t)^{-\frac{1}{2}} \oplus 1 \right) \left( H(s) - H(t) \right) \left( L(t)^{-\frac{1}{2}} \oplus 1 \right) \right\| \\ &\leq \left\| L(t)^{-\frac{1}{2}} \left( L(s) - L(t) \right) L(t)^{-\frac{1}{2}} \right\| + 2 \left\| \left( W(s) - W(t) \right) L(t)^{-\frac{1}{2}} \right\| \\ &\leq \int_{s}^{t} C(r) \, \mathrm{d}r. \end{split}$$
(5.3)

Eq. (4.1) then implies that

$$\left\| H(t)^{-\frac{1}{2}} (L(t) \oplus 1) H(t)^{-\frac{1}{2}} \right\| \le c(t).$$
 (5.4)

Putting together (5.3) and (5.4), we obtain

$$\left\|H(t)^{-\frac{1}{2}}(H(s)-H(t))H(t)^{-\frac{1}{2}}\right\| \leq c(t)\int_{s}^{t}C(r)\,\mathrm{d}r.$$

Consequently we have

$$\left| \|u\|_{\mathrm{en},s}^{2} - \|u\|_{\mathrm{en},t}^{2} \right| \leq \|u\|_{\mathrm{en},t}^{2} \left( c(t) \int_{s}^{t} C(r) \,\mathrm{d}r \right).$$

Therefore

$$\|u\|_{\text{en},s}^{2} \leq \|u\|_{\text{en},t}^{2} \left(1 + c(t) \int_{s}^{t} C(r) \, \mathrm{d}r\right)$$
$$\leq \|u\|_{\text{en},t}^{2} \exp\left(c(t) \int_{s}^{t} C(r) \, \mathrm{d}r\right)$$

and, exchanging the role of t and s, we can similarly derive

$$||u||_{\mathrm{en},s}^2 \ge ||u||_{\mathrm{en},t}^2 \exp\left(-c(t)\int_s^t C(r)\,\mathrm{d}r\right),$$

so that the inequality (5.2) for  $\alpha = 1$  follows.

For  $\alpha = -1$  the inequality follows by duality. Using interpolation, we can then extend the inequality to the remaining values of  $\alpha$ .

To show that the condition (a) of Thm. C.10 holds, we only need to show the normcontinuity of  $t \mapsto B(t)$ ; the remaining statements are obvious.

**Proposition 5.2.** With  $C \in L^1_{loc}(\mathbb{R})$  as in Assumption 1.c, c(t) as in (4.1) and  $|t-s| \leq 1$ 

$$\left\| \left( B(s) - B(t) \right) u \right\|_{\mathrm{en}^{*}, t} \leq \left\| u \right\|_{\mathrm{en}, t} \left| c(t) \int_{s}^{t} C(r) \, \mathrm{d}r \right|,$$

where we place the absolute value on the right-hand side because  $t \ge s$  or  $t \le s$ . In particular,  $t \mapsto B(t)$  is norm-continuous as an operator from  $\mathcal{H}_{en,t}$  to  $\mathcal{H}^*_{en,t}$ .

**Proof.** We reduce the problem to the inequalities

$$\begin{split} \left\| \left( \mathbb{1} \oplus L(t)^{-\frac{1}{2}} \right) \left( B(s) - B(t) \right) \left( L(t)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \right\| \\ &= \left\| Q \left( L(t)^{-\frac{1}{2}} \oplus \mathbb{1} \right) Q \left( B(s) - B(t) \right) \left( L(t)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \right\| \\ &\leq \left\| \left( L(t)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \left( H(s) - H(t) \right) \left( L(t)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \right\| \\ &\leq \left\| \int_{s}^{t} C(r) \, dr \right\| \end{split}$$

and proceed similar as in the proof of Prop. 5.1. Since the integral is continuous, the required norm-continuity follows.  $\hfill \Box$ 

It follows that we can globally define an evolution for B(t):

**Theorem 5.3.** There exists a unique, strongly continuous family of bounded operators  $\{U(t,s)\}_{s,t\in\mathbb{R}}$  on  $\mathcal{H}_{en}^*$ , the evolution generated by B(t), with the following properties:

(i) For all  $r, s, t \in \mathbb{R}$ , we have the identities

$$U(t,t) = 1, \quad U(t,r)U(r,s) = U(t,s).$$
(5.5)

(ii) For  $\alpha \in [-1,1]$ ,  $U(t,s)\mathcal{H}_{\alpha} \subset \mathcal{H}_{\alpha}$ ,  $(t,s) \mapsto U(t,s)$  is strongly  $\mathcal{H}_{\alpha}$ -continuous and satisfies the bound

$$\|U(t,r)\|_{\alpha,s} \le \exp\left(2c(t)\int_{r}^{t}C(\tau)\,\mathrm{d}\tau\right),\tag{5.6a}$$

$$\|U(r,t)\|_{\alpha,s} \le \exp\left(2c(t)\int_{r}^{t}C(\tau)\,\mathrm{d}\tau\right)$$
(5.6b)

with C, c as in Prop. 5.1 and  $r \le s \le t$  where  $|t - r| \le 1$ .

(iii) For all  $u \in \mathcal{H}_{en}$ , U(t,s)u is continuously differentiable in  $s, t \in \mathbb{R}$  with respect to the strong topology of  $\mathcal{H}_{en}^*$  and it satisfies

$$i\partial_t U(t,s)u = B(t)U(t,s)u, \qquad (5.7a)$$

$$-i\partial_s U(t,s)u = U(t,s)B(s)u.$$
(5.7b)

**Proof.** Props. 5.1 and 5.2 as well as the results of Sect. 3 show that Thm. C.10 can be applied to our operator B(t) understood as an operator from  $\mathcal{H}_{en}$  to  $\mathcal{H}_{en}^*$  (or, equivalently, as a form on  $\mathcal{H}_{dyn}$  with form domain  $\mathcal{H}_{en}$ ). We thus obtain for every sufficiently small compact interval  $I \subset \mathbb{R}$  an evolution U(t,s) with the properties (i)–(iv) of Thm. C.10. In particular, we have for  $r, t \in I$  and  $r \leq s \leq t$ 

$$\|U(t,r)\|_{\mathrm{en},s} \leq \exp\left(2c(t)\int_{r}^{t}C(\tau)\,\mathrm{d}\tau\right),\\|U(t,r)\|_{\mathrm{en}^{*},s} \leq \exp\left(2c(t)\int_{r}^{t}C(\tau)\,\mathrm{d}\tau\right).$$

The same bounds also hold for  $||U(r, t)||_{en,s}$  and  $||U(r, t)||_{en^*,s}$ . By interpolation we find (5.6).

We cover  $\mathbb{R}$  by compact intervals. Using the identity (5.5), we thereby define the evolution U(t,s) on the whole real axis by gluing. For finite *s*, *t*, it has the properties (i)–(iv) of Thm. C.10.

Eq. (5.6) states that U(t,s) is bounded for finite t,s. To obtain stronger results later, we can choose more stringent assumptions:

**Corollary 5.4.** If Assumption 2.c holds, and we set  $C_1(t) := 2(1-a)^{-1}C(t)$ , then

$$||U(t,s)||_{\alpha,r} \leq \exp\left(\int_{\mathbb{R}} C_1(\tau) \,\mathrm{d}\tau\right)$$

for all  $r, s, t \in \mathbb{R}$  and any  $\alpha \in [-1, 1]$ .

**Remark 5.5.** In Assumption 1.a we supposed that L(t) is positive and invertible all the time. The results of this section remain true, with obvious modifications, if L(t) is only bounded from below. In fact, we can shift *Y* so that L(t) is positive. Then we can apply the perturbation theorem C.11 to find the evolution for the unshifted potential.

**Remark 5.6.** Our choice of spaces (5.1) to prove Thm. 5.3 is natural, especially given our low regularity setup. Under more restrictive assumptions on the smoothness and boundedness of coefficients of the Klein–Gordon operator K, other spaces in the scale  $\mathcal{H}_{\alpha,t}$ ,  $\alpha \in \mathbb{R}$ , could be used. This would lead to improved regularity results of the type  $U(t,s)\mathcal{H}_{\alpha} \subset \mathcal{H}_{\alpha}$  and continuous differentiability of  $U(t,s)\mathcal{H}_{\alpha}$  in  $\mathcal{H}_{\alpha-2}$ .

#### 6 Solutions of the Klein–Gordon equation

Solutions of the Klein–Gordon equation are closely related to solutions of the first-order Klein–Gordon equation.

Let us introduce the projection onto the second component:

$$\pi_2 \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \coloneqq u_2,$$

We also define embeddings

$$u_2 u \coloneqq \begin{pmatrix} 0 \\ u \end{pmatrix}, \quad \rho u \coloneqq \begin{pmatrix} u \\ -(D_t + W)u \end{pmatrix}$$

A formal calculation then shows that

$$\tilde{K} = i\pi_2(\partial_t + iB)\rho \quad \text{and} \quad K = i\beta^{-\frac{1}{2}}\pi_2(\partial_t + iB)\rho\beta^{-\frac{1}{2}}.$$
(6.1)

Therefore, if Ku = f or, equivalently,  $\tilde{K}\tilde{u} = \tilde{f}$  with  $\tilde{u} = \beta^{-\frac{1}{2}}u$ ,  $\tilde{f} = \beta^{\frac{1}{2}}f$ , then

$$i(\partial_t + iB)\rho \tilde{u} = \iota_2 \tilde{f}.$$

The projection  $\pi_2$  and the embeddings  $\rho$ ,  $\iota_2$ , which relate solutions of the Klein–Gordon equation and the first-order Klein–Gordon equation, can be understood between various spaces. It follows from the definition of  $\mathcal{H}_{\alpha}$  in (3.1) that, for  $\alpha \in [-1, 1]$ ,

$$\pi_2: \mathcal{H}_a \to \mathcal{K}^{(\alpha-1)/2},\tag{6.2a}$$

$$\pi_2 Q: \mathcal{H}_a \to \mathcal{K}^{(\alpha+1)/2},\tag{6.2b}$$

$$\iota_2: \mathcal{K}^{(\alpha-1)/2} \to \mathcal{H}_{\alpha}. \tag{6.2c}$$

These projections and embeddings already allows us to easily prove an existence and uniqueness result regarding solutions of the Klein–Gordon equation with Cauchy data in the energy space:

**Theorem 6.1.** Let  $s \in \mathbb{R}$ ,  $\begin{pmatrix} u_1(s) \\ u_2(s) \end{pmatrix} \in \mathcal{H}_{en}$  and  $f \in L^1_{loc}(\mathbb{R}; \mathcal{K}^0)$ . Set  $\begin{pmatrix} \tilde{u}_1(s) \\ \tilde{u}_2(s) \end{pmatrix} = \beta(s)^{-\frac{1}{2}} \begin{pmatrix} u_1(s) \\ u_2(s) \end{pmatrix} \quad and \quad \tilde{f} = \beta^{\frac{1}{2}} f.$  Then  $u = \beta^{\frac{1}{2}} \tilde{u}$  with

$$\tilde{u}(t) = \pi_2 Q U(t,s) \begin{pmatrix} \tilde{u}_1(s) \\ \tilde{u}_2(s) \end{pmatrix} - \mathbf{i} \int_s^t \pi_2 Q U(t,r) \iota_2 \tilde{f}(r) dr$$

is the unique solution of Ku = f such that

$$u \in C(\mathbb{R}; \mathcal{K}^1) \cap C^1(\mathbb{R}; \mathcal{K}^0) \quad and \quad \rho \tilde{u}(s) = \begin{pmatrix} \tilde{u}_1(s) \\ \tilde{u}_2(s) \end{pmatrix}.$$
(6.3)

**Proof.** We have the following special cases of (6.2):

$$\iota_2: \mathcal{K}^0 \to \mathcal{H}_{en}, \tag{6.4a}$$

$$\pi_2 Q: \mathcal{H}_{en} \to \mathcal{K}^1, \tag{6.4b}$$

$$\pi_2 Q: \mathcal{H}^*_{\text{en}} \to \mathcal{K}^0. \tag{6.4c}$$

By (6.4a), (6.4b) and Assumption 1.d, *u* belongs to  $C(\mathbb{R}; \mathcal{K}^1)$ . By (6.4a), (6.4c) and Assumption 1.d,  $\partial_t u$  belongs to  $C(\mathbb{R}; \mathcal{K}^0)$ . Hence the first part of (6.3) is true. The second part of (6.3) is obvious.

Set

$$\begin{pmatrix} \tilde{u}_1(t) \\ \tilde{u}_2(t) \end{pmatrix} = U(t,s) \begin{pmatrix} \tilde{u}_1(s) \\ \tilde{u}_2(s) \end{pmatrix} - i \int_s^t U(t,r) \iota_2 \tilde{f}(r) dr.$$
(6.5)

Differentiating (6.5) we obtain

$$i\partial_t \begin{pmatrix} \tilde{u}_1(t) \\ \tilde{u}_2(t) \end{pmatrix} = B(t) \begin{pmatrix} \tilde{u}_1(t) \\ \tilde{u}_2(t) \end{pmatrix} + \iota_2 \tilde{f}(t)$$
(6.6)

Clearly,  $\tilde{u}(t) = \tilde{u}_1(t)$ . The first component of (6.6) yields  $\tilde{u}_2(t) = -(D_t + W(t))\tilde{u}_1(t)$ . Hence

$$\rho \tilde{u}(t) = \begin{pmatrix} \tilde{u}_1(t) \\ \tilde{u}_2(t) \end{pmatrix}$$
(6.7)

The second component of (6.6), and then insertion of (6.7) yield

$$\tilde{f}(t) = i\pi_2(\partial_t + iB) \begin{pmatrix} \tilde{u}_1(t) \\ \tilde{u}_2(t) \end{pmatrix} = i\pi_2(\partial_t + iB)\rho \tilde{u}(t) = \tilde{K}\tilde{u}(t),$$

whence we have shown that  $\tilde{u}$  solves  $\tilde{K}\tilde{u} = \tilde{f}$  and thus Ku = f.

Uniqueness of the solution follows from the uniqueness of the evolution U(t,s), and the linearity of  $K, \rho$  by the standard argument: If u, u' satisfy

$$Ku = Ku' = f$$
 and  $\rho \tilde{u}(s) = \rho \tilde{u}'(s) = \begin{pmatrix} \tilde{u}_1(s) \\ \tilde{u}_2(s) \end{pmatrix}$ ,

where  $\tilde{u}' = \beta^{-\frac{1}{2}}u'$ , then K(u-u') = 0,  $\rho(\tilde{u}-\tilde{u}')(s) = 0$  and thus u = u'.

It is well-known that solutions of the Klein–Gordon equation propagate at a finite speed, more exactly, slower than the speed of light. The method of evolution equations together with the freedom of the choice of the time-variable provide a rather obvious heuristic argument for the propagation at a finite speed. However, when one tries to convert this argument into a rigorous proof, technical problems appear which make such a proof difficult to formulate.

In the literature the finiteness of the speed of propagation is usually shown for the Klein–Gordon equation with smooth coefficients. In Appx. E, in particular in Thm. E.1, we show that solutions of the Klein–Gordon propagate at a finite speed also in a low-regularity setup typical for our paper.

# 7 Classical propagators

Having constructed the evolution for B(t) in Sect. 5, it is not difficult to find the classical propagators for the first-order Klein–Gordon operator  $\partial_t + iB$ . To wit, the *Pauli–Jordan* propagator  $E^{\text{PJ}}$  and the forward/backward propagator  $E^{\text{V/A}}$  are given by the integral kernels

$$E^{\mathrm{PJ}}(t,s) := U(t,s), \tag{7.1a}$$

$$E^{\vee}(t,s) \coloneqq \theta(t-s)U(t,s), \tag{7.1b}$$

$$E^{\wedge}(t,s) \coloneqq -\theta(s-t)U(t,s) \tag{7.1c}$$

via

$$(E^{\bullet}f)(t) = \int_{\mathbb{R}} E^{\bullet}(t,s)f(s) \,\mathrm{d}s.$$
(7.2)

**Theorem 7.1.** *Let*  $\alpha \in [-1, 1]$ *.* 

(i) The classical propagators  $E^{PJ}$  and  $E^{\vee/\wedge}$  are well-defined between the following spaces:

$$E^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{H}_{\alpha}) \to C(\mathbb{R}; \mathcal{H}_{\alpha}),$$
  
$$E^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{H}_{en}) \to C^{1}(\mathbb{R}; \mathcal{H}_{en}^{*}).$$

(ii) The forward and backward propagator  $E^{\vee/\wedge}$  are well-defined between the following spaces:

$$E^{\vee/\wedge}: L^{1}_{\text{loc}}(I; \mathcal{H}_{\alpha}) \to C(I; \mathcal{H}_{\alpha}),$$
  
$$E^{\vee/\wedge}: L^{1}_{\text{loc}}(I; \mathcal{H}_{\text{en}}) \to C^{1}(I; \mathcal{H}_{\text{en}}^{*}),$$

where  $I = [a, +\infty[ \text{ resp. } ]-\infty, a]$  for some  $a \in \mathbb{R}$ .

(iii) If Assumption 2 is satisfied, the classical propagators  $E^{PJ}$  and  $E^{\vee/\wedge}$  are bounded between the following spaces:

$$E^{\bullet}: L^{1}(\mathbb{R}; \mathcal{H}_{\alpha}) \to C_{b}(\mathbb{R}; \mathcal{H}_{\alpha}),$$
  
$$E^{\bullet}: L^{1}(\mathbb{R}; \mathcal{H}_{en}) \to C_{b}^{1}(\mathbb{R}; \mathcal{H}_{en}^{*}).$$

(iv)  $E^{PJ}$  is a bisolution of  $\partial_t + iB$ :

$$(\partial_t + \mathbf{i}B)E^{\mathrm{PJ}}f = 0, \quad f \in L^1_c(\mathbb{R}; \mathcal{H}_{\mathrm{en}}), \tag{7.3}$$

$$E^{\rm PJ}(\partial_t + iB)f = 0, \quad f \in L^1_{\rm c}(\mathbb{R};\mathcal{H}_{\rm en}) \cap AC_{\rm c}(\mathbb{R};\mathcal{H}_{\rm en}^*).$$
(7.4)

(v)  $E^{\vee/\wedge}$  are the unique inverses of  $\partial_t + iB$  such that

$$(\partial_t + iB)E^{\vee/\wedge}f = f, \quad f \in L^1_{loc}(I, \mathcal{H}_{en}), \tag{7.5}$$

$$E^{\vee/\wedge}(\partial_t + \mathbf{i}B)f = f, \quad f \in L^1_{\mathrm{loc}}(I; \mathcal{H}_{\mathrm{en}}) \cap AC(I, \mathcal{H}^*_{\mathrm{en}}), \tag{7.6}$$

with  $I = [a, +\infty[ \text{ resp. } ]-\infty, a]$  for some  $a \in \mathbb{R}$ .

(vi) The relation  $E^{\text{PJ}} = E^{\vee} - E^{\wedge}$  holds.

**Proof.** (i)–(iii) follow from the properties of the evolution U(t,s) (see Thm. 5.3 and Cor. 5.4) and the definition of the kernels (7.1).

Consider next (iv) and (v). We first need to check that the products contained in these properties are well-defined. Indeed, by (i), the following maps are well-defined:

$$E^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{H}_{en}) \to C(\mathbb{R}; \mathcal{H}_{en}) \cap C^{1}(\mathbb{R}; \mathcal{H}^{*}_{en}),$$
(7.7a)

$$(\partial_t + iB): C(\mathbb{R}; \mathcal{H}_{en}) \cap C^1(\mathbb{R}; \mathcal{H}_{en}^*) \to C(\mathbb{R}; \mathcal{H}_{en}^*), \tag{7.7b}$$

which shows that (7.3) and (7.5) make sense. Similarly, by (i), we have

$$(\partial_t + \mathbf{i}B) : L^1_c(\mathbb{R}; \mathcal{H}_{en}) \cap AC_c(\mathbb{R}; \mathcal{H}^*_{en}) \to L^1_c(\mathbb{R}; \mathcal{H}^*_{en}), \tag{7.8a}$$

$$E^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{H}^{*}_{en}) \to C(\mathbb{R}; \mathcal{H}^{*}_{en}),$$
(7.8b)

hence the products in (7.4) and (7.6) make sense. Then we show (7.3)–(7.6) using (7.2) and (5.7). For (7.4) and (7.6) we also need to apply an integration by parts.  $\Box$ 

We can also state an  $L^2$  version of (iii) in Thm. 7.1 above:

**Theorem 7.2.** Let  $s > \frac{1}{2}$  and  $\alpha \in [-1, 1]$ . If Assumption 2 is satisfied, the classical propagators  $E^{PJ}$  and  $E^{\vee/\wedge}$  are bounded between the following spaces:

$$E^{\bullet}: \langle t \rangle^{-s} L^{2}(\mathbb{R}; \mathcal{H}_{\alpha}) \to \langle t \rangle^{s} L^{2}(\mathbb{R}; \mathcal{H}_{\alpha}),$$
  
$$E^{\bullet}: \langle t \rangle^{-s} L^{2}(\mathbb{R}; \mathcal{H}_{en}) \to \langle t \rangle^{s} \langle \partial_{t} \rangle^{-1} L^{2}(\mathbb{R}; \mathcal{H}_{en}^{*}).$$

**Proof.** We use the embeddings

$$\langle t \rangle^{-s} L^2(\mathbb{R}; \mathcal{X}) \subset L^1(\mathbb{R}; \mathcal{X}) \text{ and } \langle t \rangle^{s} L^2(\mathbb{R}; \mathcal{X}) \supset C_b(\mathbb{R}; \mathcal{X})$$

for any Banach space  $\mathcal{X}$  and  $s > \frac{1}{2}$ .

The classical propagators for the first-order Klein–Gordon operator can also be understood between various spaces other than those considered in Thms. 7.1 and 7.2, but our choices are quite natural. At the same time, this setup leads to an almost straightforward derivation of the propagators for the Klein–Gordon operator K.

Since  $\partial_t + iB$  and K are related via (6.1), also the propagators of these operators are closely related. At least formally, it can be shown that if  $E^{\bullet}$  is a propagator for  $\partial_t + iB$ , then  $-i\pi_2 Q E^{\bullet} \iota_2$  is a propagator for  $\tilde{K}$ , and hence

$$G^{\bullet} = -i\beta^{\frac{1}{2}}\pi_2 Q E^{\bullet}\iota_2 \beta^{\frac{1}{2}}.$$
(7.9)

is a propagator for the Klein–Gordon operator K. As we shall see now, this is indeed true if the domain of  $G^{\bullet}$  is carefully chosen:

# **Theorem 7.3.** *Let* $\delta \in [0, 1]$ *.*

(i) The classical propagators  $G^{PJ}$  and  $G^{\vee/\wedge}$  are well-defined between the following spaces:

$$G^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{K}^{-\delta}) \to C(\mathbb{R}; \mathcal{K}^{1-\delta}),$$
(7.10)

$$G^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{K}^{0}) \to C^{1}(\mathbb{R}; \mathcal{K}^{0}).$$

$$(7.11)$$

(ii) The forward and backward propagators G<sup>∨/∧</sup> are well-defined between the following spaces:

$$G^{\vee/\wedge}: L^{1}_{\text{loc}}(I; \mathcal{K}^{-\delta}) \to C(I; \mathcal{K}^{1-\delta}),$$
  
$$G^{\vee/\wedge}: L^{1}_{\text{loc}}(I; \mathcal{K}^{0}) \to C^{1}(I; \mathcal{K}^{0}),$$

where  $I = [a, +\infty[ \text{ resp. } ]-\infty, a]$  for some  $a \in \mathbb{R}$ .

(iii) If Assumption 2 is satisfied, the classical propagators  $G^{PJ}$  and  $G^{\vee/\wedge}$  are bounded between the following spaces:

$$G^{\bullet}: L^{1}(\mathbb{R}; \mathcal{K}^{-\delta}) \to C_{b}(\mathbb{R}; \mathcal{K}^{1-\delta}),$$
  
$$G^{\bullet}: L^{1}(\mathbb{R}; \mathcal{K}^{0}) \to C_{b}^{1}(\mathbb{R}; \mathcal{K}^{0}).$$

(iv)  $G^{PJ}$  is a bisolution of K:

$$KG^{\mathrm{PJ}}f = 0, \quad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0), \tag{7.12}$$

$$G^{\mathrm{PJ}}Kf = 0, \quad f \in L^{1}_{\mathrm{c}}(\mathbb{R};\mathcal{K}^{1}) \cap AC_{\mathrm{c}}(\mathbb{R};\mathcal{K}^{0}) \cap AC^{1}_{\mathrm{c}}(\mathbb{R};\mathcal{K}^{-1}).$$
(7.13)

(v)  $G^{\vee/\wedge}$  are the unique inverses of K such that

$$KG^{\vee/\wedge}f = f, \quad f \in L^1_{\text{loc}}(I; \mathcal{K}^0), \tag{7.14}$$

$$G^{\vee/\wedge}Kf = f, \quad f \in L^1_{\text{loc}}(I; \mathcal{K}^1) \cap AC(\mathbb{R}; \mathcal{K}^0) \cap AC^1(I; \mathcal{K}^{-1}).$$
(7.15)

with  $I = [a, +\infty[ \text{ resp. } ]-\infty, a]$  for some  $a \in \mathbb{R}$ .

(vi) The relation  $G^{PJ} = G^{\vee} - G^{\wedge}$  holds.

**Proof.** These results are a direct consequence of Thm. 7.1. In (i)–(iii) we used (6.2) and Assumption 1.d.

Let us check that the products in (iv) and (v) are well-defined. From the definition of  $\rho$  we can read off that

$$\rho: C(\mathbb{R}; \mathcal{K}^{1}) \cap C^{1}(\mathbb{R}; \mathcal{K}^{0}) \to C(\mathbb{R}; \mathcal{H}_{en}),$$
  

$$\rho: L^{1}_{c}(\mathbb{R}; \mathcal{K}^{1}) \cap AC_{c}(\mathbb{R}; \mathcal{K}^{0}) \to L^{1}_{c}(\mathbb{R}; \mathcal{H}_{en}),$$
  

$$\rho: AC_{c}(\mathbb{R}; \mathcal{K}^{0}) \cap AC^{1}_{c}(\mathbb{R}; \mathcal{K}^{-1}) \to AC_{c}(\mathbb{R}; \mathcal{H}_{en}^{*}).$$

Then, by (i) and also using (7.7), we have

$$\begin{aligned} G^{\bullet}: L^{1}_{c}(\mathbb{R};\mathcal{K}^{0}) &\to C(\mathbb{R};\mathcal{K}^{1}) \cap C^{1}(\mathbb{R};\mathcal{K}^{0}), \\ K: C(\mathbb{R};\mathcal{K}^{1}) \cap C^{1}(\mathbb{R};\mathcal{K}^{0}) \to C^{-1}(\mathbb{R};\mathcal{K}^{0}) \cap C(\mathbb{R};\mathcal{K}^{-1}), \end{aligned}$$

where  $C^{-1}(\mathbb{R})$  denotes the space of distributional derivatives of continuous functions. This shows that (7.12) and (7.14) make sense. Similarly, by (i) and (7.8), we have

$$K: L^{1}_{c}(\mathbb{R}; \mathcal{K}^{1}) \cap AC_{c}(\mathbb{R}; \mathcal{K}^{0}) \cap AC^{1}_{c}(\mathbb{R}; \mathcal{K}^{-1}) \to L^{1}_{c}(\mathbb{R}; \mathcal{K}^{-1}),$$
  
$$G^{\bullet}: L^{1}_{c}(\mathbb{R}; \mathcal{K}^{-1}) \to C(\mathbb{R}; \mathcal{K}^{0}),$$

hence the products in (7.13) and (7.15) make sense.

Here is an  $L^2$  version of (iii) in Thm. 7.3:

**Theorem 7.4.** Let  $s > \frac{1}{2}$ . If Assumption 2 is satisfied, the classical propagators  $G^{PJ}$  and  $G^{\vee/\wedge}$  are bounded between the following spaces:

$$G^{\bullet}: \langle t \rangle^{-s} L^2(\Omega^{\frac{1}{2}}M) \to \langle t \rangle^s L(t)^{-1} L^2(\Omega^{\frac{1}{2}}M), \tag{7.16a}$$

$$G^{\bullet}: \langle t \rangle^{-s} L^2(\Omega^{\frac{1}{2}}M) \to \langle t \rangle^s \langle \partial_t \rangle^{-1} L^2(\Omega^{\frac{1}{2}}M).$$
(7.16b)

**Proof.** By (7.10), for  $\delta \in [0, 1]$  we have

$$G^{\bullet}: \langle t \rangle^{-s} L^2(\mathbb{R}; \mathcal{K}^{-\delta}) \to \langle t \rangle^{s} L^2(\mathbb{R}; \mathcal{K}^{1-\delta}).$$
(7.17)

Setting  $\delta = 0$  we obtain

$$G^{\bullet}: \langle t \rangle^{-s} L^2(\mathbb{R}; \mathcal{K}^0) \to \langle t \rangle^s L(t)^{-1} L^2(\mathbb{R}; \mathcal{K}^0).$$
(7.18)

But  $L^2(\mathbb{R}; \mathcal{K}^0) = L^2(\mathbb{R}; L^2(\Omega^{\frac{1}{2}}\Sigma))$  and  $L^2(\Omega^{\frac{1}{2}}M)$  can naturally be identified, which proves (7.16a). It follows from (7.11) that

$$G^{\bullet}: \langle t \rangle^{-s} L^2(\mathbb{R}; \mathcal{K}^0) \to \langle t \rangle^s \langle \partial_t \rangle^{-1} L^2(\mathbb{R}; \mathcal{K}^0).$$

This yields (7.16b).

Observe that in other approaches, *e.g.* [2], the retarded and advanced propagators are the central objects and the Pauli–Jordan propagator is defined as their difference. Here, instead, the Pauli–Jordan propagator follows immediately from the evolution U(t,s) and should be seen as the central object, while the retarded and advanced propagators are derived objects.

Using the Pauli–Jordan propagator  $G^{PJ}$ , we can associate to every sufficiently regular compactly supported function a solution of the homogeneous Klein–Gordon equation. In fact, as the following proposition shows, also the converse is true.

**Proposition 7.5.** Suppose that  $u \in L^1_{loc}(\mathbb{R}; \mathcal{K}^1) \cap AC(\mathbb{R}; \mathcal{K}) \cap AC^1(\mathbb{R}; \mathcal{K}^{-1})$  satisfies Ku = 0. Then there exists a (non-unique)  $f \in L^1_c(\mathbb{R}; \mathcal{K}^{-1})$  such that  $u = G^{PJ}f$ .

**Proof.** Choose any  $r, s \in \mathbb{R}$ , r < s, and  $\chi \in C^{\infty}(M)$  such that  $\chi(t) = 0$  for  $t < r, 0 \le \chi(t) \le 1$  for  $r \le t \le s$  and  $\chi(t) = 1$  for t > s. Clearly,

$$0 = Ku = K\chi u - K(\chi - 1)u$$

and thus supp $(K\chi u) \subset [r,s] \times \Sigma$ . Besides,  $K\chi u \in L^1_c(\mathbb{R}; \mathcal{K}^{-1})$ . Therefore, we can act with  $G^{PJ}$  on  $K\chi u$ , obtaining

$$G^{\mathrm{PJ}}K\chi u = G^{\vee}K\chi u - G^{\wedge}K(\chi - 1)u = u.$$

That is,  $f = K \chi u$  is the desired function.

Our construction of the classical propagators starts from the propagators for the first-order Klein–Gordon operator (*i.e.*, given  $E^{\bullet}$ , we derive  $G^{\bullet}$  using (7.9)). If, instead,  $G^{\bullet}$  is provided, then  $E^{\bullet}$  can be derived:

(i) If  $G^{\bullet}$  is an inverse of *K* then

$$E^{\bullet} = \begin{pmatrix} -\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} (D_t + \overline{W}) & -\mathrm{i}\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} \\ \mathbb{1} + \mathrm{i}(D_t + W)\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} (D_t + \overline{W}) & -(D_t + W)\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} \end{pmatrix}$$

is (formally) an inverse of  $(\partial_t + iB)$ .

(ii) If  $G^{\bullet}$  is a bisolution of *K* then

$$E^{\bullet} = \begin{pmatrix} -\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} (D_t + \overline{W}) & -\mathbf{i}\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} \\ \mathbf{i}(D_t + W)\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} (D_t + \overline{W}) & -(D_t + W)\beta^{-\frac{1}{2}} G^{\bullet} \beta^{-\frac{1}{2}} \end{pmatrix}$$

is (formally) a bisolution of  $(\partial_t + iB)$ .

Note the subtle difference in the formulas inverses and bisolutions. No such difference appears in (7.9) which yields  $G^{\bullet}$  given  $E^{\bullet}$ .

#### 8 Instantaneous non-classical propagators

Consider an arbitrary reference time  $\tau$ . According to Prop. 4.2,  $B(\tau)$  is a self-adjoint operator on  $\mathcal{H}^*_{en,\tau}$ . Therefore we can use the functional calculus to define the projections onto the positive and negative spectrum of  $B(\tau)$ :

$$\Pi_{\tau}^{(\pm)} \coloneqq \mathbb{1}_{[0,\infty[}(\pm B(\tau)). \tag{8.1}$$

Zero is in its resolvent set of  $B(\tau)$ , and therefore (8.1) are complementary.

**Proposition 8.1.**  $\Pi_{\tau}^{(\pm)}$  restrict to complementary projections on  $\mathcal{H}_{\alpha}$  for  $\alpha \in [-1, 1]$ , and have the following properties:

- (i)  $\Pi_{\tau}^{(\pm)}B(\tau) = B(\tau)\Pi_{\tau}^{(\pm)}$ ,
- (ii)  $\Pi_{\tau}^{(+)} \Pi_{\tau}^{(-)} = \operatorname{sgn} B(\tau),$
- (iii)  $\operatorname{sp}(\pm \Pi_{\tau}^{(\pm)}B(\tau)) \subset ]0, \infty[,$
- (iv)  $\Pi_{\tau}^{(\pm)}$  are self-adjoint with respect to  $\mathcal{H}_{a,\tau}$ .

Moreover, the projections  $\Pi_{\tau}^{(\pm)}$  split  $\mathcal{H}_{\alpha,\tau}$  into subspaces of positive and negative charge (with respect to the charge form Q):

**Proposition 8.2.** 

$$\pm (u | Q \Pi_{\tau}^{(\pm)} u) = \pm (\Pi_{\tau}^{(\pm)} u | Q u) = \pm (\Pi_{\tau}^{(\pm)} u | Q \Pi_{\tau}^{(\pm)} u) \ge 0$$
(8.2)

for all  $u \in \mathcal{H}_{\alpha}$  with  $\alpha \in [-1, 1]$ .

**Proof.** The proof is the same as for Prop. 6.3 in [9].

The projections  $\Pi_{\tau}^{(\pm)}$  can be used to define *instantaneous positive/negative frequency* bisolutions  $E_{\tau}^{(\pm)}$ , given by their integral kernels as

$$E_{\tau}^{(\pm)}(t,s) := \pm U(t,\tau) \Pi_{\tau}^{(\pm)} U(\tau,s).$$
(8.3)

Using step functions, we then define the kernels of the *instantaneous Feynman and anti-Feynman inverses of*  $\partial_t$  + iB:

$$\begin{split} E_{\tau}^{\mathrm{F}}(t,s) &\coloneqq \theta(t-s) E_{\tau}^{(+)}(t,s) - \theta(s-t) E_{\tau}^{(-)}(t,s), \\ E_{\tau}^{\overline{\mathrm{F}}}(t,s) &\coloneqq \theta(t-s) E_{\tau}^{(-)}(t,s) - \theta(s-t) E_{\tau}^{(+)}(t,s). \end{split}$$

It is easy to see that these kernels can also be expressed using the retarded and advanced propagators:

$$E_{\tau}^{\rm F}(t,s) = E^{\wedge}(t,s) + E_{\tau}^{(+)}(t,s) = E^{\vee}(t,s) + E_{\tau}^{(-)}(t,s), \tag{8.4a}$$

$$E_{\tau}^{\overline{F}}(t,s) = E^{\vee}(t,s) - E_{\tau}^{(+)}(t,s) = E^{\wedge}(t,s) - E_{\tau}^{(-)}(t,s).$$
(8.4b)

As before, these kernels define the corresponding propagators via (7.2):

# **Theorem 8.3.** *Let* $\alpha \in [-1, 1]$ *.*

(i) The instantaneous non-classical propagators  $E_{\tau}^{(\pm)}$  and  $E_{\tau}^{F/F}$  are well-defined between the following spaces:

$$\begin{split} E^{\bullet}_{\tau} &: L^{1}_{c}(\mathbb{R};\mathcal{H}_{\alpha}) \to C(\mathbb{R};\mathcal{H}_{\alpha}), \\ E^{\bullet}_{\tau} &: L^{1}_{c}(\mathbb{R};\mathcal{H}_{en}) \to C^{1}(\mathbb{R};\mathcal{H}^{*}_{en}). \end{split}$$

(ii) If Assumption 2 is satisfied,  $E_{\tau}^{(\pm)}$  and  $E_{\tau}^{F/F}$  are bounded between the following spaces:

$$E^{\bullet}_{\tau}: L^{1}(\mathbb{R}; \mathcal{H}_{\alpha}) \to C_{b}(\mathbb{R}; \mathcal{H}_{\alpha}),$$
  
$$E^{\bullet}_{\tau}: L^{1}(\mathbb{R}; \mathcal{H}_{en}) \to C^{1}_{b}(\mathbb{R}; \mathcal{H}^{*}_{en}).$$

(iii)  $E_{\tau}^{(\pm)}$  are a bisolutions of  $\partial_t + iB$ :

$$\begin{aligned} (\partial_t + \mathrm{i}B)E_{\tau}^{(\pm)}f &= 0, \quad f \in L^1_{\mathrm{c}}(\mathbb{R};\mathcal{H}_{\mathrm{en}}), \\ E_{\tau}^{(\pm)}(\partial_t + \mathrm{i}B)f &= 0, \quad f \in L^1_{\mathrm{c}}(\mathbb{R};\mathcal{H}_{\mathrm{en}}) \cap AC_{\mathrm{c}}(\mathbb{R};\mathcal{H}_{\mathrm{en}}^*). \end{aligned}$$

(iv)  $E_{\tau}^{\mathrm{F}/\mathrm{F}}$  are inverses of  $\partial_t + \mathrm{i}B$ :

$$(\partial_t + \mathbf{i}B)E_{\tau}^{F/F}f = f, \quad f \in L^1_c(\mathbb{R}; \mathcal{H}_{\mathrm{en}}),$$
$$E_{\tau}^{F/\overline{F}}(\partial_t + \mathbf{i}B)f = f, \quad f \in L^1_c(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \cap AC_c(\mathbb{R}; \mathcal{H}_{\mathrm{en}}^*).$$

(v) The instantaneous non-classical propagators satisfy the relations:

$$\begin{split} E_{\tau}^{\rm F} &= E^{\wedge} + E_{\tau}^{(+)} = E^{\vee} + E_{\tau}^{(-)}, \qquad E_{\tau}^{\rm F} + E_{\tau}^{\overline{\rm F}} = E^{\vee} + E^{\wedge}, \qquad E_{\tau}^{(+)} - E_{\tau}^{(-)} = E^{\rm PJ}, \\ E_{\tau}^{\overline{\rm F}} &= E^{\vee} - E_{\tau}^{(+)} = E^{\wedge} - E_{\tau}^{(-)}, \qquad E_{\tau}^{\rm F} - E_{\tau}^{\overline{\rm F}} = E_{\tau}^{(+)} + E_{\tau}^{(-)}. \end{split}$$

**Proof.** The various properties of the non-classical propagators can be shown along the same lines as in Thm. 7.1 so we will omit the proofs. Property (v) in particular follows from (8.4) and its linear combinations.

As for the classical propagators, we can also find an  $L^2$  version of (ii) in Thm. 8.3:

**Theorem 8.4.** Let  $s > \frac{1}{2}$  and  $\alpha \in [-1, 1]$ . If Assumption 2 is satisfied, the instantaneous non-classical propagators  $E_{\tau}^{(\pm)}$  and  $E_{\tau}^{F/F}$  are bounded between the following spaces:

$$E_{\tau}^{\bullet}: \langle t \rangle^{-s} L^{2}(\mathbb{R}; \mathcal{H}_{\alpha}) \to \langle t \rangle^{s} L^{2}(\mathbb{R}; \mathcal{H}_{\alpha}),$$
  

$$E_{\tau}^{\bullet}: \langle t \rangle^{-s} L^{2}(\mathbb{R}; \mathcal{H}_{en}) \to \langle t \rangle^{s} \langle \partial_{t} \rangle^{-1} L^{2}(\mathbb{R}; \mathcal{H}_{en}^{*}).$$

Similar to (7.9), we define the instantaneous non-classical propagators  $G_{\tau}^{(\pm)}$  and  $G_{\tau}^{F/\overline{F}}$  for the Klein–Gordon operator *K* by

$$G_{\tau}^{(\pm)} := \beta^{\frac{1}{2}} \pi_2 Q E_{\tau}^{(\pm)} \iota_2 \beta^{\frac{1}{2}}, \quad G_{\tau}^{F/\overline{F}} := -i\beta^{\frac{1}{2}} \pi_2 Q E_{\tau}^{F/\overline{F}} \iota_2 \beta^{\frac{1}{2}}.$$

Note the absence of the complex unit in the definition of  $G_{\tau}^{(\pm)}$  so that  $G_{\tau}^{(\pm)}$  define positive forms, see property (vi) below.

Analogously to Thm. 7.3, we find

**Theorem 8.5.** *Let*  $\delta \in [-1, 1]$ *.* 

(i) The non-classical propagators  $G_{\tau}^{(\pm)}$  and  $G_{\tau}^{F/\overline{F}}$  are well-defined between the following spaces:

$$G_{\tau}^{\bullet}: L_{c}^{1}(\mathbb{R}; \mathcal{K}^{-\delta}) \to C(\mathbb{R}; \mathcal{K}^{1-\delta}), G_{\tau}^{\bullet}: L_{c}^{1}(\mathbb{R}; \mathcal{K}^{0}) \to C^{1}(\mathbb{R}; \mathcal{K}^{0}).$$

(ii) If Assumption 2 is satisfied,  $G_{\tau}^{(\pm)}$  and  $G_{\tau}^{F/F}$  are bounded between the following spaces:

$$G_{\tau}^{\bullet}: L^{1}(\mathbb{R}; \mathcal{K}^{-\delta}) \to C_{b}(\mathbb{R}; \mathcal{K}^{1-\delta}),$$
  
$$G_{\tau}^{\bullet}: L^{1}(\mathbb{R}; \mathcal{K}^{0}) \to C_{b}^{1}(\mathbb{R}; \mathcal{K}^{0}).$$

(iii)  $G_{\tau}^{(\pm)}$  are a bisolutions of K:

$$\begin{split} & KG_{\tau}^{(\pm)}f = 0, \quad f \in L^{1}_{c}(\mathbb{R};\mathcal{K}^{0}), \\ & G_{\tau}^{(\pm)}Kf = 0, \quad f \in L^{1}_{c}(\mathbb{R};\mathcal{K}^{1}) \cap AC_{c}(\mathbb{R};\mathcal{K}^{0}) \cap AC^{1}_{c}(\mathbb{R};\mathcal{K}^{-1}). \end{split}$$

(iv)  $G_{\tau}^{F/\overline{F}}$  are inverses of K:

$$\begin{split} & KG_{\tau}^{\mathrm{F}/\mathrm{F}}f = f, \quad f \in L^{1}_{\mathrm{c}}(\mathbb{R};\mathcal{K}^{0}), \\ & G_{\tau}^{\mathrm{F}/\mathrm{F}}Kf = f, \quad f \in L^{1}_{\mathrm{c}}(\mathbb{R};\mathcal{K}^{1}) \cap AC_{\mathrm{c}}(\mathbb{R};\mathcal{K}^{0}) \cap AC_{\mathrm{c}}^{1}(\mathbb{R};\mathcal{K}^{-1}). \end{split}$$

(v) The instantaneous non-classical propagators satisfy the relations:

$$\begin{split} G_{\tau}^{\rm F} &= G^{\wedge} + {\rm i} G_{\tau}^{(+)} = G^{\vee} + {\rm i} G_{\tau}^{(-)}, \qquad G_{\tau}^{\rm F} + G_{\tau}^{\overline{\rm F}} = G^{\vee} + G^{\wedge}, \qquad \qquad G_{\tau}^{(+)} - G_{\tau}^{(-)} = -{\rm i} G^{\rm PJ}, \\ G_{\tau}^{\overline{\rm F}} &= G^{\vee} - {\rm i} G_{\tau}^{(+)} = G^{\wedge} - {\rm i} G_{\tau}^{(-)}, \qquad \qquad G_{\tau}^{\rm F} - G_{\tau}^{\overline{\rm F}} = {\rm i} G_{\tau}^{(+)} + {\rm i} G_{\tau}^{(-)}. \end{split}$$

(vi) The instantaneous positive/negative frequency bisolutions are positive:

$$(f \mid G_{\tau}^{(\pm)}f) = \int_{M} \overline{f} \ G_{\tau}^{(\pm)}f \ge 0$$

for  $f \in L^1_c(\mathbb{R}; \mathcal{K}^0)$ .

**Proof.** We only show (vi); the remaining properties follow from corresponding properties of  $E_{\tau}^{\bullet}$  in Thm. 8.3 and can be shown as in Thm. 7.3. For (vi), we note that

$$(f \mid G_{\tau}^{(\pm)}f) = \iint \left(\iota_2 f(t) \mid Q E_{\tau}^{(\pm)}(t,s)\iota_2 f(s)\right) \mathrm{d}s \,\mathrm{d}t$$
$$= \left(u(\tau) \mid Q \Pi_{\tau}^{(\pm)}u(\tau)\right) \ge 0$$

by Prop. 8.2, where we set  $u(\tau) = \int U(\tau, t)f(t) dt \in \mathcal{H}_{en}$ .

The  $L^2$  version of (ii) of Thm. 8.5 is:

**Theorem 8.6.** Let  $s > \frac{1}{2}$ . If Assumption 2 is satisfied, the instantaneous non-classical propagators  $G_{\tau}^{(\pm)}$  and  $G_{\tau}^{F/\overline{F}}$  are bounded between the following spaces:

$$\begin{split} G^{\bullet}_{\tau} &: \langle t \rangle^{-s} L^2(\Omega^{\frac{1}{2}}M) \to \langle t \rangle^s L(t)^{-1} L^2(\Omega^{\frac{1}{2}}M), \\ G^{\bullet}_{\tau} &: \langle t \rangle^{-s} L^2(\Omega^{\frac{1}{2}}M) \to \langle t \rangle^s \langle \partial_t \rangle^{-1} L^2(\Omega^{\frac{1}{2}}M). \end{split}$$

In the static case, the non-classical propagators defined above do not depend on  $\tau$ . They are the natural propagators to consider in that situation, see also our earlier work [9].

In the non-static case, however, the instantaneous non-classical propagators just defined have deficiencies from the physical point of view, see *e.g.* [13]. First of all, their definition hinges on the arbitrary choice of a fixed instance of time and, even more seriously, on the choice of a time function. Secondly, instantaneous positive frequency bisolutions usually do not satisfy the microlocal spectrum condition of [30] (in other words, they do not define Hadamard states).

Nevertheless, the situation improves if the Klein–Gordon operator is infinitesimally static at the time when the positive/negative frequency splitting is performed. In a forthcoming article [8] we will show (using methods of evolution equations) that the corresponding instantaneous positive frequency bisolutions, which we define in the following section, satisfy then the microlocal spectrum condition of [30].

# 9 Asymptotic non-classical propagators

Throughout this section we assume that Assumption 2 is satisfied. It follows, in particular, that B(t) converges to  $B(\pm\infty)$  as  $t \to \pm\infty$  in norm as an operator from  $\mathcal{H}_{en}$  to  $\mathcal{H}_{en}^*$ . We define the *out* and *in positive/negative frequency projections* 

$$\Pi_{+}^{(\pm)} := \mathbb{1}_{[0,\infty[} (\pm B(+\infty)),$$
  
$$\Pi_{-}^{(\pm)} := \mathbb{1}_{[0,\infty[} (\pm B(-\infty)).$$

Theorem 9.1. The strong limits

$$\Pi_{+}^{(\pm)}(t) \coloneqq \underset{\tau \to +\infty}{\text{s-lim}} U(t,\tau) \Pi_{+}^{(\pm)} U(\tau,t), \tag{9.1a}$$

$$\Pi_{-}^{(\pm)}(t) \coloneqq \underset{\tau \to -\infty}{\text{s-lim}} U(t,\tau) \Pi_{-}^{(\pm)} U(\tau,t)$$
(9.1b)

exist as bounded operators on  $\mathcal{H}_{\alpha}$  with  $\alpha \in [-1,1]$ . They satisfy the obvious analogs of Propositions 8.1 and 8.2. Besides,

$$U(t,s)\Pi_{+}^{(\pm)}(t)U(t,s) = \Pi_{+}^{(\pm)}(s),$$
(9.2)

$$U(t,s)\Pi_{-}^{(\pm)}(t)U(t,s) = \Pi_{-}^{(\pm)}(s).$$
(9.3)

**Proof.** We only prove the theorem for (9.1a) because the proof for (9.1b) is the same. We have

$$U(t,r)\Pi_{+}^{(\pm)}U(r,t) = U(t,r)e^{i(t-r)B(+\infty)}\Pi_{+}^{(\pm)}e^{i(r-t)B(+\infty)}U(r,t).$$

We analyze separately the limit  $r \to +\infty$  of the operators left and right of the projection. Since both operators are bounded on  $\mathcal{H}_{\alpha,\tau}$ ,  $\alpha \in [-1, 1]$ , uniformly in t, r for arbitrary  $\tau \in \mathbb{R}$ , it is sufficient to show the convergence on  $\mathcal{H}_{en}$  with respect to the norm on  $\mathcal{H}_{en,\tau}^*$ .

We may assume that r > t. For  $u \in \mathcal{H}_{en}$  we have

$$U(t,r)e^{i(t-r)B(+\infty)}u = u + \int_t^r \partial_s (U(t,s)e^{i(t-s)B(+\infty)})u \,ds$$
$$= u - i \int_t^r U(t,s)(B(s) - B(+\infty))e^{i(t-s)B(+\infty)}u \,ds,$$

by the fundamental theorem of calculus and (iii) of Thm. 5.3. Taking the norm of this expression in  $\mathcal{H}^*_{en,\tau}$ , we find

$$\begin{aligned} \left\| U(t,r) \mathrm{e}^{\mathrm{i}(t-r)B(+\infty)} u - u \right\|_{\mathrm{en}^{*},\tau} \\ &\leq C \|u\|_{\mathrm{en},\tau} \int_{t}^{r} \left\| \left( \mathbb{1} \oplus L(\tau)^{-\frac{1}{2}} \right) \left( B(s) - B(+\infty) \right) \left( L(\tau)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \right\| \mathrm{d}s, \end{aligned}$$

since U(t,s) is uniformly bounded on  $\mathcal{H}_{en,\tau}^*$ .

It follows from the proof of Prop. 5.2 that

$$\left\| \left( \mathbb{1} \oplus L(\tau)^{-\frac{1}{2}} \right) \left( B(s) - B(+\infty) \right) \left( L(\tau)^{-\frac{1}{2}} \oplus \mathbb{1} \right) \right\|$$

is uniformly bounded. Therefore,

$$\left\| U(t,r) \mathrm{e}^{\mathrm{i}(t-r)B(+\infty)} u - u \right\|_{\mathrm{en}^*,\tau} \to 0$$

as  $t, r \rightarrow +\infty$  and the desired convergence follows.

The proof for  $U(t,r)e^{i(t-r)B(+\infty)}$  is essentially the same. The main difference is that we use the uniform boundedness of U(t,s) on  $\mathcal{H}_{en,\tau}$ .

We also define

$$E_{+}^{(\pm)}(t,s) \coloneqq \pm U(t,\tau)\Pi_{+}^{(\pm)}(\tau)U(\tau,s), \tag{9.4}$$

$$E_{-}^{(\pm)}(t,s) := \pm U(t,\tau)\Pi_{-}^{(\pm)}(\tau)U(\tau,s).$$
(9.5)

Clearly, the definition above do not depend on  $\tau$ .

The kernels  $E_{\pm}^{(\pm)}(t,s)$  yield the positive/negative frequency bisolutions at future and past infinity. They are often called out and in, or jointly asymptotic. Moreover, we may use them

together with the advanced and retarded propagators to define corresponding *asymptotic Feynman* and *anti-Feynman* propagators:

$$\begin{split} E^{\rm F}_{\pm} &= E^{\wedge} + E^{(+)}_{\pm} = E^{\vee} + E^{(-)}_{\pm}, \\ E^{\rm \overline{F}}_{\pm} &= E^{\vee} - E^{(+)}_{\pm} = E^{\wedge} - E^{(-)}_{\pm}. \end{split}$$

As before, the propagators  $E_{\pm}^{\bullet}$  for  $\partial_t + iB$  induce the corresponding propagators  $G_{\pm}^{\bullet}$  for *K*. Obviously, the asymptotic non-classical propagators defined here have analogues to Thm. 8.3 and Thm. 8.5; we only have to replace occurrences of  $\tau$  with  $\pm$ .

The asymptotic propagators defined above have various advantages over the instantaneous ones of the previous section. For one, they do not depend on an arbitrarily chosen instant of time. Under rather broad assumptions one can show that they even do not depend on the choice of the time function, but only on the spacetime itself. Finally, as recently discussed in [18], if the spacetime becomes asymptotically static sufficiently fast, they satisfy the microlocal spectrum condition of [30].

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# A Second order differential operators

Consider a manifold  $\Sigma$ . Every second-order Hermitian differential operator on  $L^2(\Omega^{\frac{1}{2}}\Sigma)$  can locally be written as

$$L = D_i g^{ij}(x) D_j - A^i(x) D_i - D_i A^i(x) + Y_0(x),$$
(A.1)

where  $g^{ij} = g^{ji}$ ,  $Y_0$  and  $A^i$  are real-valued.

L can be often rewritten in the form

$$L = (D_i - A_i)g^{ij}(D_j - A_j) + Y_1.$$
(A.2)

This is possible in particular if  $g^{ij}$  is everywhere non-degenerate, *viz.*, *g* determines a (pseudo-)Riemannian structure on *M*. Then (A.2) holds with

$$A_i \coloneqq g_{ij}A^j, \quad Y_1 \coloneqq Y_0 - A^i g_{ij}A^j,$$

where  $g_{ij}$  denotes the inverse of  $g^{ij}$ .

Let  $\gamma$  be an everywhere non-zero function. Then the operator *L* can be rewritten as

$$L = \gamma^{-\frac{1}{2}} (D_i - A_i) \gamma g^{ij} (D_j - A_j) \gamma^{-\frac{1}{2}} + Y_{\gamma}, \qquad (A.3)$$

where

$$Y_{\gamma} := Y - \frac{1}{2} \left( D_i g^{ij} \gamma^{-1} (D_j \gamma) \right) - \frac{1}{4} g^{ij} \gamma^{-2} (D_i \gamma) (D_j \gamma).$$

In particular, if we set  $\gamma := |g|^{\frac{1}{2}}$ , where  $|g| := |\det[g_{ij}]|$  is the canonical density induced by the metric, and  $Y := Y_{|g|^{\frac{1}{2}}}$ , then (A.3) yields the geometric form of the operator *L*:

$$L = |g|^{-\frac{1}{4}} (D_i - A_i)|g|^{\frac{1}{2}} g^{ij} (D_j - A_j)|g|^{-\frac{1}{4}} + Y.$$
(A.4)

If g is a metric tensor, A a 1-form, and Y a scalar, then the right-hand side of (A.4) transforms covariantly and L is well-defined as a differential operator acting on half-densities. We can rewrite (A.4) using the Levi-Civita derivative  $\nabla$  for g as

$$L = g^{ij}(i\nabla_i + A_i)(i\nabla_j + A_j) + Y.$$
(A.5)

Note that in (A.5) the right  $\nabla$  acts on half-densities and the left  $\nabla$  acts on half-densitized covectors.

If the metric is Riemannian, the differential part of the operator (A.4) can be called a (magnetic) Laplace-Beltrami operator, and the full operator can be called a (magnetic) Schrödinger operator. If the metric is Lorentzian, the differential part of the operator (A.4) can be called an *(electromagnetic)* d'Alembertian, and the full operator can be called an (electromagnetic) Klein–Gordon operator.

It is however sometimes convenient to consider a density  $\gamma$  independent of the metric tensor g, i.e., to work with (A.3) instead of (A.4). Using the derivative

$$D^{A,\gamma} \coloneqq \gamma^{\frac{1}{2}} (D-A) \gamma^{-\frac{1}{2}}, \tag{A.6}$$

L can be written as a quadratic form on half-densities:

$$(u | Lv) = \int_{\Sigma} \left( (\overline{D_i^{A,\gamma} u}) g^{ij} (D_j^{A,\gamma} v) + \overline{u} Y_{\gamma} v \right).$$
(A.7)

**Assumption 3.** In the remaining part of this appendix we assume that g is a Riemannian metric. We also assume that  $\gamma^{-1}\partial_i\gamma$ ,  $A_i \in L^2_{loc}(\Sigma)$ ,  $g^{ij} \in L^{\infty}_{loc}(\Sigma)$  and  $Y_{\gamma} \in L^1_{loc}(\Sigma)$  such that  $Y_{\gamma} \geq C$  for some  $C \in \mathbb{R}$ .

We will see that under the above assumption L can be understood as a self-adjoint operator on  $L^2(\Omega^{\frac{1}{2}}\Sigma)$  in at least two natural ways. First we reinterpret (A.7) by introducing the form

$$l_{\mathrm{mx}}[u,v] = \int_{\Sigma} \left( (\overline{D_i^{A,\gamma} u}) g^{ij} (D_j^{A,\gamma} v) + \overline{u} Y_{\gamma} v \right)$$
(A.8)

on its maximal form domain

dom 
$$l_{\mathrm{mx}} = \left\{ u \in L^2(\Omega^{\frac{1}{2}}\Sigma) \mid D^{A,\gamma}u \in L^2(\Omega^{\frac{1}{2}}T^*\Sigma, g), Y_{\gamma}^{\frac{1}{2}}u \in L^2(\Omega^{\frac{1}{2}}\Sigma) \right\}.$$

Here we denote by  $L^2(\Omega^{\frac{1}{2}}T^*\Sigma, g)$  the completion of  $C_c^{\infty}(\Omega^{\frac{1}{2}}T^*\Sigma)$  with respect to the norm given by

$$\iota\mapsto \left(\int_{\Sigma}\overline{u}_i\,g^{ij}u_j\right)^{\frac{1}{2}}.$$

We remark that  $C_c^{\infty}(\Omega^{\frac{1}{2}}\Sigma) \subset \text{dom } l_{\text{mx}}$ . The following is a standard proof and has been adapted from Lem. 1 of [28].

**Lemma A.1.** The form  $l_{mx}$  is closed and Hermitian. It defines a unique self-adjoint operator  $L_{mx}$ on

$$\operatorname{Dom} L_{\operatorname{mx}} = \left\{ v \in \operatorname{dom} l_{\operatorname{mx}} \mid |l_{\operatorname{mx}}[u, v]| \le C_{v} ||u|| \text{ for all } u \in L^{2}(\Omega^{\frac{1}{2}} \Sigma) \right\}$$

satisfying

$$(u \mid L_{\mathrm{mx}}v) = l_{\mathrm{mx}}[u, v]$$

for  $u \in \text{dom} l_{\text{mx}}$  and  $v \in \text{Dom} L_{\text{mx}}$ . Moreover,  $\text{dom} l_{\text{mx}} = \text{Dom} L_{\text{mx}}^{\frac{1}{2}}$ .

**Proof.** Suppose that  $\{u_n\} \subset \text{dom } l_{\text{mx}}$  is a Cauchy sequence with respect to the norm

dom 
$$l_{mx} \ni u \mapsto (l_{mx}[u, u] + (1 - C) ||u||^2)^{\frac{1}{2}}$$
.

Then there exist  $u, v \in L^2(\Omega^{\frac{1}{2}}\Sigma)$  and  $w \in L^2(\Omega^{\frac{1}{2}}T^*\Sigma, g)$  such that

$$u_n \to u, \quad Y_{\gamma}^{\frac{1}{2}} u_n \to \nu \quad \text{in } L^2(\Omega^{\frac{1}{2}} \Sigma)$$

$$D^{A,\gamma}u_n \to w \quad \text{in } L^2(\Omega^{\frac{1}{2}}T^*\Sigma,g).$$

Moreover,  $Y_{\gamma}^{\frac{1}{2}}u_n \to Y_{\gamma}^{\frac{1}{2}}u$  and  $D^{A,\gamma}u_n \to D^{A,\gamma}u$  weakly, and thus  $v = Y_{\gamma}^{\frac{1}{2}}u$  and  $w = D^{A,\gamma}u$  because v, w must coincide with the weak limits. It follows that  $l_{mx}$  is a closed form (and manifestly Hermitian). Therefore, by the first representation theorem (Thm. VI.2.6 of [25]),  $l_{mx}$  defines a unique self-adjoint operator with the stated properties.

An alternative to  $l_{\rm mx}$  is the form  $l_{\rm mn}$  given by the completion of the form (A.8) on  $C_{\rm c}^{\infty}(\Omega^{\frac{1}{2}}\Sigma)$ , and the corresponding operator  $L_{\rm mn}$ .  $l_{\rm mn}$  may have a strictly smaller domain than  $l_{\rm mx}$  because of the boundary effects. If  $l_{\rm mn} = l_{\rm mx}$ , then  $C_{\rm c}^{\infty}(\Omega^{\frac{1}{2}}\Sigma)$  is a core of  $l_{\rm mx}$ . Note that for  $\Sigma = \mathbb{R}^3$  with the Euclidean metric this is known to be true, see *e.g.* [28].

Certainly the setting considered in this appendix is not the most general possible. For example, the assumption that *Y* is bounded from below can certainly be relaxed.

#### **B** Concrete assumptions

The objective of this appendix is to eludicate how Assumption 1.c may be realized in practice. Recall that  $(\Sigma, \tilde{g}(t))$  is a family of Riemannian manifolds,  $\gamma(t) > 0$  are densities on  $\Sigma, A(t)$  are real-valued 1-forms and  $\tilde{Y}(t)$  are real-valued scalar potentials. As in Assumption 3 in Appx. A, we assume that  $\gamma^{-1}(t)\partial_i\gamma(t)$ ,  $A_i(t) \in L^2_{loc}(\Sigma)$ ,  $\tilde{g}^{ij} \in L^\infty_{loc}(\Sigma)$ , and  $\tilde{Y} \in L^1_{loc}(\Sigma)$  is bounded from below.

Let us recall the definition of the operators W(t) and L(t) on  $L^2(\Omega^{\frac{1}{2}}\Sigma)$ :

$$W(t) \coloneqq V(t) + \frac{i}{2} (\gamma(t)^{-1} \dot{\gamma}(t)),$$
  
$$(u \mid L(t)v) \coloneqq \int_{\Sigma} \left( \left( \overline{D_i^{A,\gamma}(t)u} \right) \tilde{g}^{ij}(t) \left( D_j^{A,\gamma}(t)v \right) + \overline{u} \, \tilde{Y}(t)v \right), \tag{B.1}$$

where L(t) is interpreted, say, as the maximal operator given by (B.1), as in Appx. A. Assumption 1.c now says that there exists a positive  $C \in L^1_{loc}(\mathbb{R})$  such that for all  $|t-s| \leq 1$ 

$$\left\| L(t)^{-\frac{1}{2}} \left( L(t) - L(s) \right) L(t)^{-\frac{1}{2}} \right\| + 2 \left\| \left( W(t) - W(s) \right) L(t)^{-\frac{1}{2}} \right\| \le \left| \int_{s}^{t} C(r) \, \mathrm{d}r \right|, \tag{B.2}$$

for some  $C \in L^1_{loc}(\mathbb{R})$ .

We also introduce the family of norms

$$\|X\|_t = \left(\int_{\Sigma} \tilde{g}^{ij}(t) \overline{X}_i X_j\right)^{\frac{1}{2}}$$

for half-densitized 1-forms X on  $\Sigma$ .

**Proposition B.1.** Suppose that there are positive  $C_Y, C_g, C_W \in L^1_{loc}(\mathbb{R})$ ,  $C_A, C_{\gamma} \in L^2_{loc}(\mathbb{R})$  such that for all  $|t-s| \leq 1$ 

$$\begin{split} \left\| L(t)^{-\frac{1}{2}} \partial_s \tilde{Y}(s) L(t)^{-\frac{1}{2}} \right\| &\leq C_Y(s), \\ \left\| \partial_s W(s) L(t)^{-\frac{1}{2}} \right\| &\leq C_W(s), \\ \left\| \partial_s A(s) L(t)^{-\frac{1}{2}} \right\|_t &\leq C_A(s), \\ \left\| \partial_s \gamma(s)^{-1} d\gamma(s) L(t)^{-\frac{1}{2}} \right\|_t &\leq C_\gamma(s), \\ \left\| \partial_s \tilde{g}^{ij}(s) X_i X_j \right\| &\leq C_g(s) \tilde{g}^{ij}(t) X_i X_j, \quad X \in C(T^* \Sigma). \end{split}$$

Then (B.2) holds and thus Assumption 1.c is true.

and

**Proof.** To avoid notational clutter within this proof, we simply write  $D_i$  for  $D_i^{A,\gamma}$ . Clearly, the assumptions of the proposition imply

$$\left\| L(t)^{-\frac{1}{2}} (\tilde{Y}(t) - \tilde{Y}(s)) L(t)^{-\frac{1}{2}} \right\| \le \left| \int_{s}^{t} C_{Y}(r) dr \right|,$$
 (B.3a)

$$\left\| \left( W(t) - W(s) \right) L(t)^{-\frac{1}{2}} \right\| \le \left| \int_{s}^{t} C_{W}(r) \, \mathrm{d}r \right|,$$
 (B.3b)

$$\left\| (A(t) - A(s))L(t)^{-\frac{1}{2}} \right\|_{t} \le \left| \int_{s}^{t} C_{A}(r) dr \right|,$$
 (B.3c)

$$\left\| \left( \gamma(t)^{-1} \mathrm{d}\gamma(t) - \gamma(s)^{-1} \mathrm{d}\gamma(s) \right) L(t)^{-\frac{1}{2}} \right\|_{t} \le \left| \int_{s}^{t} C_{\gamma}(r) \mathrm{d}r \right|, \tag{B.3d}$$

$$\left|\tilde{g}^{ij}(t)X_iX_j - \tilde{g}^{ij}(s)X_iX_j\right| \le \left|\int_s^t C_g(r)\,\mathrm{d}r\right| \tilde{g}^{ij}(t)X_iX_j. \tag{B.3e}$$

We compute

$$\begin{aligned} \left(u\left|\left(L(t)-L(s)\right)u\right) \\ &= \int_{\Sigma} \tilde{g}^{ij}(t) \left(\left(\overline{D_i(t)u}\right) \left(D_j(t)u - D_j(s)u\right) + \left(\overline{D_i(t)u - D_i(s)u}\right) \left(D_j(t)u\right) \\ &\quad - \left(\overline{D_i(t)u - D_i(s)u}\right) \left(D_j(t)u - D_j(s)u\right)\right) \\ &\quad + \int_{\Sigma} \left(\tilde{g}^{ij}(t) - \tilde{g}^{ij}(s)\right) \left(\left(\overline{D_i(t)u}\right) \left(D_j(t)u\right) - \left(\overline{D_i(t)u}\right) \left(D_j(t)u - D_j(s)u\right) \\ &\quad - \left(\overline{D_i(t)u - D_i(s)u}\right) \left(D_j(t)u\right) + \left(\overline{D_i(t)u - D_i(s)u}\right) \left(D_j(t)u - D_j(s)u\right)\right) \\ &\quad + \int_{\Sigma} \left(\tilde{Y}(t) - \tilde{Y}(s)\right) |u|^2, \end{aligned}$$

where

$$D_i(t) - D_i(s) = -A_i(t) + A_i(s) + \frac{\mathrm{i}}{2}\gamma(t)^{-1}\partial_i\gamma(t) - \frac{\mathrm{i}}{2}\gamma(s)^{-1}\partial_i\gamma(s).$$

Estimating each term separately using (B.3), we find

$$\left|\left(u\left|\left(L(t)-L(s)\right)u\right)\right| \leq \tilde{C}(t,s)(u\,|\,L(t)u),\right.$$

where

$$\tilde{C}(t,s) = 2\left|\int_{s}^{t} C_{D}(r) dr\right| + \left|\int_{s}^{t} C_{D}(r) dr\right|^{2} + \left|\int_{s}^{t} C_{g}(r) dr\right| \left(1 + \left|\int_{s}^{t} C_{D}(r) dr\right|\right)^{2} + \left|\int_{s}^{t} C_{Y}(r) dr\right|$$

with  $C_D = C_A + C_{\gamma}/2$ . After two applications of

$$\left|\int_{s}^{t} C_{D}(r) \,\mathrm{d}r\right|^{2} \leq |t-s| \left|\int_{s}^{t} C_{D}(r)^{2} \,\mathrm{d}r\right| \leq \left|\int_{s}^{t} C_{D}(r)^{2} \,\mathrm{d}r\right|,$$

which is a simple consequence of the Cauchy-Schwarz inequality, we obtain

$$\tilde{C}(t,s) \leq \left| \int_{s}^{t} \left( c(t)(2C_{D}+C_{D}^{2})+C_{\gamma}+C_{g} \right) \mathrm{d}r \right|,$$

where  $c(t) := 1 + \int_{t-1}^{t+1} C_g(r) dr$ . Thus Assumption 1.c is true with  $C(t) = \tilde{C}(t) + C_W(t)$ .

The inequalities (B.3) in the last proposition were stated with respect to L(t). For a more convenient criterion, fix a (time-independent) Riemannian metric  $g_0$  on  $\Sigma$  and set  $\gamma_0 := |g_0|^{\frac{1}{2}}$ . Consider the operator  $L_0$  defined by the form

$$(u | L_0 v) \coloneqq \int_{\Sigma} \left( (\overline{D_i^{\gamma_0} u}) g_0^{ij}(t) (D_j^{\gamma_0} v) + \overline{u} v \right).$$

**Proposition B.2.** Assume that there exists a positive  $C_g \in C(\mathbb{R})$  such that

$$\tilde{g}^{ij}(t)X_iX_j \ge C_g(t)g_0^{ij}X_iX_j. \tag{B.4}$$

Further, suppose that there exist  $\varepsilon_0 \in C(\mathbb{R})$ ,  $\varepsilon_0(t) \in [0, 1[$ , and a positive  $C_0 \in C(\mathbb{R})$  such that

$$\varepsilon_0(t)\gamma_0^2\gamma(t)^{-2} \left(\partial_i\gamma_0^{-1}\gamma(t)\right)\tilde{g}^{ij}(t) \left(\partial_j\gamma_0^{-1}\gamma(t)\right) + \tilde{Y}(t) \ge C_0(t) \tag{B.5}$$

Then there exists a positive  $C \in C(\mathbb{R})$  such that  $L_0$  satisfies the inequality

$$\left\| L(t)^{\frac{1}{2}} u \right\| \ge C(t) \left\| L_0^{\frac{1}{2}} |u| \right\|, \quad u \in \text{Dom}\, L(t)^{\frac{1}{2}}.$$
 (B.6)

**Proof.** Let  $\varepsilon(t) := (1 - 4\varepsilon_0(t))^{-1}$ , so that  $\varepsilon_0(t) = \frac{1}{4}(1 - \varepsilon(t)^{-1})$ . Then

$$\begin{aligned} (u | L(t)u) &\geq \int_{\Sigma} \left( -\left( D_{i}^{\gamma}(t) | u | \right) \tilde{g}^{ij}(t) \left( D_{j}^{\gamma}(t) | u | \right) + \tilde{Y}(t) | u |^{2} \right) \\ &\geq \int_{\Sigma} \left( \varepsilon(t) - 1 \right) (D_{i}^{\gamma_{0}} | u |) \tilde{g}^{ij}(t) (D_{j}^{\gamma_{0}} | u |) \\ &\qquad + \int_{\Sigma} \left( \varepsilon_{0}(t) \gamma_{0}^{2} \gamma(t)^{-2} \left( \partial_{i} \gamma_{0}^{-1} \gamma(t) \right) \tilde{g}^{ij}(t) \left( \partial_{j} \gamma_{0}^{-1} \gamma(t) \right) + \tilde{Y}(t) \right) | u |^{2} \\ &\geq \min \left( C_{g}(t) (1 - \varepsilon(t)), C_{0}(t) \right) \left( | u | \left| L_{0} | u | \right). \end{aligned}$$

In the first step we used the diamagnetic inequality

$$\left| \left( \partial_x - iV(x) \right) f(x) \right| \ge \left| \partial_x |f(x)| \right|$$

almost everywhere for real *V* and *f* such that  $(\partial_x - iV)f$  exists almost everywhere. In the second step we used the Cauchy–Schwarz inequality.

We can apply the preceding proposition to restate Prop. B.1 using  $L_0$  instead of L(t). For this purpose we introduce another norm on half-densitized 1-forms:

$$||X|| = \left(\int_{\Sigma} g_0^{ij} \overline{X}_i X_j\right)^{\frac{1}{2}}.$$

**Proposition B.3.** In addition to (B.4) and (B.5) we suppose that for some  $C_g \in C(\mathbb{R})$ 

$$\tilde{g}^{ij}(t)X_iX_j \leq C_g(t)g_0^{ij}X_iX_j, \quad X \in C(T^*\Sigma).$$

Moreover, we assume that there are positive  $C_{Y,0}, C_{g,0}, C_{W,0} \in L^1_{loc}(\mathbb{R}), C_{A,0}, C_{\gamma,0} \in L^2_{loc}(\mathbb{R})$  such that for all  $t \in \mathbb{R}$ 

$$\begin{split} \left\| L_{0}^{-\frac{1}{2}} |\partial_{t} \tilde{Y}(t)| L_{0}^{-\frac{1}{2}} \right\| &\leq C_{Y,0}(t), \\ \left\| \partial_{t} W(t) L_{0}^{-\frac{1}{2}} \right\| &\leq C_{W,0}(t), \\ \left\| \partial_{t} A(t) L_{0}^{-\frac{1}{2}} \right\| &\leq C_{A,0}(t), \\ \left\| \partial_{t} \gamma(t)^{-1} d\gamma(t) L_{0}^{-\frac{1}{2}} \right\| &\leq C_{\gamma,0}(t), \\ \left\| \partial_{t} \tilde{g}^{ij}(t) X_{i} X_{j} \right\| &\leq C_{g,0}(t) g_{0}^{ij} X_{i} X_{j}, \quad X \in C(T^{*} \Sigma). \end{split}$$

Then Assumption 1.c is true.

# C Non-autonomous evolution in Hilbert spaces

To make this paper more self-contained, we explain in this appendix relevant aspects of the theory of linear evolution equations. We are more general than strictly necessary for the purposes of this paper, but in anticipation of our upcoming work this generality could be useful. The results stated in this appendix can be found in similar form in [24] and in the monographs [29, 31]. We also wish to refer to the appendix of the recent work [1] by Bach and Bru, which uses slightly different assumptions that essentially coincide with ours for the Hilbertian case.

Let  $\mathcal{X}$  be a Banach space. We recall that a linear operator A on  $\mathcal{X}$  is the generator of a strongly continuous (one-parameter) semigroup  $[0, \infty[ \ni t \mapsto e^{tA} \text{ if and only if } A \text{ is densely defined, closed and there exist constants } M \ge 1, \beta \in \mathbb{R}$  such that its resolvent satisfies

$$||(A-\lambda)^{-n}|| \le M(\lambda-\beta)^{-n}, \quad \lambda > \beta, \quad n = 1, 2, \dots$$

Then we have  $||e^{tA}|| \le Me^{\beta t}$  and say that  $e^{tA}$  is a semigroup of type  $(M, \beta)$ ; a semigroup of type (1, 0) is a semigroup of contractions. If both *A* and -A generate strongly continuous semigroups, they generate a strongly continuous (one-parameter) group  $\mathbb{R} \ni t \mapsto e^{tA}$ .

Let  $\mathcal{Y}$  be another Banach space, which is densely and continuously embedded in  $\mathcal{X}$ .

**Definition C.1.** By the *part of A on*  $\mathcal{Y}$  we mean the operator  $\tilde{A}$ , which is the restriction of A to the domain

$$Dom(\hat{A}) := \{ y \in Dom(A) \cap \mathcal{Y} \mid Ay \in \mathcal{Y} \}.$$

**Definition C.2.**  $\mathcal{Y}$  is called *A*-admissible if the semigroup  $e^{tA}$ ,  $t \in [0, \infty[$ , leaves  $\mathcal{Y}$  invariant and its restriction to  $\mathcal{Y}$  is a strongly continuous semigroup on  $\mathcal{Y}$ .

In the following we consider a family  $\{A(t)\}_{t \in [0,T]}$  of generators of a strongly continuous semigroup. We chose the interval [0, T] for convenience and definiteness; the generalization to other intervals is straightforward.

**Definition C.3.** The family  $\{A(t)\}_{t \in [0,T]}$  is called *stable* with stability constants  $M \ge 1, \beta \in \mathbb{R}$ , if

$$\left\|\prod_{j=1}^{\kappa} (A(t_j) - \lambda)^{-1}\right\| \leq M(\lambda - \beta)^{-1}, \quad \lambda > \beta,$$

for all finite sequences  $s \le t_1 \le t_2 \le \cdots \le t_k \le t$ ,  $k = 1, 2, \dots$  Here and below such products are time-ordered (*viz.*, factors with a larger  $t_j$  are to the left of factors with a smaller  $t_j$ ).

**Proposition C.4.** If  $\{A(t)\}_{t \in [0,T]}$  is stable with stability constants  $M, \beta$ , then

$$\left\|\prod_{j=1}^{k} \mathrm{e}^{\mu_{j}A(t_{j})}\right\| \leq M \mathrm{e}^{\beta(\mu_{1}+\cdots+\mu_{k})}, \quad \mu_{j} \geq 0.$$

**Proof.** The proof is straightforward, see *e.g.* Prop. 7.3 of [31].

With these basic definitions and results at hand, we can formulate the first theorem on the construction of evolution operators, see also Thm. 4.1 of [24] and Thm. 7.1 of [31]:

Theorem C.5. Assume that:

- (a)  $\{A(t)\}_{t \in [0,T]}$  is stable with constants  $M, \beta$ .
- (b) Y is A(t)-admissible for each t, and the part A
   (t) of A(t) in Y is stable with constants M
   , β
   .

(c)  $\mathcal{Y} \subset \text{Dom}A(t)$  so that  $A(t) \in B(\mathcal{Y}, \mathcal{X})$  for each t, and  $t \mapsto A(t)$  is norm-continuous in the norm of  $B(\mathcal{Y}, \mathcal{X})$ .

Then there exists a unique family of bounded operators  $\{U(t,s)\}_{0 \le s \le t \le T}$ , on  $\mathcal{X}$ , called the evolution (operator) generated by A(t), with the following properties:

(i) For all  $0 \le r \le s \le t \le T$ , we have the identities

$$U(t,t) = 1$$
,  $U(t,s)U(s,r) = U(t,r)$ .

- (ii)  $(t,s) \mapsto U(t,s)$  is strongly  $\mathcal{X}$ -continuous and  $||U(t,s)||_{\mathcal{X}} \leq Me^{\beta(t-s)}$ .
- (iii) For all  $y \in \mathcal{Y}$  and  $0 \le s \le t \le T$ ,

$$\partial_t^+ U(t,s)y\Big|_{t=s} = A(s)y, \tag{C.1a}$$

$$-\partial_s U(t,s)y = U(t,s)A(s)y, \qquad (C.1b)$$

where the right derivative  $\partial_t^+$  and the derivative  $\partial_s$  (right derivative if s = 0 and left derivative if s = t) are in the strong topology of  $\mathcal{X}$ .

**Proof.** We approximate A(t) by step functions: Set

$$A_n(t) = A(T \lfloor tn/T \rfloor / n),$$

where  $\lfloor \cdot \rfloor$  denotes the floor function, *viz.*, rounding to the integral part. Since  $t \mapsto A(t)$  is norm-continuous in the norm of  $B(\mathcal{Y}, \mathcal{X})$ , we have

$$\|A_n(t) - A(t)\|_{B(\mathcal{Y},\mathcal{X})} \to 0 \quad \text{as} \quad n \to \infty \tag{C.2}$$

uniformly in *t*. It follows immediately that also  $A_n(t)$  and  $\tilde{A}_n(t)$  are stable with constants  $M, \beta$  and  $\tilde{M}, \tilde{\beta}$ , respectively.

Corresponding to  $A_n(t)$  we construct approximating evolution operators  $U_n(t,s)$  by setting

$$U_n(t,s) = e^{(t-s)A_n(s)}$$

if s, t belong to the closure of an interval where  $A_n$  is constant, and by imposing the relation

$$U_n(t,s) = U_n(t,r)U_n(r,s),$$

to determine  $U_n(t,s)$  for other values of s, t. Clearly,  $U_n(t,t) = 1$  and  $(t,s) \mapsto U_n(t,s)$  is strongly  $\mathcal{X}$ -continuous. We also have

$$\|U_n(t,s)\|_{\mathcal{X}} \le M e^{\beta(t-s)}, \quad \|U_n(t,s)\|_{\mathcal{Y}} \le \tilde{M} e^{\tilde{\beta}(t-s)}$$
 (C.3)

by Prop. C.4, and  $U_n(t,s)\mathcal{Y} \subset \mathcal{Y}$  because  $\mathcal{Y}$  is A(t)-admissible. Furthermore, because  $\mathcal{Y} \subset Dom A(t)$  we have for  $y \in \mathcal{Y}$ 

$$\partial_t U_n(t,s)y = A_n(t)U_n(t,s)y, \partial_s U_n(t,s)y = -U_n(t,s)A_n(s)y,$$

for any *t* resp. *s* that is not on the boundary of an interval where  $A_n$  is constant.

Next we show that  $U_n(t,s)$  converges to U(t,s) strongly in  $\mathcal{X}$  uniformly in s, t: By the fundamental theorem of calculus, we have

$$U_n(t,r)y - U_m(t,r)y = \int_r^t U_n(t,s) (A_n(s) - A_m(s)) U_m(s,r)y \, \mathrm{d}s.$$

Applying (C.3), we thus obtain

$$\|U_n(t,r)y - U_m(t,r)y\|_{\mathcal{X}} \le M\tilde{M}\mathrm{e}^{\gamma(t-r)}\|y\|_{\mathcal{Y}}\int_r^t \|A_n(s) - A_m(s)\|_{B(\mathcal{Y},\mathcal{X})}\,\mathrm{d}s,$$

where  $\gamma = \max(\beta, \tilde{\beta})$ . Therefore it follows from (C.2) that  $U_n(t,s)y$  converges in the strong topology of  $\mathcal{X}$  uniformly in *s*, *t*. Since  $\mathcal{Y}$  is dense in  $\mathcal{X}$  and  $U_n(t,s)$  is uniformly bounded in *n*,  $U_n(t,s)$  converges strongly in  $\mathcal{X}$  and we set

$$U(t,s) = \operatorname{s-lim}_{n \to \infty} U_n(t,s).$$

It is immediate that the properties (i) and (ii) follow from the corresponding properties for  $U_n(t,s)$ .

Finally, we show uniqueness and (iii): If  $\{V(t,s)\}_{0 \le s \le t \le T}$  satisfies (i)–(iii) for a stable family of operators  $\{A'(t)\}_{t \in [0,T]}$  with the same stability constants, then we apply the fundamental theorem of calculus to find

$$U_n(t,r)y - V(t,r)y = \int_r^t U_n(t,s) (A_n(s) - A'(s)) V(s,r)y \, \mathrm{d}s,$$

and therefore

$$\|U_n(t,r)y-V(t,r)y\|_{\mathcal{X}} \leq M\tilde{M}\mathrm{e}^{\gamma(t-r)}\|y\|_{\mathcal{Y}}\int_r^t \|A_n(s)-A'(s)\|_{B(\mathcal{Y},\mathcal{X})}\,\mathrm{d}s.$$

If we set A'(t) = A(t) and let  $n \to \infty$ , we thus find that U(t,s)y = V(t,s)y and by density U(t,s) = V(t,s) on the whole of  $\mathcal{X}$ . We conclude that U(t,s) is unique.

Now we set  $A'(t) = A(\tau) = \text{const}$  for  $\tau \in [0, T]$ , divide by t - s and let  $n \to \infty$ . On the one hand, for  $\tau = s$ , we find (C.1a) in the limit  $t \to s$ . On the other hand, setting  $\tau = t$  and letting  $t \to s$ , we find

$$\partial_s^{-}U(t,s)y\Big|_{s=t} = -A(t)y.$$
(C.4)

To find (C.1b), we check the right and left derivative separately. Applying (C.1a) and (C.4), we obtain

$$\partial_{s}^{+}U(t,s)y = \underset{h\searrow 0}{\text{s-lim}} h^{-1} (U(t,s+h)y - U(t,s)y)$$
  
=  $U(t,s+h) \underset{h\searrow 0}{\text{s-lim}} h^{-1} (y - U(s+h,s)y) = -U(t,s)A(s)y,$  (C.5a)

$$\partial_{s}^{-}U(t,s)y = \underset{h\searrow 0}{\text{s-lim}} h^{-1} (U(t,s)y - U(t,s-h)y)$$
  
=  $U(t,s) \underset{h\searrow 0}{\text{s-lim}} h^{-1} (y - U(s,s-h)y) = -U(t,s)A(s)y.$  (C.5b)

Therefore we have completed the proof also for (iii).

П

We say that a Banach space  $\mathcal{Y}$  possesses a predual if there exists a Banach space  $\mathcal{Y}_*$  such that  $\mathcal{Y}$  is the dual of  $\mathcal{Y}_*$ . Having fixed a predual  $\mathcal{Y}_*$ , we can equip  $\mathcal{Y}$  with the so-called weak\* topology, which is generated by the seminorms  $y \mapsto |\xi(y)|$ , where  $\xi \in \mathcal{Y}_*$ . Note in particular that every reflexive Banach space possesses a unique predual (namely, its dual). For reflexive Banach spaces the weak\* convergence clearly coincides with the weak convergence.

For Banach spaces possessing a predual one can slightly improve the previous theorem (see also Thm. 5.1 of [24]).

**Theorem C.6.** In addition to the assumptions of Thm. C.5, assume that:

(d) *Y* possesses a predual.

Then, in addition to (i)–(iii), the evolution  $\{U(t,s)\}_{0 \le s \le t \le T}$  has the following properties:

(iv)  $U(t,s)\mathcal{Y} \subset \mathcal{Y}$ ,  $(t,s) \mapsto U(t,s)$  is weakly<sup>\*</sup> continuous and

$$\|U(t,r)\|_{\mathcal{V}} \le \tilde{M} e^{\beta(t-s)}, \quad 0 \le r \le s \le t \le T.$$

**Proof.** Note that for fixed  $s, t \in [0, T]$  and  $y \in \mathcal{Y}$ ,  $U_n(t, s)y$  is a uniformly bounded sequence in  $\mathcal{Y}$ , and thus, by the Banach–Alaoglu Theorem, it contains a weakly<sup>\*</sup> convergent subsequence. Moreover, by our previous results,  $U_n(t,s)y \rightarrow U(t,s)y$  in  $\mathcal{X}$ . But U(t,s)y must be equal to the weak<sup>\*</sup> limit, and thus lie in  $\mathcal{Y}$ , *i.e.*,  $U(t,s)\mathcal{Y} \subset \mathcal{Y}$ . The inequality then follows from (C.3).

Now, let  $(t_j)_j$ ,  $(s_j)_j$  be sequences with  $t_j \to t$ ,  $s_j \to s$  and  $y \in \mathcal{Y}$ . Recall that  $U(t_j, s_j)y \to U(t,s)y$  in  $\mathcal{X}$  because  $(t,s) \mapsto U(t,s)$  is  $\mathcal{X}$ -strongly continuous. By the Banach–Alaoglu Theorem, since  $U(t_j, s_j)$  is uniformly bounded,  $U(t_j, s_j)y$  contains a weakly\* convergent subsequence. The weak\* limit of  $U(t_j, s_j)y$  is thus U(t,s)y and must lie in  $\mathcal{Y}$ . In other words, U(t,s) is weakly\* continuous on  $\mathcal{Y}$ .

The following is a simple generalization of Prop. 3.4 in [24].

**Proposition C.7.** For each  $t \in [0, T]$ , let  $\|\cdot\|_t$  be an equivalent norm on  $\mathcal{X}$  and  $C \in L^1[0, T]$  positive such that

$$\|u\|_{s} \leq \|u\|_{t} \exp\left|\int_{s}^{t} C(r) \mathrm{d}r\right|, \quad u \in \mathcal{X}, \quad s, t \in [0, T].$$
(C.6)

If  $\{A(t)\}$  satisfies

$$\left\| \left( A(t) - \lambda \right)^{-1} \right\|_{t} \le (\lambda - \beta)^{-1}, \quad \lambda > \beta,$$
(C.7)

for all  $t \in [0, T]$ , then

$$\left\|\prod_{j=1}^{k} (A(t_j) - \lambda)^{-1}\right\|_{s} \le (\lambda - \beta)^{-k} \exp\left(\int_{t_1}^{t_k} 2C(r) dr\right), \quad t_1 \le s \le t_k,$$

for every finite sequence  $0 \le t_1 \le t_2 \le \cdots \le t_k \le T$ .

**Proof.** Repeated application of (C.6) and (C.7) yields

$$\begin{split} \left\| \prod_{j=1}^{k} (A(t_{j}) - \lambda)^{-1} u \right\|_{t_{k}} &\leq (\lambda - \beta)^{-1} \left\| \prod_{j=1}^{k-1} (A(t_{j}) - \lambda)^{-1} u \right\|_{t_{k}} \\ &\leq (\lambda - \beta)^{-1} \exp\left( \int_{t_{k-1}}^{t_{k}} C(r) dr \right) \left\| \prod_{j=1}^{k-1} (A(t_{j}) - \lambda)^{-1} u \right\|_{t_{k-1}} \\ &\leq \cdots \\ &\leq (\lambda - \beta)^{-k} \exp\left( \int_{t_{1}}^{t_{k}} C(r) dr \right) \|u\|_{t_{1}}. \end{split}$$

Applying (C.6) twice more (for *s* and  $t_k$ , as well as *s* and  $t_1$ ), we obtain the desired result.  $\Box$ 

A simple calculation shows that the proposition implies

$$\left\|\prod_{j=1}^{k} (A(t_j) - \lambda)^{-1}\right\|_{s} \le (\lambda - \beta)^{-k} \exp\left(\int_{0}^{T} 2C(r) dr\right), \quad t_1 \le s \le t_k,$$

for *any*  $s \in [0, T]$ . That is, we have found an estimate of the time-ordered product which does not depend on the time of the factors but rather the boundaries of the considered interval.

If we assume that the Banach space  $\mathcal{Y}$  is uniformly convex, stronger results can be derived. We recall that a normed space is called *uniformly convex* if for every  $\varepsilon > 0$  and unit vectors ||x|| = ||y|| = 1 there exists  $\delta > 0$  such that

$$\|x-y\| \ge \varepsilon \quad \Rightarrow \quad \left\|\frac{x+y}{2}\right\| \le 1-\delta.$$

Moreover, we note that all uniformly convex Banach spaces are reflexive, and weak convergence  $x_n \to x$  implies strong convergence if  $||x_n|| \to ||x||$  on uniformly convex Banach spaces. All Hilbert spaces are uniformly convex.

Applying also Prop. C.7, we find the following, which is part of Thm. 5.2 of [24]:

**Theorem C.8.** In addition to the assumptions of Thm. C.5, assume that:

(d)  $\mathcal{Y}$  is uniformly convex and for every t there exist on  $\mathcal{Y}$  an equivalent norm  $\|\cdot\|_{\mathcal{Y},t}$  as well as a positive  $C \in L^1[0,T]$  such that

$$\|y\|_{\mathcal{Y},s} \le \|y\|_{\mathcal{Y},t} \exp\left|\int_{s}^{t} C(r) dr\right|, \quad s,t \in [0,T].$$
 (C.8)

(e) There exists  $\tilde{\beta} \in \mathbb{R}$  such that

$$\left\|\left(A(t)-\lambda\right)^{-1}\right\|_{\mathcal{Y},t}\leq (\lambda-\tilde{\beta})^{-1}, \quad \lambda>\tilde{\beta},$$

for all  $t \in [0, T]$ .

Then, in addition to (i)–C.6, the evolution  $\{U(t,s)\}_{0 \le s \le t \le T}$  has the following properties:

(iv') In addition to C.6 of Thm. C.6 we have

$$\|U(t,r)\|_{\mathcal{Y},s} \le \exp\left(\int_{r}^{t} \left(\tilde{\beta} + 2C(\tau)\right) \mathrm{d}\tau\right), \quad 0 \le r \le s \le t \le T.$$
(C.9)

 (v) U(t,s) is Y-strongly continuous in s for fixed t and Y-strongly right-continuous in t for fixed s.

**Proof.** Since  $\mathcal{Y}$  is uniformly convex, it is also reflexive, and thus C.6 of Thm. C.6 holds. Then we use Props. C.4 and C.7 to find (C.9), which concludes the proof of C.6.

Next, we prove C.8. By C.6,  $U(t,r) \rightarrow 1$  weakly in  $\mathcal{Y}$ . The bound (C.9) then shows that

$$1 \leq \liminf_{r,t \to s} \|U(t,r)\|_{\mathcal{Y},s} \leq \limsup_{r,t \to s} \|U(t,r)\|_{\mathcal{Y},s}$$
$$\leq \limsup_{r,t \to s} \exp\left(\int_{r}^{t} (\tilde{\beta} + 2C(\tau)) d\tau\right) = 1,$$

and thus  $||U(t,r)||_{\mathcal{Y},s} \to ||U(s,s)||_{\mathcal{Y},s} = 1$ . But  $\mathcal{Y}$  is uniformly convex, so this implies that  $U(t,r) \to 1$  strongly. Let  $0 \le s \le s' \le t \le T$  and  $y \in \mathcal{Y}$ . Then

$$||U(t,s')y - U(t,s)y||_{\mathcal{Y}} \le ||U(t,s')||_{\mathcal{Y}} ||y - U(s',s)y||_{\mathcal{Y}} \to 0$$

as  $s' \to s$  or  $s \to s'$ . Similarly, for  $0 \le s \le t \le t' \le T$  we find

$$||U(t',s)y - U(t,s)y||_{\mathcal{Y}} \le ||(U(t',t) - 1)U(t,s)y||_{\mathcal{Y}} \to 0$$

as  $t' \rightarrow t$ .

In the previous theorem we still had to distinguish between between the *t*- and *s*-properties of U(t,s). If the reversed operator -A(T-t) also satisfies the assumptions of the theorems above, this distinction can be dropped, see also Remark 5.3 in [24]:

**Theorem C.9.** Suppose that both  $\{A(t)\}_{t \in [0,T]}$  and the reversed family  $\{-A(T-t)\}_{t \in [0,T]}$  satisfy the assumptions of Thms. C.5 and C.8. Then there exists a unique family of bounded operators  $\{U(t,s)\}_{s,t\in\mathbb{R}}$  such that

(i') For all  $r, s, t \in [0, T]$ , we have the identities

$$U(t,t) = 1$$
,  $U(t,s)U(s,r) = U(t,r)$ .

(iii') For all  $y \in \mathcal{Y}$  and  $s, t \in [0, T]$ ,

$$\partial_t U(t,s)y = A(t)U(t,s)y,$$
 (C.10a)

$$-\partial_s U(t,s)y = U(t,s)A(s)y, \qquad (C.10b)$$

where the derivatives (right/left derivatives at the boundaries of [0, T]) are in the strong topology of  $\mathcal{X}$ .

(v')  $(t,s) \mapsto U(t,s)$  is *Y*-strongly continuous.

**Proof.** Denote the evolution for  $\{A(t)\}_{t \in [0,T]}$  by U(t,s) and the evolution for  $\{-A(T-t)\}_{t \in [0,T]}$ by V(t,s). For  $0 \le s \le t \le T$ , we define

$$U(s,t) = V(T-s,T-t).$$

From the approximations  $U_n(t,s)$  and  $V_n(t,s)$ , it is easy to see that

$$U(t,s)U(s,t) = 1$$

for  $s, t \in \mathbb{R}$ . This proves C.9. It is clear that

$$\partial_t U(t,s)y\Big|_{t=s} = A(s)y,$$
  
 $-\partial_s U(t,s)y = U(t,s)A(s)y$ 

for  $s, t \in [0, T]$ . Then we can proceed as in (C.5) to find also

$$\partial_t U(t,s)y = A(t)U(t,s)y.$$

Finally, C.9 follows from C.8 for U(t,s) and V(t,s), which implies, in particular, that U(t,s) is strongly right- and left-continuous in t for fixed s. 

Theorem C.9 implies the following, see also Thm. 3.2 of [32]:

**Theorem C.10.** Let  $\mathcal{X}$  and  $\mathcal{Y}$  be Hilbert spaces such that  $\mathcal{Y}$  is densely and continuously embedded in  $\mathcal{X}$ . Let  $I \subset \mathbb{R}$  be a compact interval, and  $\{A(t)\}_{t \in I}$  a family of densely defined, closed operators on  $\mathcal{X}$ . Suppose that the following is satisfied:

- (a)  $\mathcal{Y} \subset \text{Dom}A(t)$  so that  $A(t) \in A(\mathcal{Y}, \mathcal{X})$  and  $t \mapsto A(t)$  is norm-continuous in the norm of  $B(\mathcal{Y}, \mathcal{X})$ .
- (b) For every  $t \in I$ , there exist on  $\mathcal{X}$  and  $\mathcal{Y}$  Hilbert structures  $(\cdot | \cdot)_{\mathcal{X},t}$  and  $(\cdot | \cdot)_{\mathcal{Y},t}$ , which are equivalent to the original ones and for a positive  $C \in L^1(I)$  and all  $s, t \in I$

$$\|x\|_{\mathcal{X},s} \le \|x\|_{\mathcal{X},t} \exp\left|\int_{s}^{t} C(r) dr\right|,$$
$$\|y\|_{\mathcal{Y},s} \le \|y\|_{\mathcal{Y},t} \exp\left|\int_{s}^{t} C(r) dr\right|.$$

Denote the corresponding Hilbert spaces  $X_t$  and  $Y_t$ .

(c) A(t) is self-adjoint with respect to  $\mathcal{X}_t$  and the part  $\tilde{A}(t)$  of A(t) in  $\mathcal{Y}_t$  is self-adjoint in  $\mathcal{Y}_t$ .

Then there exists a unique family of bounded operators  $\{U(t,s)\}_{s,t\in I}$ , in  $\mathcal{X}$ , called the evolution (operator) generated by A(t), with the following properties:

(i) For all  $r, s, t \in I$ , we have the identities

$$U(t,t) = 1$$
,  $U(t,s)U(s,r) = U(t,r)$ .

(ii) U(t,s) is  $\mathcal{X}$ -strongly continuous and

$$\|U(t,s)\|_{\mathcal{X},s} \leq \exp\left|\int_{s}^{t} 2C(r) \,\mathrm{d}r\right|, \quad s,t \in I.$$

(iii) For all  $y \in \mathcal{Y}$  and  $s, t \in I$ ,

$$i\partial_t U(t,s)y = A(t)U(t,s)y,$$
  
$$-i\partial_s U(t,s)y = U(t,s)A(s)y,$$

where the derivatives (right/left derivatives at the boundaries of I) are in the strong topology of X.

(iv)  $U(t,s)\mathcal{Y} \subset \mathcal{Y}$ , U(t,s) is  $\mathcal{Y}$ -strongly continuous and

$$\|U(t,s)\|_{\mathcal{Y},s} \leq \exp\left|\int_{s}^{t} 2C(r) dr\right|, \quad s,t \in I.$$

The following perturbation theorem is essentially Thm. 4.5 of [25]. We leave the proof as an exercise to the reader.

**Theorem C.11.** Suppose that  $\{A(t)\}_{t \in [0,T]}$  satisfies the assumptions of Thm. C.5. Let  $\{B(t)\}_{t \in [0,T]}$  be a family of bounded operators in  $\mathcal{X}$  such that  $t \mapsto B(t)$  is strongly continuous with respect to  $\mathcal{X}$ . Then there exists a unique evolution V(t,s) for  $\{A(t) + B(t)\}_{t \in [0,T]}$  satisfying the properties (i)-(iii), but with the estimate  $||V(t,s)|| \leq Me^{(\beta+KM)(t-s)}$ , where  $K = \sup_t ||B(t)||_{\mathcal{X}}$ . If  $\{A(t)\}_{t \in [0,T]}$  also satisfies the stronger assumptions of Thm. C.8 or Thm. C.9, and  $\{B(t)\}_{t \in [0,T]}$  is bounded in  $\mathcal{Y}$ , then the evolution V(t,s) for  $\{A(t) + B(t)\}_{t \in [0,T]}$  satisfies the corresponding stronger properties.

The evolution V(t,s) in the theorem above is given symbolically by

$$V = U + U * B * U + U * B * U * B * U + \cdots,$$

where \*B \* denotes a Volterra-type convolution with 'density' B(t). For example,

$$(U * B * U)(t, r) = \int_{r}^{t} U(t, s)B(s)U(s, r) \,\mathrm{d}s.$$

# D Heinz-Kato inequality

We recall the Heinz–Kato inequality [19, 23], which is an elementary but very useful result for the interpolation of operators:

**Theorem D.1.** Suppose that A, B are positive operators on Hilbert spaces  $\mathcal{X}$ ,  $\mathcal{Y}$ , respectively. If T is a bounded operator from  $\mathcal{X}$  to  $\mathcal{Y}$  such that  $T(\text{Dom}A) \subset \text{Dom}B$  and

$$||Tx|| \le C_0 ||x||, ||BTx|| \le C_1 ||Ax||,$$

for  $x \in \text{Dom}A$ , then

$$||B^{\alpha}Tx|| \le C_0^{\alpha} C_1^{1-\alpha} ||A^{\alpha}x||, \quad \alpha \in [0,1].$$
(D.1)

**Proof.** First suppose that A > 0 and B > 0. Let  $x \in Dom A$  and  $y \in Dom B^*$ . Then

$$f(z) = (TA^{-\overline{z}} x \mid B^{*z} y),$$

is analytic in the strip  $\operatorname{Re} z \in [0, 1]$  and satisfies

$$|f(i\beta)| \le C_0 ||x|| ||y||, ||f(1+i\beta)| \le C_1 ||x|| ||y||.$$

Applying Hadamard's three-lines theorem, we thus obtain for  $\alpha \in [0, 1]$ 

$$|f(\alpha)| \le C_0^{\alpha} C_1^{1-\alpha} ||x|| ||y||$$

Since  $Dom B^*$  is dense in  $\mathcal{Y}$ , (D.1) follows.

Now consider the general case. For  $\varepsilon > 0$  we have

$$\begin{aligned} \|(B+\varepsilon^2)Tx\| &\leq C_1 \|Ax\| + C_0\varepsilon^2 \|x\| \leq (C_1^2 + \varepsilon C_0^2)^{\frac{1}{2}} (\|(Ax\|^2 + \varepsilon^2 \|x\|^2)^{\frac{1}{2}} \\ &\leq (C_1^2 + \varepsilon C_0^2)^{\frac{1}{2}} \|(A+\varepsilon)x\|. \end{aligned}$$

Therefore (D.1) holds with  $A, B, C_1$  replaced by  $A + \varepsilon$ ,  $B + \varepsilon^2$  and  $(C_1^2 + \varepsilon C_0^2)^{\frac{1}{2}}$ . Using  $\text{Dom}(A + \varepsilon)^{\alpha} = \text{Dom}A^{\alpha}$  and  $(A + \varepsilon)^{\alpha} \to A^{\alpha}$  as  $\varepsilon \to 0$ , see *e.g.* Lem. A2 in [22], we find (D.1) taking the limit  $\varepsilon \to 0$ .

It is not difficult to see that the preceeding theorem implies the next one and vice versa.

**Theorem D.2.** Suppose that A, B are as in Thm. D.1. If Q is a densely defined, closed operator from  $\mathcal{X}$  to  $\mathcal{Y}$  with  $Q(\text{Dom}A) \subset \text{Dom}B$ , such that  $||Qx|| \leq ||Ax||$  and  $||Q^*y|| \leq ||By||$  holds, then

$$|(Qx|y)| \le ||A^{\alpha}x|| ||B^{1-\alpha}y||, \quad \alpha \in [0,1].$$
(D.2)

# E Finite speed of propagation

In this appendix we prove the finite speed of propagation for solutions of the Klein–Gordon equation with coefficients of low regularity.

In this section we prefer to work with the Klein-Gordon equation in the scalar formalism, given by (1.1), which can be locally written as

$$Ku := -g^{\mu\nu} (\nabla_{\mu} - iA_{\mu}) (\nabla_{\nu} - iA_{\nu})u + Yu$$
(E.1)

with pseudo-Riemannian metric g and the corresponding Levi-Civita derivative  $\nabla$ , vector potential A, and scalar potential Y. Our standing assumptions in this appendix are as follows:

**Assumption 4.**  $M = \mathbb{R} \times \Sigma$  is equipped with a continuous Lorentzian metric  $g = -\beta dt^2 + g_{\Sigma}$ , where  $\beta > 0$  and  $g_{\Sigma}$  are continuous, and  $g_{\Sigma}$  restricts to a family of Riemannian metrics on  $\Sigma$ . (Recall that every globally hyperbolic spacetime can be brought into this form.) We assume that  $A_{\mu}(t) \in L^{\infty}_{loc}(\Sigma)$  for all t, and  $A_{\mu}, \dot{A}_{\mu}, Y \in L^{\infty}_{loc}(M)$ . Moreover, in every compact neighbourhood  $U \subset M$  there is  $C_g > 0$  such that

$$|\dot{g}^{\mu\nu}X_{\mu}X_{\nu}| \le C_g |g^{\mu\nu}X_{\mu}X_{\nu}|$$

almost everywhere in U for all covectors X.

Under these assumption we will show the following thorem on the finite speed of propagation: **Theorem E.1.** If  $u \in C^1(\mathbb{R}; L^2_{loc}(\Sigma))$  with  $\partial_i u \in C(\mathbb{R}; L^2_{loc}(\Sigma))$  and  $Ku \in L^2_{loc}(M)$ , then

$$\operatorname{supp} u \subset J\left(\operatorname{supp} Ku \cup \{t\} \times \left(\operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t)\right)\right)$$

for any  $t \in \mathbb{R}$ . That is, u is supported in the causal shadow of the union of Ku and of the support of its Cauchy data on  $\{t\} \times \Sigma$ .

(E.1) can be obtained via the Euler-Lagrange equations from the Lagrangian density

$$\mathcal{L}[u] := |g|^{\frac{1}{2}} \Big( \big( (\partial_{\mu} + iA_{\mu})\overline{u} \big) g^{\mu\nu} \big( (\partial_{\nu} - iA_{\nu})u \big) + Y|u|^{2} \Big).$$

If the action for  $\mathcal{L}$  is invariant under infinitesimal time-translations, we derive from Noether's theorem the conserved momentum flux density

$$\mathcal{P}^{\mu}[u] \coloneqq \delta^{\mu}_{0}\mathcal{L}[u] - \frac{\partial \mathcal{L}[u]}{\partial (\partial_{\mu}\overline{u})} \partial_{t}\overline{u} - \frac{\partial \mathcal{L}[u]}{\partial (\partial_{\mu}u)} \partial_{t}u.$$

If the action is not time-translation invariant, we can still consider  $\mathcal{P}$  as the momentum flux density, which is, however, not conserved.

The energy density  $\mathcal{E} = \mathcal{P}^0$  is not necessarily positive. Therefore we also introduce an auxiliary Lagrangian density

$$\tilde{\mathcal{L}}[u] := |g|^{\frac{1}{2}} \left( \left( (\partial_{\mu} + iA_{\mu})\overline{u} \right) g^{\mu\nu} \left( (\partial_{\nu} - iA_{\nu})u \right) + (1 + \beta^{-1}A_0^2) |u|^2 \right)$$

and denote the corresponding momentum flux density  $\tilde{\mathcal{P}}$ . We find the energy density

$$\tilde{\mathcal{E}}[u] := \tilde{\mathcal{P}}^0[u] = |g|^{\frac{1}{2}} \left(\beta^{-1} |\dot{u}|^2 + \left((\partial_i + iA_i)\overline{u}\right)g^{ij} \left((\partial_j + iA_j)u\right) + |u|^2\right)$$

and the spatial momentum flux density

$$\tilde{\mathcal{P}}^{i}[u] = \mathcal{P}^{i}[u] = -|g|^{\frac{1}{2}} \left( \dot{\overline{u}} g^{ij} \left( (\partial_{j} - \mathbf{i} A_{j}) u \right) + \dot{u} g^{ij} \left( (\partial_{j} + \mathbf{i} A_{j}) \overline{u} \right) \right)$$

Below we will integrate  $\partial_{\mu} \tilde{\mathcal{P}}^{\mu}$  over a region which is delimited by two constant-time surfaces and the backward lightcone of a point as described in Fig. 1. To rewrite this integral as an integral over the boundary of said region via Stokes' theorem, it is useful to assume that  $\partial J_g^{\pm}(\Omega)$  is a Lipschitz topological hypersurface, see Thm. 3.9 of [3]. Here we denoted by  $J_g^{\pm}(\Omega)$  the causal future (+) or causal past (-) of  $\Omega$ , *i.e.*, the set of points which can be reached from  $\Omega$  by future- resp. past-directed causal curves with respect to the metric g. Moreover, we write  $J_g(\Omega) = J_g^+(\Omega) \cup J_g^-(\Omega)$ .

If g is not smooth (or at least  $C^2$ ), it is not guaranteed that  $\partial J_g^{\pm}(\Omega)$  is a Lipschitz topological hypersurface. However, we can approximate g by smooth metrics:

If a Lorentzian metric  $\hat{g}$  has strictly larger lightcones than g, *i.e.*, each non-vanishing g-causal vector  $X^{\mu}$  ( $g_{\mu\nu}X^{\mu}X^{\nu} \leq 0$ ) is  $\hat{g}$ -timelike ( $\hat{g}_{\mu\nu}X^{\mu}X^{\nu} < 0$ ), then we write

 $\hat{g} \succ g$ .

As shown in Prop. 1.2 of [5], there always exists a *smooth* Lorentzian metric  $\hat{g}$  with strictly larger lightcones which approximates g arbitrarily well.

**Proposition E.2.** Let  $\hat{g} \succ g$  be smooth and consider the situation depicted in Fig. 1. Then there exists C > 0 such that

$$e^{C(s-t)} \int_{K_t} \tilde{\mathcal{E}}[u](t) \le \int_{K_s} \tilde{\mathcal{E}}[u](s) + \int_{\Omega} |g|^{\frac{1}{2}} |Ku|^2.$$
 (E.2)

for all  $u \in C^1(\mathbb{R}; L^2_{\text{loc}}(\Sigma))$  with  $\partial_i u \in C(\mathbb{R}; L^2_{\text{loc}}(\Sigma))$  and  $Ku \in L^2_{\text{loc}}(M)$ ,



**Figure 1.** The truncated cone given by the backward lightcone  $J_{\hat{g}}^-(x)$  of a point, and two constant-time surfaces  $\Sigma_t = \{t\} \times \Sigma$  and  $\Sigma_s$  (with t > s). We write  $K_t = J_{\hat{g}}^-(x) \cap (\{t\} \times \Sigma)$  and  $K_s$  for the caps, and  $\Lambda = \partial J_{\hat{g}}^-(x) \cap ([s, t] \times \Sigma)$  for the mantle of the truncated cone  $\Omega = J_{\hat{g}}^-(x) \cap ([s, t] \times \Sigma)$ .

Proof. We derive

$$\begin{split} \partial_{\mu}\tilde{\mathcal{P}}^{\mu}[u] &= \partial_{t}\tilde{\mathcal{L}}[u] - \left(\partial_{\mu}\frac{\partial\tilde{\mathcal{L}}[u]}{\partial(\partial_{\mu}\overline{u})}\right)\dot{\overline{u}} - \frac{\partial\tilde{\mathcal{L}}}{\partial(\partial_{\mu}\overline{u})}\partial_{\mu}\partial_{t}\overline{u} - \left(\partial_{\mu}\frac{\partial\tilde{\mathcal{L}}}{\partial(\partial_{\mu}u)}\right)\dot{u} - \frac{\partial\tilde{\mathcal{L}}[u]}{\partial(\partial_{\mu}u)}\partial_{\mu}\partial_{t}u \\ &= \partial_{t}\tilde{\mathcal{L}}[u] + \left(|g|^{\frac{1}{2}}\tilde{K}u - \frac{\partial\tilde{\mathcal{L}}[u]}{\partial\overline{u}}\right)\dot{\overline{u}} - \frac{\partial\tilde{\mathcal{L}}[u]}{\partial(\partial_{\mu}\overline{u})}\partial_{t}\partial_{\mu}\overline{u} + \left(|g|^{\frac{1}{2}}\overline{K}u - \frac{\partial\tilde{\mathcal{L}}[u]}{\partial u}\right)\dot{u} \\ &- \frac{\partial\tilde{\mathcal{L}}[u]}{\partial(\partial_{\mu}u)}\partial_{t}\partial_{\mu}u \\ &= 2|g|^{\frac{1}{2}}\operatorname{Re}(\dot{\overline{u}}\tilde{K}u) + \frac{\partial\tilde{\mathcal{L}}[u]}{\partial g^{\mu\nu}}\dot{g}^{\mu\nu} + \frac{\partial\tilde{\mathcal{L}}[u]}{\partial A_{\mu}}\dot{A}_{\mu} + \frac{\partial\tilde{\mathcal{L}}[u]}{\partial|g|}\partial_{t}|g| \\ &= |g|^{\frac{1}{2}}\Big(2\operatorname{Re}(\dot{\overline{u}}\tilde{K}u) + \left((\partial_{\mu} + \mathrm{i}A_{\mu})\overline{u}\right)\dot{g}^{\mu\nu}((\partial_{\nu} - \mathrm{i}A_{\nu})u) - \beta^{-2}\dot{\beta}A_{0}^{2}|u|^{2} \\ &- 2\operatorname{Im}\Big(\overline{u}\dot{A}_{\mu}g^{\mu\nu}(\partial_{\nu} - \mathrm{i}A_{\nu})u\Big) + 2\beta^{-1}A_{0}\dot{A}_{0}|u|^{2} + \frac{1}{2}|g|^{-1}(\partial_{t}|g|)\tilde{\mathcal{L}}[u]\Big). \end{split}$$

where, in the second step, we used the Euler-Lagrange equations with

$$\tilde{K} = K - Y + 1 + \beta^{-1} A_0^2$$

being the Klein–Gordon operator associated to  $\tilde{\mathcal{L}}$ . Estimating each term separately using our assumptions and the Cauchy–Schwarz inequality yields

$$\partial_{\mu}\tilde{\mathcal{P}}^{\mu}[u] \leq |g|^{\frac{1}{2}} \Big( |Ku|^{2} + C_{1}\beta^{-1}|\dot{u}|^{2} + C_{2} \big( (\partial_{i} + iA_{i})\overline{u} \big) g^{ij} \big( (\partial_{j} + iA_{j})u \big) + C_{3}|u|^{2} \Big)$$

for  $C_1, C_2, C_3 > 0$  which do not depend on *u*. Therefore we find

$$\int_{\Omega} \partial_{\mu} \tilde{\mathcal{P}}^{\mu}[u] \leq \int_{\Omega} \left( |g|^{\frac{1}{2}} |Ku|^{2} + C\tilde{\mathcal{E}}[u] \right)$$
(E.3)

for some constant C > 0.

By Stokes' theorem,

$$\int_{\Omega} \partial_{\mu} \tilde{\mathcal{P}}^{\mu}[u] = \int_{\partial \Omega} n_{\mu} \tilde{\mathcal{P}}^{\mu}[u] = \int_{K_{t}} \tilde{\mathcal{E}}[u](t) - \int_{K_{s}} \tilde{\mathcal{E}}[u](s) + \int_{\Lambda} n_{\mu} \tilde{\mathcal{P}}^{\mu}[u], \quad (E.4)$$

where *n* is the outward-directed normal field to  $\partial \Omega$ . For any future-directed causal covector field  $\xi$  (*i.e.*,  $g^{\mu\nu}\xi_{\mu}\xi_{\nu} \leq 0$  and  $\xi_0 \geq 0$ ) with  $|\vec{\xi}| = (g^{ij}\xi_i\xi_j)^{\frac{1}{2}}$ ,

$$\begin{aligned} \xi_{\mu} \tilde{\mathcal{P}}^{\mu}[u] &= \xi_{0} \tilde{\mathcal{E}}[u] - 2|g|^{\frac{1}{2}} \operatorname{Re}\left(\xi_{i} \dot{\overline{u}} g^{ij} (\partial_{j} - iA_{j})u\right) \\ &\geq \xi_{0} \tilde{\mathcal{E}}[u] - |g|^{\frac{1}{2}} \beta^{\frac{1}{2}} |\vec{\xi}| \Big(\beta^{-1} |\dot{u}|^{2} + \big((\partial_{i} + iA_{i}u)\big) g^{ij} \big((\partial_{j} - iA_{j})u\big)\Big) \\ &\geq (\xi_{0} - \beta^{\frac{1}{2}} |\vec{\xi}|) \tilde{\mathcal{E}}[u] \geq 0 \end{aligned}$$

almost everywhere. Consequently, we can estimate the last term in (E.4) as  $\int_{\Lambda} n_{\mu} \tilde{\mathcal{P}}^{\mu} \ge 0$ . Combining (E.3) and (E.4), we obtain

$$\int_{K_t} \tilde{\mathcal{E}}[u](t) - \int_{K_s} \tilde{\mathcal{E}}[u](s) \leq \int_s^t \left( \int_{K_r} \left( |g|^{\frac{1}{2}} |Ku(r)|^2 + C \tilde{\mathcal{E}}[u](r) \right) \right) \mathrm{d}r,$$

and thus (E.2) by Grönwall's inequality.

Now, using the proposition above, we can show the finite speed of propagation:

**Theorem E.3.** If  $u \in C^1(\mathbb{R}; L^2_{loc}(\Sigma))$  with  $\partial_i u \in C(\mathbb{R}; L^2_{loc}(\Sigma))$  and  $Ku \in L^2_{loc}(M)$ , then

$$\operatorname{supp} u \cap M_{\pm} \subset J_{g}^{\pm} \Big( (\operatorname{supp} Ku \cap M_{\pm}) \cup \{t\} \times \big( \operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t) \big) \Big), \qquad (E.5)$$
$$\operatorname{supp} u \subset J_{g} \Big( \operatorname{supp} Ku \cup \{t\} \times \big( \operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t) \big) \Big),$$

for any  $t \in \mathbb{R}$ , where  $M_+ = [t, +\infty[ \times \Sigma, M_- = ]-\infty, t] \times \Sigma$ .

**Proof.** Note that, as a subset of  $\Sigma$ , we have  $\operatorname{supp} \tilde{\mathcal{E}}[u](t) = \operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t)$ . We show that u(x) = 0 for any

$$x \in M \setminus J^+_{\hat{\varphi}} ((\operatorname{supp} Ku \cap M_+) \cup \{t\} \times \operatorname{supp} \tilde{\mathcal{E}}[u](t))$$

by an application of Prop. E.2 for all smooth  $\hat{g} \succ g$ . For any such  $x, J_{\hat{g}}^-(x)$  does not intersect  $(\operatorname{supp} Ku \cap M_+) \cup \{t\} \times \operatorname{supp} \tilde{\mathcal{E}}[u](t)$ . Prop. E.2 now shows that u vanishes in  $J_{\hat{g}}^-(x) \cap M_+$  and thus also at x.

We have thus shown that

$$\operatorname{supp} u \cap M_{\pm} \subset J^{\pm}_{\hat{\sigma}} (\operatorname{supp} Ku \cap M_{\pm}) \cup \{t\} \times (\operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t))$$

for all smooth  $\hat{g} \succ g$ . It follows that (E.5) holds, because a vector is *g*-causal if and only if it is  $\hat{g}$ -timelike for all smooth  $\hat{g} \succ g$  by Prop. 1.5 of [5] and therefore

$$J_g^{\pm}(\Omega) = \bigcap_{\hat{g}\succ g} J_{\hat{g}}^{\pm}(\Omega), \quad \Omega \subset M.$$

The embedding for  $J^-$  follows by time reversal and remaining embedding by the union of the embeddings for  $J^+$  and  $J^-$ .

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