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# Feynman propagators and Hadamard states from scattering data for the Klein-Gordon equation on asymptotically Minkowski spacetimes

Christian GÉRARD & Michał WROCHNA

ABSTRACT. We consider the massive Klein-Gordon equation on a class of asymptotically static spacetimes. We prove the existence and Hadamard property of the *in* and *out* states constructed by scattering theory methods. Assuming in addition that the metric approaches that of Minkowski space at infinity in a short-range way, jointly in time and space variables, we define Feynman scattering data and prove the Fredholm property of the Klein-Gordon operator with the associated Atiyah-Patodi-Singer boundary conditions. We then construct a parametrix (with compact remainder terms) for the Fredholm problem and prove that it is also a Feynman parametrix in the sense of Duistermaat and Hörmander.

## 1. INTRODUCTION & SUMMARY

**1.1. Hadamard property of in/out states.** The construction of quantum states from scattering data is a subject that has been studied extensively in various contexts in Quantum Field Theory, including the case of the wave and Klein-Gordon equation — set either on Minkowski space, in external electromagnetic potentials [Is, Lu, Ru, Se], or on curved spacetimes with special asymptotic symmetries, to mention only the works [Wa1, DK1, DK2, DK3, Mo1]. On the physics side, the primary motivation is to give meaning to the notion of particles and anti-particles and to describe quantum scattering phenomena. From the mathematical point of view, the problems often discussed in this context in the literature involve existence of scattering and Møller operators, the question of asymptotic completeness, as well as specific properties of states such as the ground state or thermal condition with respect to an asymptotic dynamics, see e.g. [Dr, DD, DRS, GGH, Ni] for recent developments on curved backgrounds.

In the present paper we address the question of whether the so-called *in* and *out* states on asymptotically static spacetimes satisfy the *Hadamard condition* [KW]. Nowadays regarded as an indispensable ingredient in the perturbative construction of interacting fields (see e.g. recent reviews [HW, KM, FV2]), this property accounts for the correct short-distance behaviour of expectation values of fields. It can be conveniently formulated as a condition on the wave front set of the state's two-point functions [Ra] — a terminology that we explain in the paragraphs below. It is known that in the special case of the conformal wave equation, one can study the wave front set of the two-point functions quite directly in the geometrical setup of conformal scattering on asymptotically flat spacetimes [Mo2, GW3] (cf. [DMP1, DMP2, BJ] for generalizations on the allowed classes of spacetimes). Furthermore, propagation estimates in b-Sobolev spaces of variable order were used recently to show a similar result in the case of the wave equation on asymptotically Minkowski spacetimes [VW]. The two methods being however currently limited to a special value of the mass parameter, our focus here is instead on the proof of the Hadamard property of the *in* and *out* state for the Klein-Gordon operator  $P = -\square_g + m^2$  for any positive mass  $m$ , or more generally for  $P = -\square_g + V$  with a real-valued potential  $V \in C^\infty(M)$  satisfying an asymptotic positivity condition.

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Specifically, we first consider the special case of a  $1 + d$ -dimensional globally hyperbolic spacetime  $(M, g)$  with Cauchy surface  $\Sigma$  and metric of the form  $g = -dt^2 + h_t$ , with  $h_t$  a Riemannian metric smoothly depending on  $t$ . The Klein-Gordon operator can be written in the form

$$(1.1) \quad P = \partial_t^2 + r(t)\partial_t + a(t, x, \partial_x),$$

where  $r(t)$  is the multiplication operator  $|h_t|^{-\frac{1}{2}}\partial_t|h_t|^{\frac{1}{2}}$  and  $a(t, x, D_x) \in \text{Diff}^2(\Sigma)$  has principal symbol  $k \cdot h_t^{-1}(x)k$  (where  $\xi = (\tau, k)$  is the dual variable of  $x = (t, x)$ ) and is bounded from below. Now, supposing  $\Sigma$  is a *manifold of bounded geometry* (see Subject. 3.1), there exist uniform pseudodifferential operator classes  $\Psi^m(\Sigma)$  due to Kordyukov and Shubin [Ko, Sh2] that generalize the well-known pseudodifferential calculus of Hörmander on  $\mathbb{R}^d$  and closed manifolds. Here in addition, in order to control decay in time, we introduce  $t$ -dependent pseudodifferential operators  $\Psi_{\text{td}}^{m, \delta}(\mathbb{R}; \Sigma)$  as quantizations of  $t$ -dependent symbols  $a(t, x, k)$  that satisfy

$$|\partial_t^\alpha \partial_x^\beta \partial_k^\gamma a(t, x, k)| \leq C_{\alpha\beta\gamma} \langle t \rangle^{\delta - \alpha} \langle k \rangle^{m - |\gamma|}, \quad \alpha \in \mathbb{N}, \beta, \gamma \in \mathbb{N}^d,$$

where  $\langle t \rangle = (1 + t^2)^{\frac{1}{2}}$ ,  $\langle k \rangle = (1 + |k|^2)^{\frac{1}{2}}$ , and the constants  $C_{\alpha\beta\gamma}$  are uniform in an appropriate sense. This allows us to state a hypothesis that accounts for asymptotic ultra-staticity of  $(M, g)$  at future and past infinity. Namely, we assume that there exists  $a_{\text{out}}, a_{\text{in}} \in \Psi^2(\Sigma)$  elliptic and bounded from below (by a positive constant), such that on  $\mathbb{R}_\pm \times \Sigma$ ,

$$(1.2) \quad \begin{aligned} a(t, x, D_x) &= a_{\text{out/in}}(x, D_x) + \Psi_{\text{td}}^{2, -\delta}(\mathbb{R}; \Sigma), \quad \delta > 0, \\ r(t) &\in \Psi_{\text{td}}^{0, -1-\delta}(\mathbb{R}; \Sigma). \end{aligned}$$

In practice, in our main cases of interest  $a_{\text{out/in}}(x, D_x)$  will simply be the Laplace-Beltrami operator of some asymptotic metric  $h_{\text{out/in}}$  plus the mass or potential term.

Let now  $\mathcal{U}(t, s)$  be the Cauchy evolution of  $P$ , i.e. the operator that maps Cauchy data of  $P$  at time  $s$  to Cauchy data at time  $t$ . In this setup, what we call *time- $t$  covariances of the out state* are the pair of operators defined by

$$(1.2) \quad c_{\text{out}}^\pm(t) := \lim_{t_+ \rightarrow \infty} \mathcal{U}(t, t_+) c_{\text{out}}^{\pm, \text{vac}} \mathcal{U}(t_+, t)$$

whenever the limit exists (in a sense made precise later on), where  $c_{\text{out}}^{\pm, \text{vac}}$  equals

$$c_{\text{out}}^{\pm, \text{vac}} = \frac{1}{2} \begin{pmatrix} \mathbf{1} & \pm a_{\text{out}}^{\frac{1}{2}} \\ \pm a_{\text{out}}^{-\frac{1}{2}} & \mathbf{1} \end{pmatrix}.$$

To elucidate the interpretation of  $c_{\text{out}}^{\pm, \text{vac}}$  let us point out that  $c_{\text{out}}^{\pm, \text{vac}}$  is the spectral projection on  $\mathbb{R}^\pm$  of the generator<sup>1</sup> of the Cauchy evolution  $\mathcal{U}_{\text{out}}(t, s)$  corresponding to the asymptotic Klein-Gordon operator  $P_{\text{out}} := \partial_t^2 + a_{\text{out}}$ . On the other hand, to  $c_{\text{out}}^{\pm, \text{vac}}$ ,  $c_{\text{out}}^\pm$  we can associate pairs of operators  $\Lambda_{\text{out}}^{\pm, \text{vac}}, \Lambda_{\text{out}}^\pm : C_c^\infty(M) \rightarrow C^\infty(M)$  by

$$\begin{aligned} \Lambda_{\text{out}}^{\pm, \text{vac}}(t, s) &:= \mp \pi_0 \mathcal{U}_{\text{out}}(t, 0) c_{\text{out}}^{\pm, \text{vac}} \mathcal{U}_{\text{out}}(0, s) \pi_1^*, \\ \Lambda_{\text{out}}^\pm(t, s) &:= \mp \pi_0 \mathcal{U}(t, 0) c_{\text{out}}^\pm(0) \mathcal{U}(0, s) \pi_1^*, \end{aligned}$$

where we wrote  $\Lambda_{\text{out}}^{\pm, \text{vac}}, \Lambda_{\text{out}}^\pm$  as operator-valued Schwartz kernels in the time variable and  $\pi_0, \pi_1$  are the respective projections to the two pieces of Cauchy data. In QFT terms (strictly speaking, using the terminology for charged fields), the operators  $\Lambda_{\text{out}}^{\pm, \text{vac}}, \Lambda_{\text{out}}^\pm$  are *two-point functions*, i.e. they satisfy

$$\begin{aligned} P_{\text{out}} \Lambda_{\text{out}}^{\pm, \text{vac}} &= \Lambda_{\text{out}}^{\pm, \text{vac}} P_{\text{out}} = 0, \quad \Lambda_{\text{out}}^{+, \text{vac}} - \Lambda_{\text{out}}^{-, \text{vac}} = iG_{\text{out}}, \quad \Lambda_{\text{out}}^{\pm, \text{vac}} \geq 0, \\ P \Lambda_{\text{out}}^\pm &= \Lambda_{\text{out}}^\pm P = 0, \quad \Lambda_{\text{out}}^+ - \Lambda_{\text{out}}^- = iG, \quad \Lambda_{\text{out}}^\pm \geq 0, \end{aligned}$$

<sup>1</sup>This generator is selfadjoint for the energy scalar product.

where  $G_{\text{out}}, G$  are the *causal propagators* for respectively  $P_{\text{out}}, P$ , i.e.

$$G_{\text{out}}(t, s) = i\pi_0 \mathcal{U}_{\text{out}}(t, s)\pi_1^*, \quad G(t, s) = i\pi_0 \mathcal{U}(t, s)\pi_1^*.$$

As a consequence, using the standard apparatus of algebraic QFT one can associate states  $\omega_{\text{out}}^{\text{vac}}$ ,  $\omega_{\text{out}}$  on the corresponding CCR  $C^*$ -algebras:  $\omega_{\text{out}}^{\text{vac}}$  is then the very well studied ground state associated with  $P_{\text{out}}$  and  $\omega_{\text{out}}$  is the *out* state that we study.

Our first result can be expressed as follows in terms of the two-point functions  $\Lambda_{\text{out}}^\pm$ .

**Theorem 1.1.** *Assume (td). Then the limit (1.2) exists and  $\omega_{\text{out}}$  is a Hadamard state, i.e. the two-point functions  $\Lambda_{\text{out}}^\pm$  satisfy the Hadamard condition:*

$$(1.3) \quad \text{WF}'(\Lambda_{\text{out}}^\pm) = \bigcup_{t \in \mathbb{R}} (\Phi_t(\text{diag}_{T^*M}) \cap \pi^{-1}\mathcal{N}^\pm),$$

where  $\mathcal{N}^+, \mathcal{N}^-$  are the two connected components of the characteristic set  $\mathcal{N} \subset T^*M \setminus o$  of  $P$ ,  $\Phi_t$  is the bicharacteristic flow acting on the left component of  $\text{diag}_{T^*M}$  (the diagonal in  $(T^*M \times T^*M) \setminus o$ ), and  $\pi : \mathcal{N} \times \mathcal{N} \rightarrow \mathcal{N}$  is the projection to the left component.

Above,  $\text{WF}'(\Lambda_{\text{out}}^\pm)$  stands for the primed wave front set of  $\Lambda_{\text{out}}^\pm$ , i.e. it is the image of the wave front set of the (full) Schwartz kernel of  $\Lambda_{\text{out}}^\pm$  by the map  $(x, \xi, x', \xi') \mapsto (x, \xi, x', -\xi')$ . We refer to [Hö] for the definition and the basic properties of the wave front set of a distribution, cf. [BDH] for a concise introduction. The *bicharacteristic flow*  $\Phi_t$  is the Hamilton flow of  $p(x, \xi) = \xi \cdot g^{-1}(x)\xi$  restricted to  $\mathcal{N} = p^{-1}(\{0\})$  understood as a subset of  $T^*M \setminus o$  (where  $o$  is the zero section of the cotangent bundle), see [Hö].

The essential feature of the Hadamard condition (1.3) is that it constraints  $\text{WF}'(\Lambda_{\text{out}}^\pm)$  to the positive/negative frequency components  $\mathcal{N}^\pm \times \mathcal{N}^\pm$ . Thus, on a very heuristic level, the plausibility of this statement can be explained as follows. In a static situation,  $c_{\text{out}}^{\pm, \text{vac}}$  can be interpreted as projections that single out Cauchy data that propagate as superpositions of plane waves with positive/negative frequency, and thus with wave front set in  $\mathcal{N}^\pm$ . On a generic asymptotically flat spacetime it is not immediately clear what the analogous decomposition at finite times is, but instead one can try to use the decomposition given by  $c_{\text{out}}^{\pm, \text{vac}}$  at *infinite times*: this is what indeed motivates the definition of  $\Lambda_{\text{out}}^\pm$ . The difficulty is however to control the wave front set of the infinite time limit (1.2).

In addition to the statement of Thm. 1.1, we get in a similar vein a Hadamard state  $\omega_{\text{in}}$  by taking the analogous limit with  $t_- \rightarrow -\infty$  instead of  $t_+ \rightarrow +\infty$ ; this is the so-called *in* state.

Furthermore, our results extend to a more general class of asymptotically static spacetimes  $M = \mathbb{R} \times \Sigma$  with metric of the form

$$g = -c^2(x)dt^2 + (dx^i + b^i(x)dt)h_{ij}(x)(dx^j + b^j(x)dt),$$

where  $(\Sigma, h)$  is a manifold of bounded geometry and  $c, h, b$  as well as their inverses are bounded with all derivatives (with respect to the norm defined using a reference Riemannian metric). By *asymptotically static* we mean that there exist Riemannian metrics  $h_{\text{out/in}}$  and smooth functions  $c_{\text{out/in}}$  on  $\Sigma$ , such that on  $\mathbb{R}_\pm \times \Sigma$ ,

$$(ast) \quad \begin{aligned} h(x) - h_{\text{out/in}}(x) &\in S^{-\mu}, \\ b(x) &\in S^{-\mu'}, \text{ and } c(x) - c_{\text{out/in}}(x) \in S^{-\mu} \end{aligned}$$

for some  $\mu > 0, \mu' > 1$ ; in a similar vein the potential  $V$  is required to satisfy  $V(x) - V_{\text{out/in}}(x) \in S^{-\mu}$  for some smooth  $V_{\text{out/in}}$ . Above, the notation  $f \in S^{-\mu}$  means symbolic decay in time, i.e.  $\partial_t^\alpha f \in O(\langle t \rangle^{-\mu-|\alpha|})$  for all  $\alpha \in \mathbb{N}^{1+d}$ ; we refer to Subsect. 5.1 for the precise formulation.

In this more general situation, the Klein-Gordon operator is not necessarily of the form (1.1) considered so far. However, under a positivity assumption (pos) on  $V_{\text{out/in}}$ , it turns out that there are natural coordinates in terms of which the Klein-Gordon operator is very closely related

to an operator (1.1) satisfying (td), i.e. one is obtained from the other by conjugation with some multiplication operators. This allows us to give a very similar definition of the *out/in* state  $\omega_{\text{out/in}}$  and to prove a direct analogue of Thm. 1.1.

**1.2. Fredholm problem for the Klein-Gordon equation on asymptotically Minkowski spacetimes.** Our second main result makes use of asymptotic data at future and past infinity and at the same time relies on good control of what happens at spatial infinity, and thus requires a more refined setup.

To formulate the problem, let us first recall that in Quantum Field Theory, expectation values of time-ordered products of fields involve a *Feynman propagator*, which in the present setup is an operator of the form

$$G_{\mathbb{F},\omega} = i^{-1}\Lambda^+ + G_- = i^{-1}\Lambda^+ + G_+,$$

where  $\Lambda^\pm$  are two-point functions of a state  $\omega$  and  $G_\pm$  the retarded/advanced propagator<sup>2</sup> of  $P$ . We call any such operator  $G_{\mathbb{F},\omega}$  a *time-ordered Feynman propagator* to distinguish it from other related (approximate) inverses of  $P$ . Apart from playing an essential role in perturbative computations in interacting QFT, time-ordered Feynman propagators on curved spacetimes provide the link between the Hadamard condition (1.3) and the theory of distinguished parametrices of Duistermaat and Hörmander [DH]. In fact, Radzikowski's theorem [Ra] asserts that  $\omega$  is Hadamard if and only if the primed wave front set of  $G_{\mathbb{F},\omega}$  is the same as that of Duistermaat and Hörmander's 'Feynman parametrix', i.e. if

$$(1.4) \quad \text{WF}'(G_{\mathbb{F},\omega}) = (\text{diag}_{T^*M}) \cup \bigcup_{t \leq 0} (\Phi_t(\text{diag}_{T^*M}) \cap \pi^{-1}\mathcal{N}),$$

This plays a crucial role in applications as it implies that two-point functions of Hadamard states are unique modulo smooth terms.

Recently, a very different point of view was proposed by Gell-Redman, Haber and Vasy [GHV, Va2], basing on earlier developments [Va1, BVW, HV], who proved that the wave operator on asymptotically Minkowski spacetimes is Fredholm when interpreted as an operator acting on carefully chosen Hilbert spaces of distributions. A remarkable consequence is that it has a generalized inverse  $G_{\mathbb{F}}$  such that its primed wave front set  $\text{WF}'(G_{\mathbb{F}})$  is given precisely by (1.4) [GHV, VW]. It is however not expected to be equal  $G_{\mathbb{F},\omega}$  for some Hadamard state  $\omega$ , even in cases when  $G_{\mathbb{F}}$  is an exact inverse of  $P$ : although one could define some operators  $\Lambda^\pm$  by setting  $G_{\mathbb{F}} =: i^{-1}\Lambda^+ + G_- = i^{-1}\Lambda^+ + G_+$ , they will generically not satisfy the positivity condition  $\Lambda^\pm \geq 0$  and thus they will not be two-point functions. On the other hand, one can argue that  $G_{\mathbb{F}}$  is a canonical object (modulo finite-dimensional choices, unless some geometrical assumptions are made), and that it bears much more resemblance to elliptic inverses than the retarded and advanced propagators do. Moreover, a recent work of Bär and Strohmaier that treats the Dirac equation on a finite Lorentzian cylinder [BS1] achieves to set up a Fredholm problem which is in many ways similar to that of Gell-Redman, Haber and Vasy. Interestingly, they prove a Lorentzian analogue of the Atiyah-Patodi-Singer theorem [APS1, APS2] and relate the index to quantities of direct physical interest, in the so-called chiral anomaly [BS2].

Our aim is to set up a Fredholm problem on a class of spacetimes similar to ones considered in [GHV], but for the massive Klein-Gordon equation instead of the wave equation. On the other hand, we use an approach that is more closely related to the method of [BS1] and that in fact can be thought of as its non-compact generalization, at least if one disregards distinct features of the Dirac and Klein-Gordon equations.

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<sup>2</sup>By retarded/advanced propagator  $G_\pm$  one means the inverse of  $P$  that solves the inhomogeneous problem  $Pu = f$  for  $f$  vanishing at respectively past/future infinity.

We are primarily interested in the class of *asymptotically Minkowski spacetimes*, in the sense that  $(M, g)$  is a Lorentzian manifold (without boundary) such that  $M = \mathbb{R}^{1+d}$  and:

$$\begin{aligned} & g_{\mu\nu}(x) - \eta_{\mu\nu} \in S_{\text{std}}^{-\delta}(\mathbb{R}^{1+d}), \quad \delta > 1, \\ \text{(aM)} \quad & (\mathbb{R}^{1+d}, g) \text{ is globally hyperbolic,} \\ & (\mathbb{R}^{1+d}, g) \text{ has a time function } \tilde{t} \text{ such that } \tilde{t} - t \in S_{\text{std}}^{1-\epsilon}(\mathbb{R}^{1+d}), \quad \epsilon > 0, \end{aligned}$$

where  $\eta_{\mu\nu}$  is the Minkowski metric and  $S_{\text{std}}^{\delta}(\mathbb{R}^{1+d})$  stands for the class of smooth functions  $f$  such that

$$\partial_x^\alpha f \in O(\langle x \rangle^{\delta-|\alpha|}), \quad \alpha \in \mathbb{N}^{1+d}.$$

This way,  $g$  decays to the flat Minkowski metric simultaneously in time and in the spatial directions in a short-range<sup>3</sup> way. In a similar vein the potential is required to satisfy  $V(y) - m^2 \in S_{\text{std}}^{-\delta}(\mathbb{R}^{1+d})$ ,  $m > 0$ . Note that the definition (aM) covers a similar class of spacetimes as those considered in [BVW, GHV] (the latter are also called asymptotically Minkowski spacetimes therein), but strictly speaking they are not exactly the same. In our setup one has for instance  $(M, g)$  is globally hyperbolic, which is not clear from the outset in [BVW, GHV].

The main idea in the formulation of the Fredholm problem is to consider ‘boundary conditions’ that select asymptotic data which account for propagation of singularities within only one of the two connected components  $\mathcal{N}^\pm$  of the characteristic set of  $P$ . While in [BS1] there is indeed a boundary at finite times, here we need to consider infinite times instead, so boundary conditions are not to be understood literally as they are rather specified at the level of scattering data.

In order to define scattering data in the setting of asymptotically Minkowski spaces we first make a change of variables by means of a diffeomorphism  $\chi$  (see Subsect. 7.3), which allows to put the metric in the form

$$\chi^* g = -\hat{c}^2(t, x) dt^2 + \hat{h}(t, x) dx^2,$$

where  $\hat{c}$  tends to 1 for large  $|x|$ , while  $\hat{h}$  tends to some asymptotic metrics  $\hat{h}_{\text{in/out}}$  depending on the sign of  $t$ . In these coordinates, a convenient choice of Cauchy data is  $\varrho_s u := (u, -i\hat{c}^{-1}\partial_t u)|_{t=s}$ . On the other hand, the natural reference dynamics in this problem (at both future and past infinity) is that of the free Klein-Gordon operator

$$P_{\text{free}} = -\partial_t^2 - \Delta_x + m^2.$$

Let now  $\mathcal{U}(t, s)$ ,  $\mathcal{U}_{\text{free}}(t, s)$  be the respective Cauchy evolutions for  $P$  and  $P_{\text{free}}$ , and let us fix as reference time  $t = 0$ . We define the *Feynman* and *anti-Feynman scattering data maps*:

$$\begin{aligned} \varrho_{\text{F}} &:= \text{s-} \lim_{t_\pm \rightarrow \pm\infty} \left( c_{\text{free}}^{+, \text{vac}} \mathcal{U}_{\text{free}}(0, t_+) \varrho_{t_+} + c_{\text{free}}^{-, \text{vac}} \mathcal{U}_{\text{free}}(0, t_-) \varrho_{t_-} \right), \\ \varrho_{\overline{\text{F}}} &:= \text{s-} \lim_{t_\pm \rightarrow \pm\infty} \left( c_{\text{free}}^{+, \text{vac}} \mathcal{U}_{\text{free}}(0, t_-) \varrho_{t_-} + c_{\text{free}}^{-, \text{vac}} \mathcal{U}_{\text{free}}(0, t_+) \varrho_{t_+} \right), \end{aligned}$$

as appropriate strong operator limits, where  $c_{\text{free}}^{\pm, \text{vac}}$  is defined as  $c_{\text{out}}^{\pm, \text{vac}}$ , but with  $-\Delta_x + m^2$  in the place of  $a_{\text{out}}$ . We abbreviate the Sobolev spaces  $H^m(\mathbb{R}^d)$  by  $H^m$ . Our main result can be stated as follows.

**Theorem 1.2.** *Assume (aM) and let  $m \in \mathbb{R}$ . Consider the Hilbert space*

$$(1.5) \quad \mathcal{X}_{\text{F}}^m := \{u \in (\chi^{-1})^*(C^1(\mathbb{R}; H^{m+1}) \cap C^0(\mathbb{R}; H^m)) : Pu \in \mathcal{Y}^m, \varrho_{\overline{\text{F}}} u = 0\},$$

<sup>3</sup>This corresponds to the assumption  $\delta > 1$ .

where  $\mathcal{Y}^m := (\chi^{-1})^* (\langle t \rangle^{-\gamma} L^2(\mathbb{R}; H^m))$  and  $\frac{1}{2} < \gamma < \frac{1}{2} + \delta$ . Then  $P : \mathcal{X}_F^m \rightarrow \mathcal{Y}^m$  is Fredholm of index

$$(1.6) \quad \text{ind } P|_{\mathcal{X}_F^m \rightarrow \mathcal{Y}^m} = \text{ind}(c_{\text{free}}^{-, \text{vac}} W_{\text{out}}^{-1} + c_{\text{free}}^{+, \text{vac}} W_{\text{in}}^{-1}),$$

where  $W_{\text{out/in}}^{-1} = \lim_{t_{\pm} \rightarrow \pm\infty} \mathcal{U}_{\text{free}}(0, t_{\pm}) \mathcal{U}(t_{\pm}, 0)$ . In particular the index is independent on  $m$ . Furthermore, there exists  $G_F : \mathcal{Y}^m \rightarrow \mathcal{X}_F^m$  with  $\text{WF}'(G_F)$  as in (1.4) and such that  $\mathbf{1} - PG_F$  and  $\mathbf{1} - G_F P$  are compact and have smooth Schwartz kernels.

Note that the space  $\mathcal{X}_F^m$  is a closed subspace of the Hilbert space

$$\mathcal{X}^m = \{u \in (\chi^{-1})^*(C^1(\mathbb{R}; H^{m+1}) \cap C^0(\mathbb{R}; H^m)) : Pu \in \mathcal{Y}^m\}$$

equipped with the norm  $\|u\|_{\mathcal{X}^m}^2 = \|\varrho_0(\chi^{-1})^* u\|_{\mathcal{E}^m}^2 + \|Pu\|_{\mathcal{Y}^m}^2$ , where  $\mathcal{E}^m$  is the energy space, see Def. 6.4.

As pointed out in [BS1], the condition  $\varrho_{\overline{F}} u = 0$  can be seen as an analogue of the Atiyah-Patodi-Singer boundary condition (even though this is less evident here as we do not consider the Dirac equation). Furthermore, one could equally well consider the *anti-APS* boundary condition  $\varrho_F u = 0$ , which leads to an ‘anti-Feynman’ counterpart of Theorem 1.2 — interestingly, just as in [BS1], this differs from the Riemannian case where one boundary condition is preferred over the other. On the other hand, the kernel of  $P : \mathcal{X}_F^m \rightarrow \mathcal{Y}^m$  consists of smooth functions and  $G_F$  satisfies a positivity condition  $i^{-1}(G_F - G_F^*) \geq 0$  reminiscent of the limiting absorption principle. As pioneered in [BS1] and [BVW, Va2], this shows a striking similarity to the elliptic case.

### 1.3. Outline of proofs.

1.3.1. *Proof of Hadamard property.* The main technical ingredient that we use in the proof of both theorems is an approximate diagonalization<sup>4</sup> of the Cauchy evolution by means of elliptic pseudodifferential operators, derived in detail in [GOW] and based on the strategy developed successively in the papers [Ju, JS, GW1, GW2]. Specifically, its outcome is that the Cauchy evolution of  $P$  can be written as

$$(1.7) \quad \mathcal{U}(s, t) = T(t) \mathcal{U}^{\text{ad}}(t, s) T(s)^{-1}$$

where  $T(t)$  is a  $2 \times 2$  matrix of pseudodifferential operators (smoothly depending on  $t$ ). The superscript ad stands for ‘almost diagonal’ and indeed  $\mathcal{U}^{\text{ad}}(s, t)$  is the Cauchy evolution of a time-dependent operator of the form  $i\partial_t + H^{\text{ad}}(t)$ , where

$$H^{\text{ad}}(t) = \begin{pmatrix} \epsilon^+(t) & 0 \\ 0 & \epsilon^-(t) \end{pmatrix},$$

modulo smooth terms (more precisely, modulo terms in  $C^\infty(\mathbb{R}^2, \mathcal{W}^{-\infty}(\Sigma) \otimes \mathbb{C}^2)$ , where  $\mathcal{W}^{-\infty}(\Sigma)$  are the operators that map  $H^{-m}(\Sigma)$  to  $H^m(\Sigma)$  for each  $m \in \mathbb{N}$ ), and  $\epsilon^\pm(t)$  are elliptic pseudodifferential operators of order 1 with principal symbol  $\pm(k \cdot h_t^{-1} k)^{\frac{1}{2}}$ . Now, because of this particular form of the principal symbol, solutions of  $(i^{-1}\partial_t + \epsilon^\pm(t))$  propagate with wave front set in  $\mathcal{N}^\pm$ . This serves one to prove that if we fix some  $t_0 \in \mathbb{R}$  and set

$$c_{\text{ref}}^\pm(t_0) := T(t_0) \pi^\pm T^{-1}(t_0), \quad \text{where } \pi^+ = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & 0 \end{pmatrix}, \quad \pi^- = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix},$$

<sup>4</sup>On a side note, let us mention that a different diagonalization procedure was proposed by Ruzhansky and Wirth in the context of dispersive estimates [RW, Wi]; in their method it is the (full) symbol of the generator of the Cauchy evolution that is diagonalized (rather than the Cauchy evolution itself).

then  $\Lambda_{\text{ref}}^{\pm}(t, s) := \mp \pi_0 \mathcal{W}(t, t_0) c_{\text{ref}}^{\pm}(t_0) \mathcal{W}(t_0, s) \pi_1^*$  have wave front set only in  $\mathcal{N}^{\pm} \times \mathcal{N}^{\pm}$  and therefore satisfy the Hadamard condition (1.3). As a consequence, to prove the Hadamard condition for  $\Lambda_{\text{in/out}}^{\pm}$  it suffices to show that

$$c_{\text{in/out}}^{\pm} - c_{\text{ref}}^{\pm} \in \mathcal{W}^{-\infty}(\Sigma) \otimes B(\mathbb{C}^2).$$

To demonstrate that this is the case, we use assumption (td) to control the decay in time of various remainders in identities ‘modulo smooth’. The most crucial estimate here is

$$(1.8) \quad H^{\text{ad}}(t) - \begin{pmatrix} a(t)^{\frac{1}{2}} & 0 \\ 0 & -a(t)^{\frac{1}{2}} \end{pmatrix} \in \Psi_{\text{td}}^{0, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2),$$

which then yields time-decay of various commutators that appear in the proofs. We obtain (1.8) by revisiting the approximate diagonalization (1.7) using poly-homogeneous expansions of pseudodifferential operators in  $\Psi_{\text{td}}^{m, -\delta}(\mathbb{R}; \Sigma)$  in both  $m$  and  $\delta$ ; more details are given in Sect. 4.5.

**1.3.2. Proof of Fredholm statement.** The proof of our second result, Theorem 1.2, is based on a refinement of the above strategy. First, we show that the original problem on asymptotically Minkowski spacetimes can always be reduced to a special case of assumption (td), with  $\Sigma = \mathbb{R}^d$  and the  $\Psi_{\text{td}}^{m, \delta}$  remainders replaced by a subclass  $\Psi_{\text{std}}^{m, \delta}$  that accounts for decay in both  $t$  and  $x$  (rather than just in  $t$ ). This allows us to derive a better estimate for  $c_{\text{in/out}}^{\pm} - c_{\text{ref}}^{\pm}$ , in particular with decay in  $\langle x \rangle$  that is sufficient to get that  $c_{\text{in/out}}^{\pm} - c_{\text{ref}}^{\pm}$  is a compact operator. This way, we conclude that

$$(1.9) \quad c_{\text{in}}^+ + c_{\text{out}}^- = \mathbf{1} + \text{a compact, smoothing term,}$$

so in particular  $c_{\text{in}}^+ + c_{\text{out}}^-$  is Fredholm. From this point on we can use standard arguments from Fredholm theory, to a large extent drawing from [BS1]. To give only a rough intuition, let us point out that if we took instead of  $\varrho_{\mathbb{F}}$  standard scattering data at future or past infinity, then the associated boundary conditions would simply give rise to the forward or backward inhomogeneous problem, which is invertible. If for the sake of the argument,  $c_{\text{in}}^{\pm} = c_{\text{out}}^{\pm}$  then the same can be said about the Feynman problem. Although generically,  $c_{\text{in}}^{\pm}$  does not equal  $c_{\text{out}}^{\pm}$ , (1.9) ensures that we are in the ‘next best possible’ case, where the obstruction to invertibility of  $c_{\text{in}}^+ + c_{\text{out}}^-$  is finite dimensional.

The construction of the Feynman parametrix  $G_{\mathbb{F}}$  is then based on a formula that makes use of the approximate diagonalization again. It is interesting to note that although our techniques differ a lot from that of [VW], the final formulas are quite similar. This provides further evidence that our result can be seen as an analogue of that of [GHV] in the case of the massive Klein-Gordon equation.

It is also worth mentioning that compactness of the remainder term in (1.9) was already studied in an analogous problem for the Dirac operator on Minkowski space with external potentials [Ma1, Ma2, BH], where index formulas have also been derived and the interpretation of the index in terms of particle creation was discussed (see also [BS1, BS2]). An interesting topic of further research would thus be to find a short-hand index formula in our setting.

**1.4. Plan of the paper.** The paper is structured as follows.

In Sect. 2 we fix some basic terminology and recall the definition of two-point functions and covariances of states in the context of non-interacting Quantum Field Theory.

Sect. 3 contains a brief overview of the pseudodifferential calculus on manifolds of bounded geometry. In Sect. 4 we recall the construction of two-point functions of generic Hadamard states from [GW1, GOW]. We then introduce the time-dependent pseudodifferential operator



classes  $\Psi_{\text{td}}^{m,\delta}$ ,  $\Psi_{\text{std}}^{m,\delta}$  and state some of their properties, in particular we give a variant of Seeley's theorem on powers of pseudodifferential operators elliptic in the standard  $\Psi^m$  sense.

In Sect. 4 we first recall the approximate diagonalization of the Cauchy evolution used in [GOW] to construct generic Hadamard states. We then give a refinement in the setup of assumptions (td) and (std) (the  $\Psi_{\text{std}}^{m,\delta}$  analogue of the former) by showing decay of various remainder terms.

Sect. 5 contains the construction of *in/out* states and the proof of their Hadamard property in the case of asymptotically static spacetimes (assumptions (ast) and (pos)). The key ingredients are the reduction to the setup of assumption (td) and the estimates obtained in Sect. 4.

In Sect. 6 we set up a Fredholm problem for the Klein-Gordon operator, assuming hypothesis (std). We also construct a parametrix with Feynman type wave front set and prove that the remainder terms are compact operators. An important role is played by the approximate diagonalization and the estimates from Sect. 4.

Finally, in Sect. 7 we consider asymptotically Minkowski spacetimes (aM). We show that in this case, using the procedure from Sect. 5 one is reduced to assumption (std). This allows us to adapt the results from Sect. 6 and to prove Thm. 1.2.

Various auxiliary proofs are collected in Appendix A.

## 2. PRELIMINARIES

**2.1. Notation.** The space of differential operators (of order  $m$ ) over a smooth manifold  $M$  (here always without boundary) is denoted  $\text{Diff}(M)$  ( $\text{Diff}^m(M)$ ). The space of smooth functions on  $M$  with compact support is denoted  $C_c^\infty(M)$ .

The operator of multiplication by a function  $f$  will be denoted by  $f$ , while the operators of partial differentiation will be denoted by  $\bar{\partial}_i$ , so that  $[\bar{\partial}_i, f] = \partial_i f$ .

- If  $a, b$  are selfadjoint operators on a Hilbert space  $\mathcal{H}$ , we write  $a \sim b$  if

$$a, b > 0, \quad \text{Dom } a^{\frac{1}{2}} = \text{Dom } b^{\frac{1}{2}}, \quad c^{-1}b \leq a \leq cb,$$

for some constant  $c > 0$ .

- Similarly, if  $I \subset \mathbb{R}$  is an open interval and  $\{\mathcal{H}_t\}_{t \in I}$  is a family of Hilbert spaces with  $\mathcal{H}_t = \mathcal{H}$  as topological vector spaces, and  $a(t), b(t)$  are two selfadjoint operators on  $\mathcal{H}_t$ , we write  $a(t) \sim b(t)$  if for each  $J \Subset I$  there exist constants  $c_{1,J}, c_{2,J} > 0$  such that

$$(2.1) \quad a(t), b(t) \geq c_{1,J} > 0, \quad c_{2,J} b(t) \leq a(t) \leq c_{2,J}^{-1} b(t), \quad t \in J.$$

**2.2. Klein-Gordon operator.** Let  $(M, g)$  be a Lorentzian spacetime (we use the convention  $(-, +, \dots, +)$  for the Lorentzian signature). We consider the Klein-Gordon operator with a real-valued potential  $V \in C^\infty(M)$

$$P = -\square_g + V \in \text{Diff}^2(M),$$

Since  $V$  is real-valued we have  $P = P^*$  in the sense of formal adjoints with respect to the  $L^2(M, g)$  scalar product, naturally defined using the volume form.

For  $K \subset M$  we denote  $J^\pm(K) \subset M$  its causal future/past, see e.g. [BF, Wa2]. Let  $C_\pm^\infty(M)$  be the space of smooth functions whose support is future or past compact, that is

$$C_\pm^\infty(M) = \{f \in C^\infty(M) : \text{supp } f \subset J^\pm(K) \text{ for some compact } K \subset M\}.$$

We assume that  $(M, g)$  is globally hyperbolic, i.e. admits a foliation by Cauchy surfaces<sup>5</sup> (in the next sections we will impose more restrictive conditions on  $(M, g)$ , but these are irrelevant

<sup>5</sup>Let us recall that a Cauchy surface is a smooth hypersurface that is intersected by every inextendible, non-spacelike (i.e. causal) curve exactly once.

for the moment). It is well known that  $P$  has then unique *advanced/retarded propagators*, i.e. operators  $G_{\pm} : C_{\pm}^{\infty}(M) \rightarrow C_{\pm}^{\infty}(M)$  s.t.

$$(2.2) \quad PG_{\pm} = \mathbf{1} \quad \text{on} \quad C_{\pm}^{\infty}(M).$$

The domain of definition of  $G_{\pm}$  on which (2.2) holds true can actually be increased, this will be shown in a more specific setup in later sections.

A standard duality argument using  $P = P^*$ , (2.2), and the fact that  $C_{+}^{\infty}(M) \cap C_{-}^{\infty}(M) = C_c^{\infty}(M)$  on globally hyperbolic spacetimes, gives  $G_{+}^* = G_{-}$  as sesquilinear forms on  $C_c^{\infty}(M)$ . The *causal propagator* (often also called *Pauli-Jordan commutator function*) of  $P$  is by definition  $G := G_{+} - G_{-}$ , interpreted here as a map from  $C_c^{\infty}(M)$  to  $C_{+}^{\infty}(M) + C_{-}^{\infty}(M)$ , the space of space-compact smooth functions.

**2.3. Symplectic space of solutions.** In what follows we recall the relation between quasi-free states, two-point functions, and field quantization. The reader interested only in the analytical aspects can skip this discussion and move directly to equations (2.6)–(2.8), which can be taken as the definition of two-point functions in the present context.

By a *phase space* we will mean a pair  $(\mathcal{V}, q)$  consisting of a complex vector space  $\mathcal{V}$  and a non degenerate hermitian form  $q$  on  $\mathcal{V}$ . In our case the phase space of interest (i.e. the phase space of the classical non-interacting scalar field theory) is

$$(2.3) \quad \mathcal{V} := \frac{C_c^{\infty}(M)}{PC_c^{\infty}(M)}, \quad \bar{u}qv := i^{-1}(u|Gv),$$

where  $(\cdot|\cdot)$  is the  $L^2(M, g)$  pairing, canonically defined using the volume form. The sesquilinear form  $q$  is indeed well-defined on the quotient space  $C_c^{\infty}(M)/PC_c^{\infty}(M)$  because  $PG = GP = 0$  on test functions. Using that  $G_{+}^* = G_{-}$  one shows that  $q$  is hermitian, and it is also not difficult to show that it is non-degenerate.

Note that in contrast to most of the literature, we work with hermitian forms rather than with real symplectic ones, but the two approaches are equivalent.

**2.4. States and their two-point functions.** Let  $\mathcal{V}$  be a complex vector space,  $\mathcal{V}^*$  its anti-dual and  $L_h(\mathcal{V}, \mathcal{V}^*)$  the space of hermitian sesquilinear forms on  $\mathcal{V}$ . If  $q \in L_h(\mathcal{V}, \mathcal{V}^*)$  then we can define the polynomial CCR  $*$ -algebra  $\text{CCR}^{\text{pol}}(\mathcal{V}, q)$  (see e.g. [DG2, Sect. 8.3.1])<sup>6</sup>. It is constructed as the span of the so-called *abstract complex fields*  $\mathcal{V} \ni v \mapsto \psi(v), \psi^*(v)$ , which are taken to be anti-linear, resp. linear in  $v$  and are subject to the canonical commutation relations

$$[\psi(v), \psi(w)] = [\psi^*(v), \psi^*(w)] = 0, \quad [\psi(v), \psi^*(w)] = \bar{v}qw\mathbf{1}, \quad v, w \in \mathcal{V}.$$

Our main object of interests are the states<sup>7</sup> on  $\text{CCR}^{\text{pol}}(\mathcal{V}, q)$ .

The *complex covariances*  $\Lambda^{\pm} \in L_h(\mathcal{V}, \mathcal{V}^*)$  of a state  $\omega$  on  $\text{CCR}^{\text{pol}}(\mathcal{V}, q)$  are defined in terms of the abstract field operators by

$$(2.4) \quad \bar{v}\Lambda^{+}w = \omega(\psi(v)\psi^*(w)), \quad \bar{v}\Lambda^{-}w = \omega(\psi^*(w)\psi(v)), \quad v, w \in \mathcal{V}$$

Note that both  $\Lambda^{\pm}$  are positive and by the canonical commutation relations one always has  $\Lambda^{+} - \Lambda^{-} = q$ . We are interested in the reverse construction, namely if one has a pair of hermitian forms  $\Lambda^{\pm}$  such that  $\Lambda^{+} - \Lambda^{-} = q$  and  $\Lambda^{\pm} \geq 0$  then there is a unique *quasi-free* state  $\omega$  such that (2.4) holds. We will thus further restrict our attention to quasi-free states and more specifically to their complex covariances  $\Lambda^{\pm}$ .

<sup>6</sup>See also [GW1, Wr] for remarks on the transition between real and complex vector space terminology.

<sup>7</sup>Let us recall that a state  $\omega$  is a linear functional on  $\text{CCR}^{\text{pol}}(\mathcal{V}, q)$  such that  $\omega(a^*a) \geq 0$  for all  $a$  in  $\text{CCR}^{\text{pol}}(\mathcal{V}, q)$ , and  $\omega(\mathbf{1}) = 1$ .

In QFT (at least for scalar fields) the phase space of interest is the one defined in (2.3). In that specific case it is convenient to consider instead of complex covariances a pair of operators  $\Lambda^\pm : C_c^\infty(M) \rightarrow C^\infty(M)$  such that

$$(2.5) \quad (v|\Lambda^+w) = \omega(\psi(v)\psi^*(w)), \quad (v|\Lambda^-w) = \omega(\psi^*(w)\psi(v)), \quad v, w \in C_c^\infty(M).$$

We call  $\Lambda^\pm$  the *two-point functions* of the state  $\omega$  and identify them with the associated complex covariances whenever possible. Note that because  $(\cdot|\Lambda^\pm\cdot)$  has to induce a hermitian form on the quotient space  $C_c^\infty(M)/PC_c^\infty(M)$ , the two-point functions have to satisfy  $P\Lambda^\pm = \Lambda^\pm P = 0$  on  $C_c^\infty(M)$ . By the Schwartz kernel theorem we can further identify  $\Lambda^\pm$  with a pair of distributions on  $M \times M$ , these are then bi-solutions of the Klein-Gordon equation.

In QFT on curved spacetime one is especially interested in the subclass of quasi-free *Hadamard states* [KW, Ra]. These can be defined as in the introduction (1.3), or equivalently just by requiring that the primed wave front set of the Schwartz kernel of  $\Lambda^\pm$  is contained in  $\mathcal{N}^\pm \times \mathcal{N}^\pm$  (cf. [SV, Sa]),  $\mathcal{N}^\pm \subset T^*M \setminus o$  being the two connected components of the characteristic set of  $P$  (and  $o \subset T^*M$  the zero section). To sum this up, specifying a Hadamard state amounts to constructing a pair of operators  $\Lambda^\pm : C_c^\infty(M) \rightarrow C^\infty(M)$  satisfying the properties<sup>8</sup>:

$$(2.6) \quad P\Lambda^\pm = \Lambda^\pm P = 0, \quad \Lambda^+ - \Lambda^- = iG,$$

$$(2.7) \quad \Lambda^\pm \geq 0,$$

$$(2.8) \quad \text{WF}'(\Lambda^\pm) \subset \mathcal{N}^\pm \times \mathcal{N}^\pm.$$

Existence of generic two-point functions as above was proved in [FNW], and an alternative argument was given in [GW1]. Here we will be interested in showing (2.8) for specific two-point functions with prescribed asymptotic properties.

**2.5. Cauchy data of two-point functions.** We will need a version of two-point functions acting on Cauchy data of  $P$  instead of spacetime quantities such as  $\Lambda^\pm$ . To this end, let  $\{\Sigma_s\}_{s \in \mathbb{R}}$  be a foliation of  $M$  by Cauchy surfaces (since all  $\Sigma_s$  are diffeomorphic we occasionally write  $\Sigma$  instead). We define the map

$$\varrho_s u := (u, i^{-1}n^a \nabla_a u)|_{\Sigma_s},$$

acting on distributions  $u$  such that the restriction  $\upharpoonright_{\Sigma_s}$  makes sense, where  $n^a$  is the unit normal vector to  $\Sigma_s$ . It is well-known that  $\varrho_s \circ G$  maps  $C_c^\infty(M)$  to  $C_c^\infty(\Sigma_s)$  and that there exists an operator  $G(s)$  acting on  $C_c^\infty(\Sigma) \otimes \mathbb{C}^2$  (not to be confused with  $G$ ) that satisfies

$$(2.9) \quad G =: (\varrho_s G)^* \circ G(s) \circ \varrho_s G,$$

where  $(\varrho_s G)^*$  is the formal adjoint of  $\varrho_s \circ G$  wrt. the  $L^2$  inner product on  $\Sigma_s \sqcup \Sigma_s$  respective to some density (that can depend on  $s$ , later on we will make that choice more specific). We also set

$$q(s) := i^{-1}G(s),$$

so that  $q(s)^* = q(s)$ .

The next result provides a Cauchy surface analogue of the two-point functions  $\Lambda^\pm$ , cf. [GW2] for the proof.

**Proposition 2.1.** *For any  $s \in \mathbb{R}$  the maps:*

$$(2.10) \quad \lambda^\pm(s) \mapsto \Lambda^\pm := (\varrho_s G)^* \lambda^\pm(s) (\varrho_s G),$$

<sup>8</sup>Especially in the literature on QFT on curved spacetimes one uses frequently the following alternative convention: one assumes that the Schwartz kernel  $\Lambda^-(x, y)$  equals  $\Lambda^+(y, x)$  (this can be always ensured by taking an appropriate average if necessary), in which case one positivity condition  $\Lambda^+ \geq 0$  implies the other one. One rather speaks then of one two-point function (often denoted  $\omega_2(x, y)$  or  $W_2(x, y)$ ) instead of a pair.

and

$$(2.11) \quad \Lambda^\pm \mapsto \lambda^\pm(s) := (\varrho_s^* G(s))^* \Lambda^\pm (\varrho_s^* G(s))$$

are bijective and inverse from one another.

It is actually convenient to make one more definition and set:

$$(2.12) \quad c^\pm(s) = \pm i^{-1} G(s) \lambda^\pm(s) : C_c^\infty(\Sigma) \otimes B(\mathbb{C}^2) \rightarrow C^\infty(\Sigma) \otimes B(\mathbb{C}^2).$$

We will simply call  $c^\pm(s)$  the (*time-s*) *covariances of the state*  $\omega$ . A pair of operators  $c^\pm(s)$  are covariances of a state iff the operators  $\Lambda^\pm$  defined by (2.10) and (2.12) satisfy (2.6)-(2.7), which is equivalent to the conditions

$$(2.13) \quad c^+(s) + c^-(s) = \mathbf{1},$$

$$(2.14) \quad \lambda^\pm(s) \geq 0,$$

where we identified the operators  $\lambda^\pm(s)$  with hermitian forms using the same pairing as when we took the formal adjoint in (2.9). Note that (2.13) can also be expressed as  $\lambda^+(s) - \lambda^-(s) = q(s)$ .

Additionally, a state (recall that we consider only quasi-free states) is *pure* iff its covariances  $c^\pm(s)$  extend to projections on the completion of  $C_c^\infty(\Sigma) \otimes \mathbb{C}^2$  w.r.t. the inner product given by  $\lambda^+ + \lambda^-$ . In practice it is sufficient to construct  $c^\pm(s)$  as projections acting on a space that is big enough to contain  $C_c^\infty(\Sigma) \otimes \mathbb{C}^2$ , but small enough to be contained in the Hilbert space associated to  $\lambda^+ + \lambda^-$ .

**2.6. Propagators for the Cauchy evolution.** Recall that we have defined the operator  $G(s)$  via the identity

$$(2.15) \quad G =: (\varrho_s G)^* \circ G(s) \circ \varrho_s G.$$

A direct consequence is that the operator  $G^* \varrho_s G(s)$  assigns to Cauchy data on  $\Sigma_s$  the corresponding solution. Similarly, for  $t, s \in \mathbb{R}$  the operator

$$(2.16) \quad \mathcal{U}(s, t) := \varrho_s G^* \varrho_t^* G(t)$$

produces Cauchy data of a solution on  $\Sigma_s$  given Cauchy data on  $\Sigma_t$ . We will call  $\{\mathcal{U}(s, t)\}_{s, t \in \mathbb{R}}$  the *Cauchy evolution* of  $P$ . A straightforward computation gives the group property

$$(2.17) \quad \mathcal{U}(t, t) = \mathbf{1}, \quad \mathcal{U}(s, t') \mathcal{U}(t', t) = \mathcal{U}(s, t), \quad t' \in \mathbb{R};$$

and the conservation of the symplectic form by the evolution

$$(2.18) \quad \mathcal{U}^*(s, t) q(s) \mathcal{U}(s, t) = q(t).$$

These identities allow to conclude that the covariances  $c^\pm(t)$  (and two-point functions  $\lambda^\pm(t)$ ) at different ‘times’ of a quasi-free state are related by

$$(2.19) \quad \begin{aligned} \lambda^\pm(t) &= \mathcal{U}(s, t)^* \lambda^\pm(s) \mathcal{U}(s, t), \\ c^\pm(t) &= \mathcal{U}(t, s) c^\pm(s) \mathcal{U}(s, t). \end{aligned}$$

Notice that this induces a splitting of the evolution in two parts:

$$\mathcal{U}(s, t) = \mathcal{U}^+(s, t) + \mathcal{U}^-(s, t), \quad \text{with } \mathcal{U}^\pm(s, t) = \mathcal{U}(s, t) c^\pm(t).$$

If the state is pure then  $c^\pm(t)$  are projections for all  $t$  and the operators  $\mathcal{U}^\pm(s, t)$  obey the composition formula

$$\mathcal{U}^\pm(s, t') \mathcal{U}^\pm(t', t) = \mathcal{U}^\pm(s, t), \quad \mathcal{U}^\pm(s, t') \mathcal{U}^\mp(t', t) = 0, \quad t' \in \mathbb{R}.$$

Let us stress that  $\mathcal{U}^\pm(t, t)$  is not the identity, but rather equals  $c^\pm(t)$ . Furthermore, if the state is Hadamard then  $\mathcal{U}(s, t) c^\pm(t)$  propagate singularities along  $\mathcal{N}^\pm$  (see the discussion in [GW2]). In Sect. 4 we will be interested in the reversed argument, namely we will construct

covariances  $c^\pm(t)$  of pure Hadamard states from a splitting of the evolution  $\mathcal{U}(t, s)$  into two parts that propagate singularities along respectively  $\mathcal{N}^+$ ,  $\mathcal{N}^-$ .

### 3. PSEUDODIFFERENTIAL CALCULUS ON MANIFOLDS OF BOUNDED GEOMETRY

**3.1. Manifolds of bounded geometry.** In the present section we introduce manifolds of bounded geometry and review the pseudodifferential calculus of Kordyukov and Shubin [Ko, Sh2], making also use of some results from [GOW].

Let us denote by  $\delta$  the flat metric on  $\mathbb{R}^d$  and by  $B_d(y, r) \subset \mathbb{R}^d$  the open ball of center  $y$  and radius  $r$ .

If  $(\Sigma, h)$  is a  $d$ -dimensional Riemannian manifold and  $X$  is a  $(p, q)$  tensor on  $\Sigma$ , we can define the canonical norm of  $X(x)$ ,  $x \in \Sigma$ , denoted by  $\|X\|_x$ , using appropriate tensor powers of  $h(x)$  and  $h^{-1}(x)$ .  $X$  is *bounded* if  $\sup_{x \in \Sigma} \|X\|_x < \infty$ .

If  $U \subset \Sigma$  is open, we denote by  $\text{BT}_q^p(U, \delta)$  the Fréchet space of  $(p, q)$  tensors on  $U$ , bounded with all covariant derivatives in the above sense. Among several equivalent definitions of manifolds of bounded geometry (see [Sh2, GOW]), the one below is particularly useful in applications.

**Definition 3.1.** *A Riemannian manifold  $(\Sigma, h)$  is of bounded geometry iff for each  $x \in \Sigma$ , there exists an open neighborhood of  $x$ , denoted  $U_x$ , and a smooth diffeomorphism*

$$\psi_x : U_x \xrightarrow{\sim} B_d(0, 1) \subset \mathbb{R}^d$$

with  $\psi_x(x) = 0$ , and such that if  $h_x := (\psi_x^{-1})^* h$  then:

(C1) the family  $\{h_x\}_{x \in \Sigma}$  is bounded in  $\text{BT}_2^0(B_d(0, 1), \delta)$ ,

(C2) there exists  $c > 0$  such that :

$$c^{-1}\delta \leq h_x \leq c\delta, \quad x \in \Sigma.$$

A family  $\{U_x\}_{x \in \Sigma}$  resp.  $\{\psi_x\}_{x \in \Sigma}$  as above will be called a family of good chart neighborhoods, resp. good chart diffeomorphisms.

A known result (see [Sh2, Lemma 1.2]) says that one can find a covering  $\Sigma = \bigcup_{i \in \mathbb{N}} U_i$  by good chart neighborhoods  $U_i = U_{x_i}$  ( $x_i \in \Sigma$ ) which is *uniformly finite*, i.e. there exists  $N \in \mathbb{N}$  such that  $\bigcap_{i \in I} U_i = \emptyset$  if  $\#I > N$ . Setting  $\psi_i = \psi_{x_i}$ , we will call the sequence  $\{U_i, \psi_i\}_{i \in \mathbb{N}}$  a *good chart covering* of  $\Sigma$ .

Furthermore, by [Sh2, Lemma 1.3] one can associate to a good chart covering a partition of unity:

$$1 = \sum_{i \in \mathbb{N}} \chi_i^2, \quad \chi_i \in C_c^\infty(U_i)$$

such that  $\{(\psi_i^{-1})^* \chi_i\}_{i \in \mathbb{N}}$  is a bounded sequence in  $C_b^\infty(B_d(0, 1))$ . Such a partition of unity will be called a *good partition of unity*.

### 3.2. Bounded tensors and bounded diffeomorphisms.

**Definition 3.2.** *Let  $(\Sigma, h)$  be of bounded geometry. We denote by  $\text{BT}_q^p(\Sigma, h)$  the spaces of smooth  $(q, p)$  tensors  $X$  on  $\Sigma$  such that if  $X_x = (\exp_x^h \circ e_x)^* X$ , where  $e_x : (\mathbb{R}^d, \delta) \rightarrow (T_x \Sigma, h(x))$  is an isometry, then the family  $\{X_x\}_{x \in \Sigma}$  is bounded in  $\text{BT}_q^p(B_d(0, \frac{r}{2}), \delta)$ . We equip  $\text{BT}_q^p(\Sigma, h)$  with its natural Fréchet space topology.*

We denote by  $C_b^\infty(\mathbb{R}; \text{BT}_q^p(\Sigma, h))$  the space of smooth maps  $\mathbb{R} \in t \mapsto X(t)$  such that  $\partial_t^n X(t)$  is uniformly bounded in  $\text{BT}_q^p(\Sigma, h)$  for  $n \in \mathbb{N}$ .

We denote by  $S^\delta(\mathbb{R}; \text{BT}_q^p(\Sigma, h))$ ,  $\delta \in \mathbb{R}$  the space of smooth maps  $\mathbb{R} \in t \mapsto X(t)$  such that  $(t)^{-\delta+n} \partial_t^n X(t)$  is uniformly bounded in  $\text{BT}_q^p(\Sigma, h)$  for  $n \in \mathbb{N}$ .

It is well known (see e.g. [GOW, Subsect. 2.3]) that we can replace in Def. 3.2 the geodesic maps  $\exp_x^h \circ e_x$  by  $\psi_x^{-1}$ , where  $\{\psi_x\}_{x \in \Sigma}$  is any family of good chart diffeomorphisms as in Thm. 3.1.

**Definition 3.3.** Let  $(\Sigma, h)$  be an  $n$ -dimensional Riemannian manifold of bounded geometry and  $\chi : \Sigma \rightarrow \Sigma$  a smooth diffeomorphism. One says that  $\chi$  is a bounded diffeomorphism of  $(\Sigma, h)$  if for some family of good chart diffeomorphisms  $\{U_x, \psi_x\}_{x \in \Sigma}$ , the maps

$$\chi_x = \psi_{\chi(x)} \circ \chi \circ \psi_x^{-1}, \quad \chi_x^{-1} = \psi_{\chi^{-1}(x)} \circ \chi^{-1} \circ \psi_x : B_n(0, 1) \rightarrow B_n(0, 1)$$

are bounded in  $C_b^\infty(B_n(0, 1))$  uniformly with respect to  $x \in M$ .

It is easy to see that if the above properties are satisfied for some family of good chart diffeomorphisms then they are satisfied for any such family, furthermore bounded diffeomorphisms are stable under composition.

**3.3. Symbol classes.** We recall some well-known definitions about symbol classes on manifolds of bounded geometry, following [Sh2, Ko, ALNV].

**3.3.1. Symbol classes on  $\mathbb{R}^n$ .** Let  $U \subset \mathbb{R}^d$  be an open set, equipped with the flat metric  $\delta$  on  $\mathbb{R}^d$ .

We denote by  $S^m(T^*U)$ ,  $m \in \mathbb{R}$ , the space of  $a \in C^\infty(U \times \mathbb{R}^d)$  such that

$$\langle k \rangle^{-m+|\beta|} \partial_x^\alpha \partial_\xi^\beta a(x, k) \text{ is bounded on } U \times \mathbb{R}^d, \quad \forall \alpha, \beta \in \mathbb{N}^n,$$

equipped with its canonical semi-norms  $\|\cdot\|_{m, \alpha, \beta}$ .

We set

$$S^{-\infty}(T^*U) := \bigcap_{m \in \mathbb{R}} S^m(T^*U), \quad S^\infty(T^*U) := \bigcup_{m \in \mathbb{R}} S^m(T^*U),$$

with their canonical Fréchet space topologies. If  $m \in \mathbb{R}$  and  $a_{m-i} \in S^{m-i}(T^*U)$  we write  $a \simeq \sum_{i \in \mathbb{N}} a_{m-i}$  if for each  $p \in \mathbb{N}$

$$(3.1) \quad r_p(a) := a - \sum_{i=0}^p a_{m-i} \in S^{m-p-1}(T^*U).$$

It is well-known (see e.g. [Sh3, Sect. 3.3]) that if  $a_{m-i} \in S^{m-i}(T^*U)$ , there exists  $a \in S^m(T^*U)$ , unique modulo  $S^{-\infty}(T^*U)$  such that  $a \simeq \sum_{i \in \mathbb{N}} a_{m-i}$ .

We denote by  $S_h^m(T^*U) \subset S^m(T^*U)$  the space of  $a$  such that  $a(x, \lambda k) = \lambda^m a(x, k)$ , for  $x \in U$ ,  $|k| \geq C$ ,  $C > 0$  and by  $S_{\text{ph}}^m(T^*U) \subset S^m(T^*U)$  the space of  $a$  such that  $a \simeq \sum_{i \in \mathbb{N}} a_{m-i}$  for a sequence  $a_{m-i} \in S_h^{m-i}(T^*U)$  ( $a$  is then called a *poly-homogeneous*<sup>9</sup> symbol). Following [ALNV] one equips  $S_{\text{ph}}^m(T^*U)$  with the topology defined by the semi-norms of  $a_{m-i}$  in  $S^{m-i}(T^*U)$  and  $r_p(a)$  in  $S^{m-p-1}(T^*U)$ , (see (3.1)). This topology is strictly stronger than the topology induced by  $S^m(T^*U)$ .

The space  $S_{\text{ph}}^m(T^*U)/S_{\text{ph}}^{m-1}(T^*U)$  is isomorphic to  $S_h^m(T^*U)$ , and the image of  $a$  under the quotient map is called the *principal symbol* of  $a$  and denoted by  $\sigma_{\text{pr}}(a)$ .

If  $U = B_n(0, 1)$  (more generally, if  $U$  is relatively compact with smooth boundary), there exists a continuous extension map  $E : S^m(T^*U) \rightarrow S^m(T^*\mathbb{R}^d)$  such that  $Ea|_{T^*U} = a$ . Moreover  $E$  maps  $S_{\text{ph}}^m(T^*U)$  into  $S_{\text{ph}}^m(T^*\mathbb{R}^d)$  and is continuous for the topologies of  $S_{\text{ph}}^m(T^*U)$  and  $S_{\text{ph}}^m(T^*\mathbb{R}^d)$ , which means that all the maps

$$a \mapsto (Ea)_{m-i}, \quad a \mapsto r_p(Ea),$$

are continuous.

<sup>9</sup>These are also called classical symbols in the literature.

3.3.2. *Time-dependent symbol classes on  $\mathbb{R}^d$ .* We will also need to consider various classes of *time-dependent* symbols  $a(t, x, k) \in C^\infty(\mathbb{R} \times T^*U)$ . First of all the space  $C^\infty(\mathbb{R}; S^m(T^*U))$  is defined as the space of  $a \in C^\infty(\mathbb{R} \times T^*U)$  such that

$$\langle k \rangle^{-m+|\beta|} \partial_t^\gamma \partial_x^\alpha \partial_k^\beta a(t, x, k) \text{ is bounded on } I \times U \times \mathbb{R}^d, \forall \alpha, \beta \in \mathbb{N}^n, \gamma \in \mathbb{N},$$

for any interval  $I \Subset \mathbb{R}$ . We denote by  $C_b^\infty(\mathbb{R}; S^m(T^*U))$  the subspace of symbols which are uniformly bounded in  $S^m(T^*U)$  with all time derivatives.

Furthermore, anticipating the need for some additional decay in  $t$  in Sect. 4.5, we denote by  $S^\delta(\mathbb{R}; S^m(T^*U))$  the space of  $a \in C^\infty(\mathbb{R} \times T^*U)$  such that

$$\langle t \rangle^{\delta-\gamma} \langle k \rangle^{-m+|\beta|} \partial_t^\gamma \partial_x^\alpha \partial_k^\beta a(t, x, k) \text{ is bounded on } \mathbb{R} \times U \times \mathbb{R}^d, \forall \alpha, \beta \in \mathbb{N}^n, \gamma \in \mathbb{N}.$$

The notation  $a \sim \sum_i a_{m-i}$  and the poly-homogeneous spaces

$$C_{(b)}^\infty(\mathbb{R}; S_{\text{ph}}^m(T^*U)), \quad S^\delta(\mathbb{R}; S_{\text{ph}}^m(T^*U)),$$

are defined analogously, by requiring estimates on the time derivatives of the  $a_{m-i}$  and  $r_p$  in (3.1).

3.3.3. *Symbol classes on  $\Sigma$ .* Let  $(\Sigma, h)$  be a Riemannian manifold of bounded geometry and  $\{\psi_x\}_{x \in \Sigma}$  a family of good chart diffeomorphisms.

**Definition 3.4.** We denote by  $S^m(T^*\Sigma)$  for  $m \in \mathbb{R}$  the space of  $a \in C^\infty(T^*\Sigma)$  such that for each  $x \in \Sigma$ ,  $a_x := (\psi_x^{-1})^* a \in S^m(T^*B_n(0, 1))$  and the family  $\{a_x\}_{x \in \Sigma}$  is bounded in  $S^m(T^*B_n(0, 1))$ . We equip  $S^m(T^*\Sigma)$  with the semi-norms

$$\|a\|_{m, \alpha, \beta} = \sup_{x \in \Sigma} \|a_x\|_{m, \alpha, \beta}.$$

Similarly we denote by  $S_{\text{ph}}^m(T^*\Sigma)$  the space of  $a \in S^m(T^*\Sigma)$  such that for each  $x \in \Sigma$ ,  $a_x \in S_{\text{ph}}^m(T^*B_n(0, 1))$  and the family  $\{a_x\}_{x \in \Sigma}$  is bounded in  $S_{\text{ph}}^m(T^*B_n(0, 1))$ . We equip  $S_{\text{ph}}^m(T^*\Sigma)$  with the semi-norms

$$\|a\|_{m, i, p, \alpha, \beta} = \sup_{x \in \Sigma} \|a_x\|_{m, i, p, \alpha, \beta}.$$

where  $\|\cdot\|_{m, i, p, \alpha, \beta}$  are the semi-norms defining the topology of  $S_{\text{ph}}^m(T^*B_n(0, 1))$ .

We also set  $S_{(\text{ph})}^\infty(T^*\Sigma) = \bigcup_{m \in \mathbb{R}} S_{(\text{ph})}^m(T^*\Sigma)$ .

The definition of  $S^m(T^*\Sigma)$ ,  $S_{\text{ph}}^m(T^*\Sigma)$  and their Fréchet space topologies are independent on the choice of the family  $\{\psi_x\}_{x \in \Sigma}$  of good chart diffeomorphisms.

The notation  $a \simeq \sum_{i \in \mathbb{N}} a_{m-i}$  for  $a_{m-i} \in S_{\text{ph}}^{m-i}(T^*\Sigma)$  is defined as before. If  $a \in S_{\text{ph}}^m(T^*\Sigma)$ , we denote again by  $a_{\text{pr}}$  the image of  $a$  in  $S_{\text{ph}}^m(T^*\Sigma)/S_{\text{ph}}^{m-1}(T^*\Sigma)$ .

The spaces  $C_{(b)}^\infty(\mathbb{R}; S_{(\text{ph})}^m(T^*\Sigma))$ ,  $S^\delta(\mathbb{R}; S_{(\text{ph})}^m(T^*\Sigma))$  are defined as in 3.3.2 and equipped with their natural Fréchet space topologies.

3.4. **Sobolev spaces and smoothing operators.** Using the metric  $h$  one defines the Sobolev spaces  $H^m(\Sigma)$  as follows.

**Definition 3.5.** For  $s \in \mathbb{R}$  the Sobolev space  $H^s(\Sigma)$  is:

$$H^s(\Sigma) := \langle -\Delta_h \rangle^{-s/2} L^2(\Sigma),$$

with its natural Hilbert space topology, where  $-\Delta_h$  is the Laplace-Beltrami operator on  $(\Sigma, h)$ , strictly speaking the closure of its restriction to  $C_c^\infty(\Sigma)$ .

We further set

$$H^\infty(\Sigma) := \bigcap_{m \in \mathbb{Z}} H^m(\Sigma), \quad H^{-\infty}(\Sigma) := \bigcup_{m \in \mathbb{Z}} H^m(\Sigma),$$

equipped with their Fréchet space topologies.

We denote by  $\mathcal{W}^{-\infty}(\Sigma)$  the Fréchet space  $B(H^{-\infty}(\Sigma), H^\infty(\Sigma))$  with its Fréchet space topology, given by the semi-norms

$$\|a\|_m = \|a\|_{B(H^{-m}(\Sigma), H^m(\Sigma))}, \quad m \in \mathbb{N}.$$

This allows us to define  $C_{(b)}^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ ,  $S^\delta(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ , the latter consisting of operator-valued functions  $a(t)$  such that

$$\|\partial_t^\gamma a(t)\|_m \in O(\langle t \rangle^{\delta-\gamma}), \quad \forall \gamma, m \in \mathbb{N}.$$

**3.5. Pseudodifferential operators.** Starting from the well-known Weyl quantization on open subsets of  $\mathbb{R}^d$ , one constructs a quantization map  $\text{Op}$  for symbols in  $S^m(T^*\Sigma)$  using a good chart covering of  $\Sigma$  and good chart diffeomorphisms. More precisely let  $\{U_i, \psi_i\}_{i \in \mathbb{N}}$  be a good chart covering of  $M$  and

$$\sum_{i \in \mathbb{N}} \chi_i^2 = \mathbf{1}$$

a subordinate good partition of unity, see Subsect. 3.1. If

$$(\psi_i^{-1})^* dg =: m_i dx,$$

we set

$$\begin{aligned} T_i : L^2(U_i, dg) &\rightarrow L^2(B_n(0, 1), dx), \\ u &\mapsto m_i^{\frac{1}{2}} (\psi_i^{-1})^* u, \end{aligned}$$

so that  $T_i : L^2(U_i, dg) \rightarrow L^2(B_n(0, 1), dx)$  is unitary. We then fix an extension map

$$E : S_{\text{ph}}^m(T^*B_d(0, 1)) \rightarrow S_{\text{ph}}^m(T^*\mathbb{R}^d).$$

**Definition 3.6.** Let  $a = a(t) \in C^\infty(\mathbb{R}; S_{\text{ph}}^m(T^*M))$ . We set

$$\text{Op}(a) := \sum_{i \in \mathbb{N}} \chi_i T_i^* \circ \text{Op}^w(Ea_i) \circ T_i \chi_i,$$

where  $a_i \in S_{\text{ph}}^m(T^*B_d(0, 1))$  is the push-forward of  $a|_{T^*U_i}$  by  $\psi_i$  and  $\text{Op}^w$  is the Weyl quantization.

If  $\text{Op}'$  is another such quantization map for different choices of  $U_i, \psi_i, \chi_i$  and  $E$  then

$$S_{\text{ph}}^m(T^*\Sigma) \rightarrow \mathcal{W}^{-\infty}(\Sigma)$$

$$\text{Op} - \text{Op}' : C_{(b)}^\infty(\mathbb{R}; S_{\text{ph}}^m(T^*\Sigma)) \rightarrow C_{(b)}^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma)),$$

$$S^\delta(\mathbb{R}; S_{\text{ph}}^m(T^*\Sigma)) \rightarrow S^\delta(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma)),$$

are bounded. Then one defines the classes

$$\Psi^m(\Sigma) := \text{Op}(S_{\text{ph}}^m(T^*\Sigma)) + \mathcal{W}^{-\infty}(\Sigma),$$

$$C_{(b)}^\infty(\mathbb{R}; \Psi^m(\Sigma)) := \text{Op}(C_{(b)}^\infty(\mathbb{R}; S_{\text{ph}}^m(T^*\Sigma))) + C_{(b)}^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma)),$$

$$S^\delta(\mathbb{R}; \Psi^m(\Sigma)) := \text{Op}(S^\delta(\mathbb{R}; S_{\text{ph}}^m(T^*\Sigma)) + S^\delta(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma)).$$

Thanks to including the ideal  $\mathcal{W}^{-\infty}(\Sigma)$  of smoothing operators, the so-obtained pseudodifferential classes are stable under composition, for example  $\Psi^{m_1}(\Sigma) \circ \Psi^{m_2}(\Sigma) \subset \Psi^{m_1+m_2}(\Sigma)$ .



Note that  $S^\delta(\mathbb{R}; \Psi^m(\Sigma)) = \langle t \rangle^\delta S^0(\mathbb{R}; \Psi^m(\Sigma))$  and similarly with  $\Psi^m(\Sigma)$  replaced by  $\mathcal{W}^{-\infty}(\Sigma)$  so in what follows one can assume without loss of generality that  $\delta = 0$ .

The spaces  $\mathcal{W}^{-\infty}(\Sigma)$ ,  $C_{(b)}^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$  and  $S^\delta(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$  have natural Fréchet space topologies. If necessary we equip the spaces  $\Psi^m(\Sigma)$ ,  $C_{(b)}^\infty(\mathbb{R}; \Psi^m(\Sigma))$  and  $S^\delta(\mathbb{R}; \Psi^m(\Sigma))$  with the quotient topology obtained from the map:

$$(c, R) \mapsto \text{Op}(c) + R$$

between the appropriate spaces.

If  $a \in \Psi^m(\Sigma)$ , the *principal symbol*  $\sigma_{\text{pr}}(a) \in S_{\text{h}}^m(T^*\Sigma)$  is defined in analogy to the case  $\Sigma = \mathbb{R}^d$ . The operator  $a$  is *elliptic* if there exists  $C > 0$  such that

$$(3.2) \quad |\sigma_{\text{pr}}(a)| \geq C|k|^m, \quad |k| \geq 1,$$

uniformly in the chart open sets. If  $a \in C^\infty(\mathbb{R}; \Psi^m(\Sigma))$  we say that  $a$  is *elliptic* if  $a(t)$  is elliptic for all  $t \in \mathbb{R}$  and the constant  $C$  in (3.2) is locally uniform in  $t$ . For  $a \in C_{(b)}^\infty(\mathbb{R}; \Psi^m(\Sigma))$  or  $S^0(\mathbb{R}; \Psi^m(\Sigma))$  there is also a corresponding notion of ellipticity, where we require  $C$  to be uniform in  $t$ .

As shown in [GOW], the pseudodifferential classes  $\Psi^m(\Sigma)$  fit into the general framework of Ammann, Lauter, Nistor and Vasy [ALNV], and consequently they have many convenient properties that generalize well-known facts for say, pseudodifferential operators on closed manifolds, such as the existence of complex powers for elliptic, bounded from below operators.

We state below a particular case of *Seeley's theorem* for real powers, partly proved in [GOW, Sect. 5], based on a general result from [ALNV].

**Theorem 3.7** (Seeley's theorem). *Let  $a \in C^\infty(\mathbb{R}; \Psi^m(\Sigma))$  be elliptic, selfadjoint with  $a(t) \geq c(t)\mathbf{1}$ ,  $c(t) > 0$ . Then  $a^\alpha \in C^\infty(\mathbb{R}; \Psi^{m\alpha}(\Sigma))$  for any  $\alpha \in \mathbb{R}$  and  $\sigma_{\text{pr}}(a^\alpha)(t) = \sigma_{\text{pr}}(a(t))^\alpha$ .*

*The same result holds replacing  $C^\infty(\mathbb{R}; \Psi^m(\Sigma))$  by  $C_{(b)}^\infty(\mathbb{R}; \Psi^m(\Sigma))$  or  $S^0(\mathbb{R}; \Psi^m(\Sigma))$  if one assumes  $a(t) \geq c_0\mathbf{1}$  for  $c_0 > 0$ .*

**Proof.** The  $C_{(b)}^\infty$  cases are proved in [GOW, Thm. 5.12], by checking that the general framework of [ALNV] applies to these two situations. The  $S^\delta$  case can be proved similarly. The only point deserving special care is the *spectral invariance* of the ideal  $S^\delta(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ , which we explain in some detail. Let  $r_{-\infty} \in S^0(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ , considered as a bounded operator on  $L^2(\mathbb{R}_t \times \Sigma_x)$ . The spectral invariance property is the fact that if  $\mathbf{1} - r_{-\infty}$  is invertible in  $B(L^2(\mathbb{R}_t \times \Sigma_x))$  then  $(\mathbf{1} - r_{-\infty})^{-1} = \mathbf{1} - r_{1,-\infty}$  for  $r_{1,-\infty} \in S^0(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ . This can be however proved exactly as in [GOW, Lemma 5.5].  $\square$

**3.6. Egorov's theorem.** If  $b(t) \in C^\infty(\mathbb{R}; \Psi^m(\Sigma))$  (or more generally, if  $b(t)$  is a square matrix consisting of elements of  $C^\infty(\mathbb{R}; \Psi^m(\Sigma))$  and  $H^{-\infty}(\Sigma)$  is tensorized by powers of  $\mathbb{C}$  accordingly) we denote by

$$\mathcal{U}_b(t, s) : H^{-\infty}(\Sigma) \rightarrow H^{-\infty}(\Sigma)$$

the evolution generated by  $b(t)$ , i.e. the Cauchy evolution of  $\bar{\partial}_t - ib(t)$ , or put in other words, the unique solution (if it exists) of the system

$$(3.3) \quad \begin{cases} \frac{\partial}{\partial t} \mathcal{U}_b(t, s) = ib(t)\mathcal{U}_b(t, s), \\ \frac{\partial}{\partial s} \mathcal{U}_b(t, s) = -i\mathcal{U}_b(t, s)b(s), \\ \mathcal{U}_b(t, s) = \mathbf{1}. \end{cases}$$

The existence of  $\mathcal{U}_b(t, s)$  can typically be established if  $b(t)$  defines a differentiable family of self-adjoint operators on a Hilbert space, or a small perturbation of such family. Specifically,

consider  $b(t) \in C^\infty(\mathbb{R}; \Psi^1(\Sigma))$  such that  $b(t) = b_1(t) + b_0(t)$  with  $b_i(t) \in C^\infty(\mathbb{R}; \Psi^i(\Sigma))$  and:

(E)  $b_1(t)$  is elliptic and bounded from below on  $H^\infty(\Sigma)$ , locally uniformly in  $t$ .

Using [ALNV, Prop. 2.2] it follows that  $b(t)$  is closed with domain  $\text{Dom } b(t) = H^1(\Sigma)$ . Moreover the map  $\mathbb{R} \ni t \mapsto b(t) \in B(H^1(\Sigma), L^2(\Sigma))$  is norm continuous. It follows that we can define  $\mathcal{U}_b(t, s)$ , using for instance [RS, Thm. X.70]. In the present setup one can prove a result known generally as Egorov's theorem, we refer to [GOW] for the details and proofs.

**Lemma 3.8.** *Assume (E). Then:*

- (1)  $\mathcal{U}_b(t, s) \in B(H^m(\Sigma))$  for  $m \in \mathbb{R}$  or  $m = \pm\infty$ .
- (2) if  $r \in \mathcal{W}^{-\infty}(\Sigma)$  then  $\mathcal{U}_b(t, s)r, r\mathcal{U}_b(s, t) \in C^\infty(\mathbb{R}_{t,s}^2, \mathcal{W}^{-\infty}(\Sigma))$ .
- (3) if moreover  $b(t) \in S^0(\mathbb{R}; \Psi^1(\Sigma))$  and  $b(t) - b^*(t) \in S^{-1-\delta}(\mathbb{R}; \Psi^0(\Sigma))$  for  $\delta > 0$  then  $\mathcal{U}_b(t, s)$  is uniformly bounded in  $B(L^2(\Sigma))$ .

**Theorem 3.9** (Egorov's theorem). *Let  $c \in \Psi^m(\Sigma)$  and  $b(t)$  satisfying (E). Then*

$$c(t, s) := \mathcal{U}_b(t, s)c\mathcal{U}_b(s, t) \in C^\infty(\mathbb{R}_{t,s}^2, \Psi^m(\Sigma)).$$

Moreover

$$\sigma_{\text{pr}}(c)(t, s) = \sigma_{\text{pr}}(c) \circ \Phi(s, t),$$

where  $\Phi(t, s) : T^*\Sigma \rightarrow T^*\Sigma$  is the flow of the time-dependent Hamiltonian  $\sigma_{\text{pr}}(b)(t)$ .

**3.7. Scattering pseudodifferential calculus on  $\mathbb{R}^d$ .** In this subsection we consider a smaller class of pseudodifferential calculus for  $\Sigma = \mathbb{R}^d$  which is the natural class on asymptotically Minkowski spacetimes. For  $m, \delta \in \mathbb{R}$  we denote by  $S_{\text{std}}^{m, \delta}(\mathbb{R}; T^*\mathbb{R}^d)$  the space of functions  $a(t, x, k)$  such that

$$\partial_t^\gamma \partial_x^\alpha \partial_k^\beta a(t, x, k) \in O(\langle t \rangle + \langle x \rangle)^{\delta - \gamma - |\alpha|} \langle k \rangle^{m - |\beta|}, \quad \gamma \in \mathbb{N}, \quad \alpha, \beta \in \mathbb{N}^d.$$

The subscript *std* refers to the space-time decay properties of symbols in  $(t, x)$ . The subspace of symbols which are poly-homogeneous in  $k$  will be denoted by  $S_{\text{std,ph}}^{m, \delta}(\mathbb{R}; T^*\mathbb{R}^d)$ .

We denote by  $\mathcal{W}_{\text{std}}^{-\infty}(\mathbb{R}; \mathbb{R}^d)$  the space of operator-valued functions  $a(t)$  such that

$$\|(D_x^2 + x^2)^m \partial_t^\gamma a(t) (D_x^2 + x^2)^m\|_{B(L^2(\mathbb{R}^d))} \in O(\langle t \rangle^{-n}), \quad \forall m, n \in \mathbb{N}.$$

Finally we set:

$$\Psi_{\text{std}}^{m, \delta}(\mathbb{R}; \mathbb{R}^d) := \text{Op}^w(S_{\text{std,ph}}^{m, \delta}(\mathbb{R}; T^*\mathbb{R}^d)) + \mathcal{W}_{\text{std}}^{-\infty}(\mathbb{R}; \mathbb{R}^d),$$

where  $\text{Op}^w$  is the Weyl quantization.

Omitting the variable  $t$  in the above conditions, we also obtain classes of (time-independent) symbols and pseudodifferential operators on  $\mathbb{R}^d$ , which will be denoted by  $S_{\text{sd}}^{m, \delta}(T^*\mathbb{R}^d)$ ,  $\Psi_{\text{sd}}^{m, \delta}(\mathbb{R}^d)$  and  $\mathcal{W}_{\text{sd}}^{-\infty}(\mathbb{R}^d)$ , where the subscript *sd* refers to space decay properties of the symbols or operators.

The classes  $\Psi_{\text{sd}}^{m, \delta}(\mathbb{R}^d)$  are the well-known 'scattering pseudodifferential operators', see e.g. [Co, Pa, Sh1].

We will only need the definitions of the principal symbol and of ellipticity on  $\Psi_{\text{sd}}^{m, 0}(\mathbb{R}^d)$  resp.  $\Psi_{\text{std}}^{m, 0}(\mathbb{R}; \mathbb{R}^d)$ , which are taken here to be identical<sup>10</sup> with the ones in  $\Psi^2(\mathbb{R}^2)$ , resp.  $C_b^\infty(\mathbb{R}; \Psi^2(\mathbb{R}^d))$ . Seeley's theorem is still valid for the  $\Psi_{\text{std}}^{m, 0}(\mathbb{R}; \mathbb{R}^d)$  classes, proved similarly as before by a reduction to [ALNV], see the arguments in [GOW, Subsect. 5.3].

**Theorem 3.10.** *Let  $a \in \Psi_{\text{std}}^{m, 0}(\mathbb{R}; \mathbb{R}^d)$  be elliptic, selfadjoint with  $a(t) \geq c_0 \mathbf{1}$  with  $c_0 > 0$ . Then  $a^\alpha \in C_{(b)}^\infty(\mathbb{R}; \Psi^{m\alpha}(\Sigma))$  for any  $\alpha \in \mathbb{R}$  and  $\sigma_{\text{pr}}(a^\alpha)(t) = \sigma_{\text{pr}}(a(t))^\alpha$ .*

<sup>10</sup>Thus, we do *not* consider here ellipticity in the sense of scattering pseudodifferential calculus.

**3.8. Some auxiliary results.** For the sake of unifying the notation with the classes  $\Psi_{\text{std}}^{m,\delta}(\mathbb{R}; \mathbb{R}^d)$  introduced in Subsect. 3.7 we set for  $(\Sigma, h)$  of bounded geometry:

$$\Psi_{\text{td}}^{m,\delta}(\mathbb{R}; \Sigma) := S^\delta(\mathbb{R}; \Psi^m(\Sigma)).$$

for pseudodifferential operator classes with time decay (td) of the symbols. When writing  $\Psi_{\text{std}}^{m,\delta}(\mathbb{R}; \Sigma)$  it is assumed implicitly that  $\Sigma = \mathbb{R}^d$ .

**3.8.1. Difference of fractional powers.** We now state an auxiliary result about fractional powers of elliptic operators that will be needed later on.

**Proposition 3.11.** *Let  $a_i \in \Psi_{(*)}^{2,0}(\mathbb{R}; \Sigma)$  for  $* = \text{td}, \text{std}$ ,  $i = 1, 2$  elliptic with  $a_i = a_i^*$  and  $a_i(t) \geq c_0 \mathbf{1}$  for some  $c_0 > 0$ . Assume that  $a_1 - a_2 \in \Psi_{(*)}^{k,-\delta}(\mathbb{R}; \Sigma)$  with  $\delta > 0$ ,  $k = 0, 1, 2$ . Then for each  $\alpha \in \mathbb{R}$  one has:*

$$a_1^\alpha - a_2^\alpha \in \Psi_{(*)}^{2(\alpha-1)+k,-\delta}(\mathbb{R}; \Sigma).$$

Prop. 3.11 is proved in Subsect. A.1.

**3.8.2. Resummation of symbols.** We now examine the resummation of symbols. In the (td) case one can think of this as a statement about the uniform symbol classes on  $\mathbb{R}^d$ , after applying a chart diffeomorphism.

We denote  $\Psi_{(*)}^{-\infty,-\delta}(\mathbb{R}; \Sigma) := \bigcap_{m \in \mathbb{R}} \Psi_{(*)}^{m,-\delta}(\mathbb{R}; \Sigma)$  for  $* = \text{td}, \text{std}$ .

**Lemma 3.12.** *Let  $\delta \in \mathbb{R}$  and let  $(m_j)$  be a real sequence decreasing to  $-\infty$ . Then if  $a_j \in \Psi_{(*)}^{m_j,\delta}(\mathbb{R}; \Sigma)$  for  $* = \text{td}, \text{std}$  there exists  $a \in \Psi_{(*)}^{m_0,\delta}(\mathbb{R}; \Sigma)$ , unique modulo  $\Psi_{(*)}^{-\infty,-\delta}(\mathbb{R}; \Sigma)$ , such that*

$$a \sim \sum_{j=0}^{\infty} a_j, \text{ i.e. } a - \sum_{j=0}^N a_j \in \Psi_{(*)}^{m_{N+1},\delta}(\mathbb{R}; \Sigma), \quad \forall N \in \mathbb{N}.$$

**Proof.** By introducing the new variable  $s = \int_0^t \langle \sigma \rangle^{-1} d\sigma$  (so that  $\langle t \rangle \partial_t = \partial_s$ ) and putting the extra variable  $s$  together with the  $x$  variables we can reduce ourselves to the situation covered by the standard proof (see e.g. [Sh3, Prop. 3.5]).  $\square$

#### 4. PARAMETRIX FOR THE CAUCHY EVOLUTION AND HADAMARD STATES

**4.1. Model Klein-Gordon equation.** In the present section we outline the approximate diagonalization and the parametrix construction that are used in [GOW] to construct covariances of generic Hadamard states. We fix a  $d$ -dimensional manifold  $\Sigma$  equipped with a reference Riemannian metric  $k$  such that  $(\Sigma, k)$  is of bounded geometry. We equip  $M = \mathbb{R} \times \Sigma$ , whose elements are denoted by  $x = (t, x)$ , with a Lorentzian metric  $g$  and a real function  $V$  such that:

$$(4.1) \quad \begin{aligned} g &= -dt^2 + h_{ij}(t, x) dx^i dx^j, \\ h &\in C^\infty(\mathbb{R}, \text{BT}_2^0(\Sigma, k)), \quad h^{-1} \in C^\infty(\mathbb{R}; \text{BT}_0^2(\Sigma, k)), \\ V &\in C^\infty(\mathbb{R}; \text{BT}_0^0(\Sigma, k)). \end{aligned}$$

Although the first assumption may look restrictive, we will give in Subsects. 5.2, 7.3 a reduction procedure that will allow us to treat more general cases.

The Klein-Gordon operator  $P = -\square_g + V$  equals

$$(4.2) \quad \begin{aligned} P &= |h|^{-\frac{1}{2}} \bar{\partial}_t |h|^{\frac{1}{2}} \bar{\partial}_t - |h|^{-\frac{1}{2}} \bar{\partial}_i h^{ij} |h|^{\frac{1}{2}} \bar{\partial}_j + V \\ &= \bar{\partial}_t^2 + r(t, x) \bar{\partial}_t + a(t, x, \bar{\partial}_x), \end{aligned}$$

where

$$a(t, \mathbf{x}, \overline{\partial}_{\mathbf{x}}) = -|h|^{-\frac{1}{2}} \overline{\partial}_i h^{ij} |h|^{\frac{1}{2}} \overline{\partial}_j + V(t, \mathbf{x})$$

is formally self-adjoint with respect to the  $t$ -dependent  $L^2(\Sigma, |h|^{\frac{1}{2}} dx)$ -inner product and

$$r(t, \mathbf{x}) = |h|^{-\frac{1}{2}} \partial_t (|h|^{\frac{1}{2}})(t, \mathbf{x}).$$

Note that the above function is closely related to the extrinsic curvature of  $\Sigma$  in  $M$ .

In the sequel we will often abbreviate  $a(t, \mathbf{x}, \overline{\partial}_{\mathbf{x}})$  by  $a(t)$  or  $a$ .

**4.2. Construction of parametrix.** Following [GOW] we now explain how one obtains a parametrix for the Cauchy evolution (and a splitting of it) by means of an approximate time-dependent diagonalization. We will then adapt it to the setup of scattering theory.

The first step consists of observing that the Klein-Gordon equation  $(\partial_t^2 + r(t)\partial_t + a(t))\phi(t) = 0$  is equivalent to

$$(4.3) \quad \mathbf{i}^{-1} \partial_t \psi(t) = H(t) \psi(t), \quad \text{where } H(t) = \begin{pmatrix} 0 & \mathbf{1} \\ a(t) & ir(t) \end{pmatrix},$$

by setting

$$(4.4) \quad \psi(t) = \begin{pmatrix} \phi(t) \\ \mathbf{i}^{-1} \partial_t \phi(t) \end{pmatrix}.$$

Let us denote by  $\mathcal{U}(s, t)$  the evolution generated by  $H(t)$ , cf. (3.3). Recall that on Cauchy data on  $\Sigma_s = \{s\} \times \Sigma$ , we have a symplectic form induced from an operator  $G(s)$ , defined by:

$$G = (\varrho_s G)^* \circ G(s) \circ (\varrho_s G).$$

Here the formal adjoint will be always taken wrt. the  $L^2(\Sigma, |h|^{\frac{1}{2}} dx)$ -inner product. We have also introduced the hermitian operator  $q(s) = \mathbf{i}G(s)$ . It is well known that with these choices,  $q(s)$  equals specifically

$$(4.5) \quad q(s) = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix},$$

in particular it does not depend on  $s$ . Furthermore,

$$(4.6) \quad \mathcal{U}^*(t, s) q(s) \mathcal{U}(t, s) = q(t),$$

(the Cauchy evolution is symplectic).

**4.2.1. Riccati equation.** The approximate diagonalization of  $\mathcal{U}(s, t)$  will be based on solving the Riccati equation

$$(4.7) \quad \mathbf{i} \partial_t b - b^2 + a + irb = 0,$$

modulo smoothing terms, where the unknown is  $b(t) \in C^\infty(\mathbb{R}; \Psi^1(\Sigma))$ . By repeating the arguments in [GW1, GW2] this can be solved modulo terms in  $C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ . Concretely, supposing for the moment that  $a(t) \geq c(t)\mathbf{1}$  for  $c(t) > 0$ , one sets  $\epsilon = a^{\frac{1}{2}}$ ,  $b = \epsilon + b_0$  and obtains the equations:

$$b_0 = \frac{\mathbf{i}}{2} (\epsilon^{-1} \partial_t \epsilon + \epsilon^{-1} r \epsilon) + F(b_0),$$

$$F(b_0) = \frac{1}{2} \epsilon^{-1} (\mathbf{i} \partial_t b_0 + [\epsilon, b_0] + irb_0 - b_0^2).$$

These can be solved by substituting a poly-homogeneous expansion of the symbol of  $b_0$ , yielding an approximate solution of (4.7) in the sense that

$$(4.8) \quad \mathbf{i} \partial_t b - b^2 + a + irb = r_{-\infty} \in C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma)).$$

Set

$$(4.9) \quad b^+ = b, \quad b^- = -b^*.$$

Taking the adjoint of the (4.8) with respect to the  $t$ -dependent inner product  $L^2(\Sigma, |h|^{\frac{1}{2}} dx)$  and using that

$$(\partial_t b)^* = \partial_t(b^*) + rb^* - b^*r,$$

we obtain

$$(4.10) \quad i\partial_t b^\pm - b^{\pm 2} + a + irb^\pm = r_\pm^\pm,$$

with  $r_{-\infty}^+ = r_{-\infty}$ ,  $r_{-\infty}^- = r_{-\infty}^* \in C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ .

In general we can, using the locally uniform ellipticity of  $a(t)$ , find a cutoff function  $\chi \in C_c^\infty(\mathbb{R})$  such that  $a(t) + \chi(a(t)) \geq c(t)\mathbf{1}$  for  $c(t)$  as above. Since  $\chi(a(t))$  is a smoothing operator, replacing  $a(t)$  by  $a(t) + \chi(a(t))$  is a harmless modification.

A redefinition of  $b(t)$  involving a cutoff in low frequencies as in [GW2, GOW] gives then control of the norm sufficient to obtain in addition

$$(4.11) \quad (b^+(t) - b^-(t))^{-1} \geq C(t)\epsilon(t)^{-1}$$

for some  $C(t) > 0$ , while keeping the property that  $b^\pm(t) = \pm\epsilon(t) + C^\infty(\mathbb{R}; \Psi^0(\Sigma))$ , and with (4.10) still valid for some  $r_\pm^\pm \in C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ .

Observe now that the Riccati equation (4.10) implies the following approximate factorization of the Klein-Gordon operator:

$$(4.12) \quad (\bar{\partial}_t + ib^\pm(t) + r(t)) \circ (\bar{\partial}_t - ib^\pm(t)) = \bar{\partial}_t^2 + r\bar{\partial}_t + a - r_{-\infty}^\pm.$$

The benefits of having such a factorization were already recognized by Junker and Schrohe [Ju, JS] in the context of Hadamard states (although it was obtained only in the special case of FRLW spacetimes with compact Cauchy hypersurface). Here we use (4.12) to diagonalize (4.3) by setting

$$\tilde{\psi}(t) := \begin{pmatrix} \bar{\partial}_t - ib^-(t) \\ \bar{\partial}_t - ib^+(t) \end{pmatrix} \phi(t).$$

A direct computation yields then  $\tilde{\psi}(t) = S^{-1}(t)\psi(t)$  with

$$(4.13) \quad S^{-1}(t) = i \begin{pmatrix} -b^-(t) & \mathbf{1} \\ -b^+(t) & \mathbf{1} \end{pmatrix}, \quad S(t) = i^{-1} \begin{pmatrix} \mathbf{1} & -\mathbf{1} \\ b^+(t) & -b^-(t) \end{pmatrix} (b^+(t) - b^-(t))^{-1},$$

where well-definiteness and invertibility of  $S(t)$  rely on the fact that  $b^+(t) - b^-(t)$  is invertible by (4.11). We obtain from (4.12) that

$$\begin{aligned} \begin{pmatrix} \bar{\partial}_t + ib^- + r & 0 \\ 0 & \bar{\partial}_t + ib^+ + r \end{pmatrix} \tilde{\psi}(t) &= \begin{pmatrix} \bar{\partial}_t^2 + a + r\bar{\partial}_t - r_{-\infty}^- \\ \bar{\partial}_t^2 + a + r\bar{\partial}_t - r_{-\infty}^+ \end{pmatrix} \phi(t) \\ &= \begin{pmatrix} r_{-\infty}^- & 0 \\ r_{-\infty}^+ & 0 \end{pmatrix} S(t)\tilde{\psi}(t) = i^{-1} \begin{pmatrix} r_{-\infty}^- & -r_{-\infty}^- \\ r_{-\infty}^+ & -r_{-\infty}^+ \end{pmatrix} (b^+ - b^-)^{-1} \tilde{\psi}(t). \end{aligned}$$

Therefore,  $\tilde{\psi}(t)$  solves a diagonal matrix equation modulo smooth terms. More precisely, we have  $\tilde{\psi}(t) = \mathcal{U}_B(t, s)\tilde{\psi}(s)$  for

$$(4.14) \quad B(t) = \tilde{B}(t) + R_{-\infty}(t),$$

$$(4.15) \quad \tilde{B}(t) = \begin{pmatrix} -b^- + ir & 0 \\ 0 & -b^+ + ir \end{pmatrix}, \quad R_{-\infty}(t) = - \begin{pmatrix} r_{-\infty}^- & -r_{-\infty}^- \\ r_{-\infty}^+ & -r_{-\infty}^+ \end{pmatrix} (b^+ - b^-)^{-1},$$

Ultimately, we can thus conclude that

$$(4.16) \quad \mathcal{U}(t, s) = S(t)\mathcal{U}_B(t, s)S(s)^{-1}.$$

**4.3. Improved approximate diagonalization.** It is convenient to modify  $S(t)$  to obtain a simple formula for the symplectic form  $S^*(t)q(t)S(t)$  preserved by the almost diagonalized evolution. Namely, setting

$$(4.17) \quad \begin{aligned} T(t) &:= S(t)(b^+ - b^-)^{\frac{1}{2}}(t) = i^{-1} \begin{pmatrix} \mathbf{1} & -\mathbf{1} \\ b^+ & -b^- \end{pmatrix} (b^+ - b^-)^{-\frac{1}{2}}, \\ T^{-1}(t) &= i(b^+ - b^-)^{-\frac{1}{2}} \begin{pmatrix} -b^- & \mathbf{1} \\ -b^+ & \mathbf{1} \end{pmatrix}, \end{aligned}$$

we find that for  $q(t)$  defined in (4.5) one has:

$$T^*(t)q(t)T(t) = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} =: q^{\text{ad}}.$$

We define

$$(4.18) \quad \mathcal{U}(t, s) =: T(t)\mathcal{U}^{\text{ad}}(t, s)T(s)^{-1},$$

and we obtain that  $\mathcal{U}^{\text{ad}}(t, s)^*q^{\text{ad}}\mathcal{U}^{\text{ad}}(t, s) = q^{\text{ad}}$ , and the generator of  $\{\mathcal{U}^{\text{ad}}(t, s)\}_{t, s \in \mathbb{R}}$  is:

$$(4.19) \quad \begin{aligned} H^{\text{ad}}(t) &= (b^+ - b^-)^{-\frac{1}{2}}B(t)(b^+ - b^-)^{\frac{1}{2}} - i\partial_t(b^+ - b^-)^{-\frac{1}{2}}(b^+ - b^-)^{\frac{1}{2}} \\ &= \begin{pmatrix} -b^- + r_b^- & 0 \\ 0 & -b^+ + r_b^+ \end{pmatrix} - (b^+ - b^-)^{-\frac{1}{2}} \begin{pmatrix} r_{-\infty}^- & -r_{-\infty}^- \\ r_{-\infty}^+ & -r_{-\infty}^+ \end{pmatrix} (b^+ - b^-)^{-\frac{1}{2}}, \end{aligned}$$

where  $r_{-\infty}^{\pm} \in C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$  are the remainder terms from (4.10), and

$$(4.20) \quad r_b^{\pm} = ir + [(b^+ - b^-)^{-\frac{1}{2}}, b^{\pm}] - i\partial_t(b^+ - b^-)^{-\frac{1}{2}}(b^+ - b^-)^{\frac{1}{2}} \in \Psi^0(\Sigma).$$

This way, denoting by  $H^{\text{d}}$  the diagonal part of  $H^{\text{ad}}(t)$  we have, using that  $H^{\text{ad}}(t)^*q^{\text{ad}} = q^{\text{ad}}H^{\text{ad}}(t)$ :

$$H^{\text{d}}(t) = H^{\text{d}*}(t), \quad H^{\text{d}}(t) = \begin{pmatrix} \epsilon^+(t) & 0 \\ 0 & \epsilon^-(t) \end{pmatrix},$$

where

$$\epsilon^{\pm} = -b^{\mp} + r_b^{\mp} + C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma)),$$

and  $H^{\text{ad}}(t) = H^{\text{d}}(t) + V_{-\infty}^{\text{ad}}(t)$ , where  $V_{-\infty}^{\text{ad}}(t) \in C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma) \otimes B(\mathbb{C}^2))$ . The evolution  $\mathcal{U}^{\text{d}}(t, s)$  generated by  $H^{\text{d}}(t)$  is diagonal, in fact:

$$(4.21) \quad \mathcal{U}^{\text{d}}(t, s) = \begin{pmatrix} \mathcal{U}_{\epsilon^+}(t, s) & 0 \\ 0 & \mathcal{U}_{\epsilon^-}(t, s) \end{pmatrix}.$$

Moreover:

$$(4.22) \quad \begin{aligned} \mathcal{U}(t, s) &= T(t)\mathcal{U}^{\text{ad}}(t, s)T(s)^{-1} \\ &= T(t)\mathcal{U}^{\text{d}}(t, s)T(s)^{-1} + C^\infty(\mathbb{R}^2; \mathcal{W}^{-\infty}(\Sigma)). \end{aligned}$$

This is shown by an ‘interaction picture’ argument explained in detail in [GOW], we omit the proof here.

**Remark 4.1.** *One easily sees that  $S(t)$  is an isomorphism from  $L^2(\Sigma) \oplus L^2(\Sigma)$  to  $H^1(\Sigma) \oplus L^2(\Sigma)$  (the so-called energy space of Cauchy data of (4.3)), while  $T(t)$  is an isomorphism from  $L^2(\Sigma) \oplus L^2(\Sigma)$  to  $H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$  (this is the charge space that appears naturally in the quantization of the Klein-Gordon equation).*

4.4. **Splitting of the parametrix and of the Cauchy evolution.** Let us set

$$(4.23) \quad \pi^+ = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & 0 \end{pmatrix}, \quad \pi^- = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix}.$$

Since  $\mathcal{U}^d(t, s)$  is diagonal we have:

$$\mathcal{U}^d(t, s) = \mathcal{U}^d(t, s)\pi^+ + \mathcal{U}^d(t, s)\pi^-,$$

with  $\mathcal{U}^d(t, s)\pi^\pm$  propagating with wave front set contained in  $\mathcal{N}^\pm$  (this follows from  $b^\pm$  being  $\pm\epsilon$  modulo terms of lower order). This suggests that at least modulo smoothing terms, the splitting of  $\mathcal{U}(t, s)$  at time  $s$  should be given by a pair of operators  $c_{\text{ref}}^\pm(s)$  defined as follows. We first fix a reference time  $t_0 \in \mathbb{R}$ .

**Definition 4.2.** *We set:*

$$c_{\text{ref}}^\pm(t_0) := T(t_0)\pi^\pm T^{-1}(t_0) = \begin{pmatrix} \mp(b^+ - b^-)^{-1}b^\mp & \pm(b^+ - b^-)^{-1} \\ \mp b^\pm(b^+ - b^-)^{-1}b^- & \pm b^\pm(b^+ - b^-)^{-1} \end{pmatrix}(t_0).$$

Then  $c_{\text{ref}}^\pm(t_0)$  is a  $2 \times 2$  matrix of pseudodifferential operators and

$$c_{\text{ref}}^\pm(t_0)^2 = c_{\text{ref}}^\pm(t_0), \quad c_{\text{ref}}^+(t_0) + c_{\text{ref}}^-(t_0) = \mathbf{1}.$$

We set:

$$(4.24) \quad \mathcal{U}^\pm(t, s) := \mathcal{U}(t, t_0)c_{\text{ref}}^\pm(t_0)\mathcal{U}(t_0, s),$$

so that

$$(4.25) \quad \mathcal{U}(t, s) = \mathcal{U}^+(t, s) + \mathcal{U}^-(t, s).$$

This splitting has the following properties (see [GOW]):

**Proposition 4.3.**

$$(4.26) \quad \begin{aligned} & i) \quad \mathcal{U}^\pm(t, s)\mathcal{U}^\pm(s, t') = \mathcal{U}^\pm(t, t'), \\ & ii) \quad (\bar{\partial}_t - iH(t))\mathcal{U}^\pm(t, s) = \mathcal{U}^\pm(t, s)(\bar{\partial}_s + iH(s)) = 0, \\ & iii) \quad \text{WF}(\mathcal{U}^\pm(t, s))' = \{(X, X') \in T^*\Sigma \times T^*\Sigma : X = \Phi^\pm(t, s)(X')\}, \end{aligned}$$

where  $\Phi^\pm(t, s) : T^*\Sigma \rightarrow T^*\Sigma$  is the symplectic flow generated by the time-dependent Hamiltonian  $\pm(h^{ij}(t, x)k_i k_j)^{\frac{1}{2}}$ .

If we set for  $t \in \mathbb{R}$ :

$$(4.27) \quad \mathcal{U}^\pm(t, t) =: c_{\text{ref}}^\pm(t) = \mathcal{U}(t, t_0)c_{\text{ref}}^\pm(t_0)\mathcal{U}(t_0, t),$$

then

$$c_{\text{ref}}^\pm(t)^2 = c_{\text{ref}}^\pm(t), \quad c_{\text{ref}}^+(t) + c_{\text{ref}}^-(t) = \mathbf{1}, \quad c_{\text{ref}}^\pm(t) = \mathcal{U}(t, s)c_{\text{ref}}^\pm(s)\mathcal{U}(s, t).$$

As a consequence, one gets that  $c_{\text{ref}}^\pm(t)$  are the time- $t$  covariances of a Hadamard state [GOW]. In general, we say that a state is a *regular Hadamard state* if its time- $t$  covariances differ from  $c_{\text{ref}}^\pm(t)$  by terms in  $\mathcal{W}^{-\infty}(\Sigma) \otimes B(\mathbb{C}^2)$ , and one can show that it suffices to check that property for one value of  $t$  [GOW]. In summary:

**Theorem 4.4** ([GOW]). *The pair of operators  $c_{\text{ref}}^\pm(t)$  defined in (4.27) are the covariances of a pure, regular Hadamard state.*

We stress that in general  $c_{\text{ref}}^\pm(t)$  are not ‘canonical’ nor ‘distinguished’, because they depend on the choice of the reference time  $t_0$  and on the precise choice of the operators  $b^\pm(t)$  (to which one can always add suitable regularizing terms). On the other hand, in Sect. 4.5 we will construct covariances  $c_{\text{in}}^\pm(t)$  and  $c_{\text{out}}^\pm(t)$  of the distinguished *in* and *out* states, and the operators  $c_{\text{ref}}^\pm(t)$  will play an important role in the proof of their Hadamard property: a suitable sufficient condition for that is in fact that

$$(4.28) \quad c_{\text{out/in}}^\pm(t) - c_{\text{ref}}^\pm(t) \in \mathcal{W}^{-\infty}(\Sigma) \otimes B(\mathbb{C}^2)$$

for some (and hence all)  $t \in \mathbb{R}$ .

**4.5. Further estimates in scattering settings.** In what follows we give a refinement of the constructions in Sect. 4 for the model Klein-Gordon equation in a scattering situation, corresponding to a situation when the metric  $g$ , resp. the potential  $V$  converge to ultra-static metrics  $g_{\text{out/in}} = -dt^2 + h_{\text{out/in},ij}(x)dx^i dx^j$ , resp. time-independent potentials  $V_{\text{out/in}}$  as  $t \rightarrow \pm\infty$ . We start by fixing two classes of assumptions on the model Klein-Gordon equation (4.2).

We will often abbreviate the classes  $\Psi_{(*)}^{m,\delta}$  (introduced in Subsect. 3.5-3.8) for  $(*) = \text{td}, \text{std}$  by  $\Psi_{(*)}^{m,\delta}$ . We make the following assumptions in the two respective cases.

*Case (td):*

$$\begin{aligned} & a(t, x, D_x) = a_{\text{out/in}}(x, D_x) + \Psi_{\text{td}}^{2,-\delta}(\mathbb{R}; \Sigma) \text{ on } \mathbb{R}_\pm \times \Sigma, \quad \delta > 0, \\ (\text{td}) \quad & r(t) \in \Psi_{\text{td}}^{0,-1-\delta}(\mathbb{R}; \Sigma), \\ & a_{\text{out/in}}(x, D_x) \in \Psi^2(\Sigma) \text{ elliptic, } a_{\text{out/in}}(x, D_x) = a_{\text{out/in}}(x, D_x)^* \geq C_\infty > 0. \end{aligned}$$

*Case (std):*  $\Sigma = \mathbb{R}^d$  and

$$\begin{aligned} & a(t, x, D_x) = a_{\text{out/in}}(x, D_x) + \Psi_{\text{std}}^{2,-\delta}(\mathbb{R}_\pm; \mathbb{R}^d) \text{ on } \mathbb{R}_\pm \times \Sigma, \quad \delta > 0, \\ (\text{std}) \quad & r(t) \in \Psi_{\text{std}}^{0,-1-\delta}(\mathbb{R}; \mathbb{R}^d), \\ & a_{\text{out/in}}(x, D_x) \in \Psi_{\text{sd}}^{2,0}(\mathbb{R}^d) \text{ elliptic, } a_{\text{out/in}}(x, D_x) = a_{\text{out/in}}(x, D_x)^* \geq C_\infty > 0, \end{aligned}$$

From the definitions of  $\Psi_{\text{std}}^{m,\delta}$  and  $\Psi_{\text{td}}^{m,\delta}$  one easily sees that (std) is a special case of (td).

Below, we give estimates on the solution of the Riccati equation, taking now into account the decay in time that follows from either (td) or (std). To simplify notation we write simply  $a(t) = b(t) + \Psi_{(*)}^{m,\delta}(\mathbb{R}_\pm; \Sigma)$  when  $a(t) = b(t) + \Psi_{(*)}^{m,\delta}(\mathbb{R}; \Sigma)$  in  $\mathbb{R}_\pm \times \Sigma$ . We also abbreviate  $\Psi_{(*)}^{m,\delta}(\mathbb{R}_\pm; \Sigma)$  by  $\Psi_{(*)}^{m,\delta}$  when it is clear from the context whether the future or past case is meant.

From hypotheses  $(*)$  there exists  $c(t) \in C_c^\infty(\mathbb{R})$  such that  $a(t) + c(t)\mathbf{1} \sim a_{\text{out/in}}$ , uniformly in  $t \in \mathbb{R}_\pm$ . By functional calculus we can find  $\chi \in C_c^\infty(\mathbb{R})$  such that  $a(t) + \chi(\frac{a(t)}{c(t)}) \sim a_{\text{out/in}}$ , uniformly in  $t \in \mathbb{R}_\pm$ . The error term  $\chi(\frac{a(t)}{c(t)})$  belongs to  $C_c^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ , resp.  $C_c^\infty(\mathbb{R}; \mathcal{W}_{\text{sd}}^{-\infty}(\Sigma))$ .

We can hence replace  $a(t)$  by  $a(t) + \chi(\frac{a(t)}{c(t)})$  in the Riccati equation (4.7) and assume that

$$a(t) \sim a_{\text{out/in}} \text{ uniformly in } t \in \mathbb{R}_\pm.$$

If  $\epsilon_{\text{out/in}} := a_{\text{out/in}}^{\frac{1}{2}}$ , then from Prop. 3.11 we deduce that if  $(*)$  holds then

$$(4.1) \quad \epsilon(t) := a(t)^{\frac{1}{2}} = \epsilon_{\text{out/in}} + \Psi_{(*)}^{1,-\delta}, \quad * = \text{td}, \text{std}.$$



**Proposition 4.5.** Case (td): *There exists  $b(t) = \epsilon(t) + \Psi_{\text{td}}^{0,-1-\delta}(\mathbb{R}; \Sigma) = \epsilon_{\text{out/in}} + \Psi_{\text{td}}^{1,-\delta}(\mathbb{R}_{\pm}; \Sigma)$  that solves*

$$i\partial_t b - b^2 + a + irb \in \Psi_{\text{td}}^{-\infty,-1-\delta}(\mathbb{R}; \Sigma).$$

Case (std): *There exists  $b(t) = \epsilon(t) + \Psi_{\text{std}}^{0,-1-\delta}(\mathbb{R}; \Sigma) = \epsilon_{\text{out/in}} + \Psi_{\text{std}}^{1,-\delta}(\mathbb{R}_{\pm}; \Sigma)$  that solves*

$$i\partial_t b - b^2 + a + irb \in \Psi_{\text{std}}^{-\infty,-1-\delta}(\mathbb{R}; \Sigma).$$

The proof is given in Appendix A.2.

**Proposition 4.6.** *Assume (\*) for  $*$  = td, std and let  $r_b^{\pm}$  be defined in (4.20) and  $r_{-\infty}^{\pm}$  in (4.10). Then*

$$r_b^{\pm} \in \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma), \quad r_{-\infty}^{\pm} \in \Psi_{(*)}^{-\infty,-1-\delta}(\mathbb{R}; \Sigma).$$

The proof is given in Appendix A.3.

## 5. THE out/in STATES ON ASYMPTOTICALLY STATIC SPACETIMES

**5.1. Assumptions.** In what follows we introduce a class of asymptotically static spacetimes on which we will construct the *out/in* states and prove their Hadamard property. One of the key ingredients is the reduction to a model Klein-Gordon operator that satisfies the assumptions (td) considered in Subsect. 4.5.

We will use the framework of manifolds and diffeomorphisms of bounded geometry introduced in Defs. 3.2, 3.3.

We fix a  $d$ -dimensional manifold  $\Sigma$  equipped with a reference Riemannian metric  $k$  such that  $(\Sigma, k)$  is of bounded geometry, and consider  $M = \mathbb{R}_t \times \Sigma_y$ , setting  $y = (t, y)$ ,  $n = 1 + d$ . We equip  $M$  with a Lorentzian metric  $g$  of the form

$$(5.1) \quad g = -c^2(y)dt^2 + (dy^i + b^i(y)dt)h_{ij}(y)(dy^j + b^j(y)dt),$$

where we assume:

$$\begin{aligned} & h_{ij} \in C_b^\infty(\mathbb{R}; \text{BT}_2^0(\Sigma, k)), \quad h_{ij}^{-1} \in C_b^\infty(\mathbb{R}; \text{BT}_0^2(\Sigma, k)), \\ \text{(bg)} \quad & b \in C_b^\infty(\mathbb{R}; \text{BT}_0^1(\Sigma, k)), \\ & c, \quad c^{-1} \in C_b^\infty(\mathbb{R}; \text{BT}_0^0(\Sigma, k)). \end{aligned}$$

We recall that  $\tilde{t} \in C^\infty(M)$  is called a *time function* if  $\nabla \tilde{t}$  is a timelike vector field. It is called a *Cauchy time function* if its level sets are Cauchy hypersurfaces. By [CC, Thm. 2.1] we know that  $(M, g)$  is globally hyperbolic and  $t$  is a Cauchy time function.

We will consider the Klein-Gordon operator on  $(M, g)$ :

$$(5.2) \quad P = -\square_g + V,$$

with  $V \in C_b^\infty(\mathbb{R}; \text{BT}_0^0(\Sigma, k))$  a smooth real-valued function. We consider two static metrics

$$g_{\text{out/in}} = -c_{\text{out/in}}^2(y)dt^2 + h_{\text{out/in}}(y)dy^2$$

and time-independent potentials  $V_{\text{out/in}}$  and assume the following conditions:

$$\begin{aligned} & h(y) - h_{\text{out/in}}(y) \in S^{-\mu}(\mathbb{R}_{\pm}; \text{BT}_2^0(\Sigma, k)), \\ \text{(ast)} \quad & b(y) \in S^{-\mu'}(\mathbb{R}; \text{BT}_0^1(\Sigma, k)), \\ & c(y) - c_{\text{out/in}}(y) \in S^{-\mu}(\mathbb{R}_{\pm}; \text{BT}_0^0(\Sigma, k)), \\ & V(y) - V_{\text{out/in}}(y) \in S^{-\mu}(\mathbb{R}_{\pm}; \text{BT}_0^0(\Sigma, k)), \\ \text{(pos)} \quad & \frac{n-2}{4(n-1)} (R_{c_{\text{out/in}}^{-2} h_{\text{out/in}}} - c_{\text{out/in}}^2 R_{g_{\text{out/in}}}) + c_{\text{out/in}}^2 V_{\text{out/in}} \geq m^2. \end{aligned}$$

for some  $\mu > 0$ ,  $\mu' > 1$  and  $m > 0$ . Above,  $R_g$ , resp.  $R_h$  denotes the scalar curvature of  $g$ , resp.  $h$ .

Condition (ast) means that  $g$ , resp.  $V$  are asymptotic to the static metrics  $g_{\text{out/in}}$ , resp. to the time-independent potentials  $V_{\text{out/in}}$  as  $t \rightarrow \pm\infty$ . Condition (pos) means that the asymptotic Klein-Gordon operators  $\bar{\partial}_t^2 + a_{\text{out/in}}(x, \bar{\partial}_x)$  introduced in Lemma 5.2 below are *massive*.

It follows from (bg) that  $h_{\text{out/in}} \in \text{BT}_2^0(\Sigma, k)$ ,  $h_{\text{out/in}}^{-1} \in \text{BT}_0^2(\Sigma, k)$  and  $V_{\text{out/in}}, V_{\text{out/in}}^{-1} \in \text{BT}_0^0(\Sigma, k)$ .

**5.2. Reduction to the model case.** In this subsection we perform the reduction of the Klein-Gordon operator  $P$  to the model case considered in Sect. 4.5. We start with the well-known orthogonal decomposition of  $g$  associated with the time function  $t$ . Namely, we set

$$v := \frac{g^{-1}dt}{dt \cdot g^{-1}dt} = \bar{\partial}_t + b^i \bar{\partial}_{y^i},$$

which using (bg) is a complete vector field. Furthermore, we denote by  $\phi_t$  its flow, so that

$$\phi_t(x) = (t, 0, y(t, 0, x)), \quad t \in \mathbb{R}, \quad x \in \Sigma,$$

where  $x(t, s, \cdot)$  is the flow of the time-dependent vector field  $b$  on  $\Sigma$ . We also set

$$(5.3) \quad \chi : \mathbb{R} \times \Sigma \ni (t, x) \mapsto (t, y(t, 0, x)) \in \mathbb{R} \times \Sigma.$$

**Lemma 5.1.** *Assume (bg), (ast). Then*

$$\hat{g} := \chi^* g = -\hat{c}^2(t, x) dt^2 + \hat{h}(t, x) dy^2, \quad \chi^* V = \hat{V},$$

where:

$$\begin{aligned} \hat{c}, \hat{c}^{-1}, \hat{V} &\in C_b^\infty(\mathbb{R}; \text{BT}_0^0(\Sigma, k)), \\ \hat{h} &\in C_b^\infty(\mathbb{R}; \text{BT}_2^0(\Sigma, k)), \quad \hat{h}^{-1} \in C_b^\infty(\mathbb{R}; \text{BT}_0^2(\Sigma, k)). \end{aligned}$$

Moreover there exist bounded diffeomorphisms  $y_{\text{out/in}}$  of  $(\Sigma, k)$  such that if:

$$\begin{aligned} \hat{h}_{\text{out/in}} &:= y_{\text{out/in}}^* h_{\text{out/in}}, \\ \hat{c}_{\text{out/in}} &:= y_{\text{out/in}}^* c_{\text{out/in}}, \quad \hat{V}_{\text{out/in}} := y_{\text{out/in}}^* V_{\text{out/in}}, \end{aligned}$$

then we have:

$$\begin{aligned} \hat{h}_{\text{out/in}} &\in \text{BT}_2^0(\Sigma, k), \quad \hat{h}_{\text{out/in}}^{-1} \in \text{BT}_0^2(\Sigma, k), \\ \hat{c}_{\text{out/in}}, \hat{c}_{\text{out/in}}^{-1}, \hat{V}_{\text{out/in}} &\in \text{BT}_0^0(\Sigma, k), \end{aligned}$$

and furthermore,

$$\begin{aligned} \hat{h} - \hat{h}_{\text{out/in}} &\in S^{-\min(1-\mu', \mu)}(\mathbb{R}_\pm, \text{BT}_2^0(\Sigma, k)), \\ \hat{c} - \hat{c}_{\text{out/in}} &\in S^{-\min(1-\mu', \mu)}(\mathbb{R}_\pm, \text{BT}_0^0(\Sigma, k)), \\ \hat{V} - \hat{V}_{\text{out/in}} &\in S^{-\mu}(\mathbb{R}_\pm, \text{BT}_0^0(\Sigma, k)). \end{aligned}$$

Lemma 5.1 is proved in Appendix A.4.

Writing  $P$  as  $-\square_g + \frac{n-2}{4(n-1)} R_g + W$  for  $W = V - \frac{n-2}{4(n-1)} R_g$ , and using the conformal invariance of  $-\square_g + \frac{n-2}{4(n-1)} R_g$  and the estimates in Lemma 5.1, we obtain the following result, which completes the reduction to the model case.

**Lemma 5.2.** *Assume (bg), (ast), (pos) and consider the Klein-Gordon operator  $P$  in (5.2). Let  $\hat{h}, \hat{c}, \hat{V}$  be as in Lemma 5.1 and set:*

$$\hat{P} := \chi^* P, \quad \tilde{P} := \hat{c}^{1-n/2} \hat{P} \hat{c}^{1+n/2}, \quad \tilde{g} = \hat{c}^{-2} \hat{g}, \quad \tilde{h} = \hat{c}^{-2} \hat{h}.$$

Then

$$\tilde{P} = \bar{\partial}_t^2 + r(t, \mathbf{x})\bar{\partial}_t + a(t, \mathbf{x}, \bar{\partial}_\mathbf{x}),$$

for

$$\begin{aligned} a(t, \mathbf{x}, \bar{\partial}_\mathbf{x}) &= -\Delta_{\tilde{h}_t} + \tilde{V}, \quad r = |\tilde{h}_t|^{-\frac{1}{2}} \partial_t |\tilde{h}_t|^{\frac{1}{2}}, \\ \tilde{V} &= \frac{n-2}{4(n-1)} (R_{\tilde{g}} - \hat{c}^2 R_{\hat{g}}) + \hat{c}^2 \hat{V}. \end{aligned}$$

Moreover  $a, r$  satisfy (td) with  $\delta = \min(\mu, \mu' - 1)$  and

$$a_{\text{out/in}}(\mathbf{x}, \bar{\partial}_\mathbf{x}) = -\Delta_{\tilde{h}_{\text{out/in}}} + \tilde{V}_{\text{out/in}}(\mathbf{x}),$$

where

$$\tilde{V}_{\text{out/in}} = \left( \frac{n-2}{4(n-1)} (R_{c_{\text{out/in}}^{-2} h_{\text{out/in}}} - c_{\text{out/in}}^2 R_{g_{\text{out/in}}}) + c_{\text{out/in}}^2 V_{\text{out/in}} \right) \circ y_{\text{out/in}}.$$

Note that condition (pos) simply means that  $\tilde{V}_{\text{out/in}} \geq m^2 > 0$ .

**5.3. Cauchy evolutions.** In this subsection we relate the Cauchy evolutions of  $P$  and of the model Klein-Gordon operator  $\tilde{P}$ .

The trace operator for  $P$  associated to the time function  $t$  is given by:

$$(5.4) \quad \varrho_t \phi = \begin{pmatrix} u(t, \cdot) \\ \mathbf{i}^{-1} n \cdot \nabla \phi(t, \cdot) \end{pmatrix},$$

where  $n$  is the future directed unit normal to  $\Sigma_t$ . The corresponding trace operator for  $\hat{P} = \chi^* P$  is:

$$\hat{\varrho}_t \phi = \begin{pmatrix} \phi(t, \cdot) \\ \mathbf{i}^{-1} \hat{c}^{-1} \partial_t \phi(t, \cdot) \end{pmatrix},$$

so that denoting  $\chi^* \phi = \phi \circ \chi$ , we have:

$$\hat{\varrho}_t \chi^* \phi = \chi_t^* \varrho_t \phi \quad \text{for} \quad \chi_t^* \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} u_0 \circ \chi_t \\ u_1 \circ \chi_t \end{pmatrix},$$

and  $\chi_t(\mathbf{x}) = y(t, 0, \mathbf{x})$ , see (5.3). Finally the trace operator for  $\tilde{P}$  as in Lemma 5.2 is

$$\tilde{\varrho}_t \phi = \begin{pmatrix} \phi(t, \cdot) \\ \mathbf{i}^{-1} \phi(t, \cdot) \end{pmatrix}$$

so that if  $\tilde{\phi} = \hat{c}^{n/2-1} \phi$  is the conformal transformation in Lemma 5.2 we have:

$$\tilde{\varrho}_t \tilde{\phi} = R(t) \hat{\varrho}_t \phi, \quad \text{for} \quad R(t) = \hat{c}^{n/2-1} \begin{pmatrix} 1 & 0 \\ -\mathbf{i}(n/2-1) \partial_t \ln(\hat{c}) & 1 \end{pmatrix}.$$

Let us denote by  $\mathcal{U}(t, s)$  the Cauchy evolution for  $P$  associated to  $\varrho_t$  and by  $\mathcal{U}^{\text{ad}}(t, s)$  the almost diagonal Cauchy evolution introduced in Subsect. 4.3 for the model Klein-Gordon operator  $\tilde{P}$ . The following lemma follows from the above computations and (4.18).

**Lemma 5.3.** *Let  $Z(t) := (\chi_t^*)^{-1} R(t) T(t)$ , where  $T(t)$  is defined in (4.17). Then*

$$(5.5) \quad \mathcal{U}(t, s) = Z(t) \mathcal{U}^{\text{ad}}(t, s) Z^{-1}(s).$$

We have a similar reduction for the asymptotic Klein-Gordon operators:

$$P_{\text{out/in}} = -\square_{g_{\text{out/in}}} + \frac{n-2}{4(n-1)} R_{g_{\text{out/in}}} + V_{\text{out/in}},$$

for  $g_{\text{out/in}} = -c_{\text{out/in}}^2(y) dt^2 + h_{\text{out/in}}(y) dy^2$ , where  $h_{\text{out/in}}, c_{\text{out/in}}, V_{\text{out/in}}$  were introduced in (ast). The associated trace operator is

$$\varrho_{t, \text{out/in}} \phi = \begin{pmatrix} \phi(t, \cdot) \\ \mathbf{i}^{-1} c_{\text{out/in}}^{-1} \partial_t \phi(t, \cdot) \end{pmatrix}.$$

We also set

$$\chi_{\text{out/in}}^* \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} u_0 \circ Y_{\text{out/in}} \\ u_1 \circ Y_{\text{out/in}} \end{pmatrix}, \quad R_{\text{out/in}} = \hat{c}_{\text{out/in}}^{(d-1)/2} \mathbf{1},$$

and for  $\epsilon_{\text{out/in}} = a_{\text{out/in}}^{\frac{1}{2}}$ :

$$T_{\text{out/in}} = (i\sqrt{2})^{-1} \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} \\ \epsilon_{\text{out/in}}^{\frac{1}{2}} & \epsilon_{\text{out/in}}^{\frac{1}{2}} \end{pmatrix}, \quad Z_{\text{out/in}} = (\chi_{\text{out/in}}^*)^{-1} R_{\text{out/in}} T_{\text{out/in}},$$

so that the Cauchy evolution of  $P_{\text{out/in}}$  is given by

$$(5.6) \quad \mathcal{U}_{\text{out/in}}(t, s) = Z_{\text{out/in}} \circ \mathcal{U}_{\text{out/in}}^{\text{ad}}(t, s) \circ Z_{\text{out/in}}^{-1},$$

where  $\mathcal{U}_{\text{out/in}}^{\text{ad}}$  stands for the evolution generated by

$$(5.7) \quad H_{\text{out/in}}^{\text{ad}} = \begin{pmatrix} \epsilon_{\text{out/in}} & 0 \\ 0 & \epsilon_{\text{out/in}} \end{pmatrix}.$$

The following fact will be needed in the sequel.

**Lemma 5.4.** *We have:*

$$Z^{-1}(t)Z_{\text{out/in}} - \mathbf{1}, \quad Z_{\text{out/in}}^{-1}Z(t) - \mathbf{1} \rightarrow 0 \text{ in } B(L^2(\Sigma) \otimes \mathbb{C}^2) \text{ as } t \rightarrow \pm\infty.$$

**Proof.** From Prop. 4.5 we obtain that  $T_{\text{out/in}}^{-1}T(t) - \mathbf{1}$  tends to 0 in norm as  $t \rightarrow \pm\infty$ . By Lemma 5.1,  $R(t)$  tends to  $R_{\text{out/in}}$  in norm. Finally, from the proof of Lemma 5.1, see in particular (A.10), we obtain that  $(\chi_{\text{out/in}}^*)^{-1}\chi_t^*$  tends to  $\mathbf{1}$  in norm. This implies the lemma.  $\square$

**5.4. Construction of Hadamard states by scattering theory.** In this subsection we construct the *out/in* states  $\omega_{\text{out/in}}$  for the Klein-Gordon operator  $P$  and show that they are Hadamard states. We assume hypotheses (bg), (ast), (pos).

By the positivity condition (pos), the asymptotic Klein-Gordon operators  $P_{\text{out/in}}$  admit *vacuum states* (that is, *ground states* for the dynamics  $\mathcal{U}_{\text{out/in}}$ )  $\omega_{\text{out/in}}^{\text{vac}}$ . In terms of  $t = 0$  Cauchy data their covariances are the projections:

$$c_{\text{out/in}}^{\pm, \text{vac}} = Z_{\text{out/in}} \pi^{\pm} Z_{\text{out/in}}^{-1},$$

where  $\pi^{\pm}$  are defined in (4.23). Clearly we have

$$\mathcal{U}_{\text{out/in}}(t, s) c_{\text{out/in}}^{\pm, \text{vac}} \mathcal{U}_{\text{out/in}}(s, t) = c_{\text{out/in}}^{\pm, \text{vac}},$$

i.e.  $\omega_{\text{out/in}}^{\text{vac}}$  are invariant under the asymptotic dynamics. For  $t \in \mathbb{R}$  we now consider the projections:

$$(5.8) \quad \begin{aligned} c_{\text{out/in}}^{\pm, t}(0) &:= \mathcal{U}(0, t) c_{\text{out/in}}^{\pm, \text{vac}} \mathcal{U}(t, 0) \\ &= \mathcal{U}(0, t) \mathcal{U}_{\text{out/in}}(t, 0) c_{\text{out/in}}^{\pm, \text{vac}} \mathcal{U}_{\text{out/in}}(0, t) \mathcal{U}(t, 0). \end{aligned}$$

By taking the  $t \rightarrow \pm\infty$  limit of  $c_{\text{out/in}}^{\pm, t}(0)$  we obtain the time-0 covariances  $c_{\text{out/in}}^{\pm}(0)$  of a state  $\omega_{\text{out/in}}$  (for the Klein-Gordon operator  $P$ ) that ‘equal  $\omega_{\text{out/in}}^{\text{vac}}$  asymptotically’ at  $t = \pm\infty$ . The main new result that we prove is that  $\omega_{\text{out/in}}$  are Hadamard states.

Before stating the theorem let us recall that the Sobolev spaces  $H^m(\Sigma)$  are naturally defined using the reference Riemannian metric  $k$  on  $\Sigma$ . The *charge space*  $H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$  is the natural space of Cauchy data in connection with quantized Klein-Gordon fields.

**Theorem 5.5.** *Assume hypotheses (bg), (ast), (pos). Then*

$$(5.9) \quad \lim_{t \rightarrow \pm\infty} c_{\text{out/in}}^{\pm,t}(0) =: c_{\text{out/in}}^{\pm}(0) = c_{\text{ref}}^{\pm}(0) + \mathcal{W}^{-\infty}(\Sigma), \text{ in } B(H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)),$$

where  $c_{\text{ref}}^{\pm}(0) = Z(0)\pi^{\pm}Z^{-1}(0)$ . The operators  $c_{\text{out/in}}^{\pm}(0)$  are pairs of projections defining a pure state  $\omega_{\text{out/in}}$  for the Klein-Gordon operator  $P$ . Moreover  $\omega_{\text{out/in}}$  is a Hadamard state.

**Proof.** From (5.5), (5.6) we obtain:

$$(5.10) \quad \begin{aligned} \mathcal{U}_{\text{out/in}}(0,t)\mathcal{U}(t,0) &= Z_{\text{out/in}}(0)\mathcal{U}_{\text{out/in}}^{\text{ad}}(0,t)Z_{\text{out/in}}^{-1}(0)Z(t)\mathcal{U}^{\text{ad}}(t,0)Z^{-1}(0), \\ \mathcal{U}(0,t)\mathcal{U}_{\text{out/in}}(t,0) &= Z(0)\mathcal{U}^{\text{ad}}(0,t)Z^{-1}(t)Z_{\text{out/in}}\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,0)Z_{\text{out/in}}^{-1}. \end{aligned}$$

It follows that:

$$(5.11) \quad \begin{aligned} c_{\text{out/in}}^{\pm,t}(0) &= Z(0)\mathcal{U}^{\text{ad}}(0,t)Z^{-1}(t)Z_{\text{out/in}}\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,0) \\ &\quad \times \pi^{\pm}\mathcal{U}_{\text{out/in}}^{\text{ad}}(0,t)Z_{\text{out/in}}^{-1}Z(t)\mathcal{U}^{\text{ad}}(t,0)Z^{-1}(0). \end{aligned}$$

Since  $Z(0) : L^2(\Sigma) \otimes \mathbb{C}^2 \rightarrow H^{\frac{1}{2}}(\Sigma) \oplus H^{-\frac{1}{2}}(\Sigma)$  is boundedly invertible it suffices to show the existence of the limit

$$d_{\text{out/in}}^{\pm} = \lim_{t \rightarrow \pm\infty} \mathcal{U}^{\text{ad}}(0,t)Z^{-1}(t)Z_{\text{out/in}}\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,0)\pi^{\pm}\mathcal{U}_{\text{out/in}}^{\text{ad}}(0,t)Z_{\text{out/in}}^{-1}Z(t)\mathcal{U}^{\text{ad}}(t,0)$$

in  $B(L^2(\Sigma) \otimes \mathbb{C}^2)$ .

By Prop. 5.6 (1) below we know that  $\mathcal{U}^{\text{ad}}(t,s)$ ,  $\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,s)$  are uniformly bounded in  $B(L^2(\Sigma) \otimes \mathbb{C}^2)$ . Hence using Lemma 5.4 we can replace  $Z^{-1}(t)Z_{\text{out/in}}$  and  $Z_{\text{out/in}}^{-1}Z(t)$  by  $\mathbf{1}$  in the rhs of (5.11), modulo an error of size  $o(t^0)$  in  $B(L^2(\Sigma) \otimes \mathbb{C}^2)$ , i.e. we are reduced to prove the existence of the limit

$$\begin{aligned} d_{\text{out/in}}^{\pm} &:= \lim_{t \rightarrow \pm\infty} \mathcal{U}^{\text{ad}}(0,t)\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,0)\pi^{\pm}\mathcal{U}_{\text{out/in}}^{\text{ad}}(0,t)\mathcal{U}^{\text{ad}}(t,0) \\ &= \lim_{t \rightarrow \pm\infty} W_{\text{out/in}}(t)\pi^{\pm}W_{\text{out/in}}^{-1}(t), \end{aligned}$$

where  $W_{\text{out/in}}(t) = \mathcal{U}^{\text{ad}}(0,t)\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,0)$ . By Prop. 5.6 the limit exists in  $B(L^2(\Sigma) \otimes \mathbb{C}^2)$  and equals  $\pi^{\pm} + \mathcal{W}^{-\infty}(\Sigma)$ . The limit operators  $d_{\text{out/in}}^{\pm}$  are projections as norm limits of projections. It follows that

$$(5.12) \quad c_{\text{out/in}}^{\pm}(0) = Z(0)d_{\text{out/in}}^{\pm}Z(0)^{-1} + \mathcal{W}^{-\infty}(\Sigma) = c_{\text{ref}}^{\pm}(0) + \mathcal{W}^{-\infty}(\Sigma)$$

is a projection. The conditions (2.13), (2.14) are satisfied by  $c_{\text{out/in}}^{\pm}(0)$  since they are satisfied by  $c_{\text{out/in}}^{\pm,t}(0)$  for each finite  $t$ . Therefore  $c_{\text{out/in}}^{\pm}$  are the covariances of two pure states  $\omega_{\text{out/in}}$  for  $P$ . Finally as in [GOW] we obtain from (5.12) that  $\omega_{\text{out/in}}$  are Hadamard states.  $\square$

In the proof of Thm. 5.5, the crucial ingredient is the following proposition.

**Proposition 5.6.** *Let  $H^{\text{ad}}(t), H_{\text{out/in}}^{\text{ad}}$  be as in (4.19), (5.7). Then:*

- (1)  $\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,s)$  and  $\mathcal{U}^{\text{ad}}(t,s)$  are uniformly bounded in  $B(H^m(\Sigma) \otimes \mathbb{C}^2)$ , for all  $m \in \mathbb{R}$ .
- (2) Let  $W_{\text{out/in}}(t) = \mathcal{U}^{\text{ad}}(0,t)\mathcal{U}_{\text{out/in}}^{\text{ad}}(t,0)$ . Then

$$\lim_{t \rightarrow +\infty} W_{\text{out/in}}(t)\pi^{\pm}W_{\text{out/in}}(t)^{-1} = \pi^{\pm} + \mathcal{W}^{-\infty}(\Sigma) \otimes L(\mathbb{C}^2), \text{ in } B(L^2(\Sigma) \otimes \mathbb{C}^2).$$

**Proof.** *Proof of (1):* we can assume without loss of generality that  $s = 0$ . The statement for  $\mathcal{W}_{\text{out/in}}^{\text{ad}}(t, 0)$  is obvious since  $H_{\text{out/in}}^{\text{ad}} = \begin{pmatrix} \epsilon_{\text{out/in}} & 0 \\ 0 & -\epsilon_{\text{out/in}} \end{pmatrix}$ . Let us prove it for  $\mathcal{W}^{\text{ad}}(t, 0)$ . We have:

$$(5.13) \quad \begin{aligned} H^{\text{ad}}(t) &= \begin{pmatrix} -b^-(t) + ir_b^-(t) & 0 \\ 0 & -b^+(t) + ir_b^+(t) \end{pmatrix} + \Psi_{\text{td}}^{-\infty, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2) \\ &= \begin{pmatrix} \epsilon(t) & 0 \\ 0 & -\epsilon(t) \end{pmatrix} + \Psi_{\text{td}}^{0, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2), \end{aligned}$$

by Props. 4.5, 4.6. Since  $\epsilon(t)$  is selfadjoint, this implies that  $\mathcal{W}^{\text{ad}}(t, 0)$  is uniformly bounded in  $B(L^2(\Sigma))$ , which proves (1) for  $m = 0$ .

We now note that  $\|u\|_{H^m(\Sigma)} \sim \|\epsilon^m(t)u\|_{L^2(\Sigma)}$ , uniformly for  $t \in \mathbb{R}$ , since  $\epsilon(t)$  is elliptic uniformly for  $t \in \mathbb{R}$ . Therefore to prove (1) it suffices, using the uniform boundedness of  $\mathcal{W}^{\text{ad}}(t, 0)$  in  $B(L^2(\Sigma))$ , to show that

$$(5.14) \quad \mathcal{W}^{\text{ad}}(0, t) (\epsilon(t)^m \otimes \mathbf{1}_{\mathbb{C}^2}) \mathcal{W}^{\text{ad}}(t, 0) (\epsilon(0)^{-m} \otimes \mathbf{1}_{\mathbb{C}^2}) \text{ is uniformly bounded in } B(L^2(\Sigma)).$$

We have by (5.13):

$$\begin{aligned} &\partial_t \mathcal{W}^{\text{ad}}(0, t) (\epsilon(t)^m \otimes \mathbf{1}_{\mathbb{C}^2}) \mathcal{W}^{\text{ad}}(t, 0) (\epsilon(0)^{-m} \otimes \mathbf{1}_{\mathbb{C}^2}) \\ &= \mathcal{W}^{\text{ad}}(0, t) (\partial_t \epsilon^m(t) \otimes \mathbf{1}_{\mathbb{C}^2} + i[H^{\text{ad}}(t), \epsilon^m(t) \otimes \mathbf{1}_{\mathbb{C}^2}]) \mathcal{W}^{\text{ad}}(t, 0) (\epsilon(0)^{-m} \otimes \mathbf{1}_{\mathbb{C}^2}) \\ &= \mathcal{W}^{\text{ad}}(0, t) (\partial_t \epsilon^m(t) \otimes \mathbf{1}_{\mathbb{C}^2} + i[H^{\text{ad}}(t), \epsilon^m(t) \otimes \mathbf{1}_{\mathbb{C}^2}]) (\epsilon(t)^{-m} \otimes \mathbf{1}) \mathcal{W}^{\text{ad}}(t, 0) \\ &\quad \times \mathcal{W}^{\text{ad}}(0, t) (\epsilon(t)^m \otimes \mathbf{1}_{\mathbb{C}^2}) \mathcal{W}^{\text{ad}}(t, 0) (\epsilon(0)^{-m} \otimes \mathbf{1}_{\mathbb{C}^2}) \\ &=: M(t) \mathcal{W}^{\text{ad}}(0, t) (\epsilon(t)^m \otimes \mathbf{1}_{\mathbb{C}^2}) \mathcal{W}^{\text{ad}}(t, 0) (\epsilon(0)^{-m} \otimes \mathbf{1}_{\mathbb{C}^2}). \end{aligned}$$

By (td) and Prop. 3.11 we see that  $\partial_t \epsilon^m(t) \in \Psi_{\text{td}}^{m, -1-\delta}$ , and by (5.13) that  $[H^{\text{ad}}(t), \epsilon^m(t) \otimes \mathbf{1}_{\mathbb{C}^2}] \in \Psi_{\text{td}}^{m, -1-\delta}$ . Therefore  $\|M(t)\|_{B(L^2(\Sigma) \otimes \mathbb{C}^2)} \in O(\langle t \rangle^{-1-\delta})$ . Hence, setting

$$f(t) := \|\mathcal{W}^{\text{ad}}(0, t) (\epsilon(t)^m \otimes \mathbf{1}_{\mathbb{C}^2}) \mathcal{W}^{\text{ad}}(t, 0) (\epsilon(0)^{-m} \otimes \mathbf{1}_{\mathbb{C}^2})\|_{B(L^2(\Sigma))},$$

we have  $f(0) = 1$ ,  $|\partial_t f(t)| \in O(\langle t \rangle^{-1-\delta})f(t)$ . If  $f(t) \neq +\infty$  for each  $t$ , an application of Gronwall's inequality would immediately imply (5.14). If  $m \leq 0$  the use of Gronwall's inequality is justified by applying the above time dependent operator to a vector  $u \in H^m(\Sigma)$ . If  $m > 0$  we replace the unbounded operator  $A = \epsilon(t) \otimes \mathbf{1}_{\mathbb{C}^2}$  by the bounded operator  $A_\delta = A(1+i\delta A)$ , for  $\delta > 0$ . For the corresponding function  $f_\delta(t)$  we obtain that  $f_\delta(0) \leq 1$ ,  $|\partial_t f_\delta(t)| \in O(\langle t \rangle^{-1-\delta})f_\delta(t)$  uniformly for  $0 < \delta \leq 1$ . Then (5.14) follows using that  $\|A^m u\| = \sup_{0 < \delta \leq 1} \|A_\delta^m u\|$ .

*Proof of (2):* note first that  $[\pi^+, A] = 0$  for any diagonal operator  $A$ . Therefore:

$$W_{\text{out/in}}(t) \pi^+ W_{\text{out/in}}(t)^{-1} = \mathcal{W}(0, t) \pi^+ \mathcal{W}(t, 0),$$

and by (5.13)

$$(5.15) \quad \begin{aligned} \partial_t (W_{\text{out/in}}(t) \pi^+ W_{\text{out/in}}(t)^{-1}) &= -i \mathcal{W}(0, t) [H^{\text{ad}}(t), \pi^+] \mathcal{W}(t, 0) \\ &= \mathcal{W}(0, t) [R_{-\infty}(t), \pi^+] \mathcal{W}(t, 0), \quad R_{-\infty} \in \Psi_{\text{td}}^{-\infty, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2). \end{aligned}$$

By (1), this implies that  $\partial_t (W_{\text{out/in}}(t) \pi^+ W_{\text{out/in}}(t)^{-1}) \in \Psi_{\text{td}}^{-\infty, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2)$ , hence:

$$\lim_{t \rightarrow +\infty} W_{\text{out/in}}(t) \pi^+ W_{\text{out/in}}(t) = \pi^+ + \int_0^{+\infty} \partial_t (W_{\text{out/in}}(t) \pi^+ W_{\text{out/in}}(t)^{-1}) dt \text{ in } B(L^2(\Sigma) \otimes \mathbb{C}^2).$$

The integral term belongs to  $\mathcal{W}^{-\infty}(\Sigma)$ .  $\square$

## 6. FEYNMAN INVERSES FROM SCATTERING DATA FOR MODEL KLEIN-GORDON EQUATIONS

6.1. **Setup.** In this section we consider again the model Klein-Gordon operator studied in Subsect. 4.1:

$$(6.1) \quad P = \bar{\partial}_t^2 + r(t, x)\bar{\partial}_t + a(t, x, \bar{\partial}_x),$$

and denote by  $P_{\text{out/in}}$  the asymptotic Klein-Gordon operators

$$P_{\text{out/in}} := \bar{\partial}_t^2 + a_{\text{out/in}}(x, \bar{\partial}_x).$$

We will assume conditions (std) for  $\delta > 1$ , which corresponds to a *short-range* situation. Recall that in particular  $\Sigma = \mathbb{R}^d$ .

By a parametrix for  $P$  we will mean an operator  $G_I$  such that  $PG_I - \mathbf{1}$  and  $G_IP - \mathbf{1}$  have smooth Schwartz kernel. Duistermaat and Hörmander proved the existence of a Feynman parametrix  $G_F$ , or parametrix with *Feynman type wave front set*, i.e.

$$\text{WF}'(G_F) = (\text{diag}_{T^*M}) \cup \bigcup_{t \leq 0} (\Phi_t(\text{diag}_{T^*M}) \cap \pi^{-1}\mathcal{N}).$$

This means that up to singularities on the full diagonal  $\text{diag}_{T^*M}$  of  $T^*M \times T^*M$ ,  $\text{WF}'(G_F)$  is contained in the backward flowout of  $\text{diag}_{T^*M}$  by the bicharacteristic flow (here acting on the left component of  $T^*M \times T^*M$ , accordingly  $\pi$  is the projection to that component).

Our primary goal will be to prove that for suitably chosen Hilbert spaces of distributions  $\mathcal{X}_I^m, \mathcal{Y}^m$ , the operator  $P : \mathcal{X}_I^m \rightarrow \mathcal{Y}^m$  is Fredholm, i.e. its kernel and cokernel are of finite dimension. This guarantees the existence of pseudo-inverses, i.e. operators  $G_I : \mathcal{Y}^m \rightarrow \mathcal{X}_I^m$  such that  $PG_I - \mathbf{1}$  and  $G_IP - \mathbf{1}$  are compact.

We will be interested in constructing a pseudo-inverse that is at the same time a Feynman parametrix. This will be based on the reduction to the almost diagonalized dynamics  $\mathcal{U}^{\text{ad}}(t, s)$  obtained in Subsect. 4.3.

6.2. **Notation.** As a rule, all objects related to the almost diagonalized situation will be decorated with a superscript ad. We recall that  $L^2(\mathbb{R}^{1+d})$  is equipped with the scalar product

$$(u|v) := \int \bar{u}v|h_t|^{\frac{1}{2}} dt dx.$$

6.2.1. *Operators.* Let us recall that the operators  $H(t), H^{\text{ad}}(t), T(t)$  are defined respectively in (4.3), (4.19), (4.17).

- We set for  $u \in C^\infty(\mathbb{R}; \mathcal{D}'(\mathbb{R}^d)), u^{\text{ad}} \in C^\infty(\mathbb{R}; \mathcal{D}'(\mathbb{R}) \oplus \mathcal{D}'(\mathbb{R}))$ :

$$\begin{aligned} \varrho_t u &= (u(t), i^{-1}\partial_t u(t)), & \varrho_t^{\text{ad}} u^{\text{ad}} &= u^{\text{ad}}(t), \\ (Tu^{\text{ad}})(t) &:= T(t)u^{\text{ad}}(t), & (\varrho u)(t) &:= \varrho_t u(t). \end{aligned}$$

Setting also  $\pi_i(u_0, u_1) = u_i$  we have:

$$(6.2) \quad P = -\pi_1(D_t - H(t))\varrho,$$

where as usual  $D_t = i^{-1}\bar{\partial}_t$ .

- We set:

$$P^{\text{ad}} := D_t - H^{\text{ad}}(t),$$

and an easy computation shows that:

$$(6.3) \quad TP^{\text{ad}}T^{-1} = D_t - H(t), \text{ hence } P = -\pi_1 TP^{\text{ad}}T^{-1}\varrho.$$

- We denote by  $H_{\text{out/in}}, H_{\text{out/in}}^{\text{ad}}, T_{\text{out/in}}$ , the analogues of  $H(t), H^{\text{ad}}(t), T(t)$  with  $a(t), r(t)$  replaced by  $a_{\text{out/in}}, 0$ .

- The Cauchy evolutions generated by  $H(t)$ ,  $H_{\text{out/in}}$ ,  $H^{\text{ad}}(t)$ ,  $H_{\text{out/in}}^{\text{ad}}$  are denoted by  $\mathcal{U}(t, s)$ ,  $\mathcal{U}_{\text{out/in}}(t, s)$ ,  $\mathcal{U}^{\text{ad}}(t, s)$ ,  $\mathcal{U}_{\text{out/in}}^{\text{ad}}(t, s)$ . We recall that:

$$(6.4) \quad \mathcal{U}(t, s) = T(t)\mathcal{U}^{\text{ad}}(t, s)T^{-1}(s), \quad \mathcal{U}_{\text{out/in}}(t, s) = T_{\text{out/in}}\mathcal{U}_{\text{out/in}}^{\text{ad}}(t, s)T_{\text{out/in}}^{-1}.$$

- The symplectic forms for  $P$ ,  $P^{\text{ad}}$  are denoted by

$$q := \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}, \quad q^{\text{ad}} := \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix},$$

and we have:

$$(6.5) \quad T^*(t)qT(t) = q^{\text{ad}},$$

i.e.  $T$  is symplectic.

The adjoint of an operator  $A$  for  $q, q^{\text{ad}}$  will be denoted by  $A^\dagger$ . We recall that  $\mathcal{U}_{(\text{out/in})}^{(\text{ad})}(t, s)$ ,  $\mathcal{U}_{(\text{out/in})}^{(\text{ad})}(t, s)$  are symplectic for  $q^{(\text{ad})}$ .

- If  $a$  acting on  $\mathcal{D}'(\mathbb{R}^d)$  is a 'scalar' operator, the operator  $a \otimes \mathbf{1}_{\mathbb{C}^2}$  will be abbreviated by  $a$  for simplicity.

6.2.2. *Properties of  $H^{\text{ad}}(t)$ .* Let us summarize the properties of  $H^{\text{ad}}(t)$  in the (std) case, that follow from identity (4.19) and Props. 4.5, 4.6, namely:

$$(6.6) \quad H^{\text{ad}}(t) = \begin{pmatrix} -b^-(t) + r_b^-(t) & 0 \\ 0 & -b^+(t) + r_b^+(t) \end{pmatrix} + R_{-\infty}(t), \quad \text{where} \\ R_{-\infty}(t) \in \Psi_{\text{std}}^{-\infty, -1-\delta}(\mathbb{R}; \mathbb{R}^d) \otimes B(\mathbb{C}^2),$$

$$(6.7) \quad H^{\text{ad}}(t) = \begin{pmatrix} \epsilon(t) & 0 \\ 0 & -\epsilon(t) \end{pmatrix} + \Psi_{\text{std}}^{0, -1-\delta}(\mathbb{R}; \mathbb{R}^d) \otimes B(\mathbb{C}^2),$$

$$(6.8) \quad b^\pm(t) \mp \epsilon(t), r_b^\pm(t) \in \Psi_{\text{std}}^{0, 1-\delta}(\mathbb{R}; \mathbb{R}^d), \\ \epsilon(t) - \epsilon_{\text{out/in}} \in \Psi_{\text{std}}^{1, -\delta}(\mathbb{R}; \mathbb{R}^d).$$

6.2.3. *Function spaces.* We will abbreviate by  $H^m$  the Sobolev spaces  $H^m(\mathbb{R}^d)$ . Furthermore we set:

$$\mathcal{E}^m := H^{m+1} \oplus H^m, \quad \mathcal{H}^m := H^m \oplus H^m, \quad m \in \mathbb{R}.$$

As usual we define  $\mathcal{E}^\infty := \bigcap_{m \in \mathbb{R}} \mathcal{E}^m$ ,  $\mathcal{E}^{-\infty} := \bigcup_{m \in \mathbb{R}} \mathcal{E}^m$  and similarly for  $\mathcal{H}^\infty$ ,  $\mathcal{H}^{-\infty}$ , equipped with their canonical topologies.

We will frequently use the fact that  $T(t) : \mathcal{E}^m \rightarrow \mathcal{H}^{m+\frac{1}{2}}$  is boundedly invertible with  $\|T(t)\|, \|T^{-1}(t)\|$  uniformly bounded in  $t$ . Using Prop. 5.6, we also obtain that:

$$(6.9) \quad \sup_{t, s \in \mathbb{R}} \|\mathcal{U}^{\text{ad}}(t, s)\|_{B(\mathcal{H}^m)} < \infty, \quad \sup_{t, s \in \mathbb{R}} \|\mathcal{U}(t, s)\|_{B(\mathcal{E}^m)} < \infty.$$

- If  $\mathcal{E}$  is a Banach space,  $k \in \mathbb{N}$ , we denote by  $C^k(\mathbb{R}; \mathcal{E})$  the Banach space of  $\mathcal{E}$ -valued functions with norm

$$\|u\|_{C^k(\mathbb{R}; \mathcal{E})} = \sum_{0 \leq l \leq k} \sup_{t \in \mathbb{R}} \|\partial_t^l u(t)\|_{\mathcal{E}}.$$



**6.3. Møller (wave) operators.** We will consider  $t = 0$  as our fixed reference time. It is a standard fact, derived using (6.7), (6.8) and the so-called Cook argument (see e.g. [DG1]), that the Møller operators

$$(6.10) \quad W_{\text{out/in}}^{\text{ad}} := \lim_{t \rightarrow \pm\infty} \mathcal{U}^{\text{ad}}(0, t) \mathcal{U}_{\text{out/in}}^{\text{ad}}(t, 0) \in B(\mathcal{H}^m)$$

exist and are invertible with inverses given by

$$(6.11) \quad (W_{\text{out/in}}^{\text{ad}})^{-1} = (W_{\text{out/in}}^{\text{ad}})^\dagger = \lim_{t \rightarrow \pm\infty} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \mathcal{U}^{\text{ad}}(t, 0) \in B(\mathcal{H}^m).$$

Using then (6.4) and that fact that  $T^{-1}(t)T_{\text{out/in}} - \mathbf{1}$  tends to 0 in  $B(\mathcal{H}^m)$  when  $t \rightarrow \pm\infty$ , we obtain the existence of

$$(6.12) \quad W_{\text{out/in}} := \lim_{t \rightarrow \pm\infty} \mathcal{U}(0, t) \mathcal{U}_{\text{out/in}}(t, 0) \in B(\mathcal{E}^m),$$

with inverses

$$(6.13) \quad (W_{\text{out/in}})^{-1} = (W_{\text{out/in}})^\dagger = \lim_{t \rightarrow \pm\infty} \mathcal{U}_{\text{out/in}}(0, t) \mathcal{U}(t, 0) \in B(\mathcal{E}^m),$$

and satisfying the identities

$$(6.14) \quad W_{\text{out/in}} = T(0)W_{\text{out/in}}^{\text{ad}}T_{\text{out/in}}^{-1}.$$

**Remark 6.1.** *Strictly speaking  $W_{\text{out/in}}^{(\text{ad})}$  acting on  $\mathcal{E}^m$  or  $\mathcal{H}^m$  should be denoted by, e.g.,  $W_{\text{out/in}}^{(\text{ad}),m}$  to indicate its dependence on  $m$ . However since  $W_{\text{out/in}}^{(\text{ad}),m}$  is the closure of  $W_{\text{out/in}}^{(\text{ad}),m'}$  for any  $m' > m$ , we will often dispense with the exponent  $m$  in the sequel. The same remark applies to  $(W_{\text{out/in}}^{(\text{ad})})^{-1}$ .*

**6.4. Compactness properties of  $W_{\text{out/in}}^{\text{ad}}$ .** The additional space decay properties implied by conditions (std) have the following important consequence:

**Proposition 6.2.** *Assume condition (std) and let  $\alpha < \delta/2$ . Then*

$$W_{\text{out/in}}^{\text{ad}} \pi^+ (W_{\text{out/in}}^{\text{ad}})^{-1} - \pi^+ \in \langle x \rangle^{-\alpha} \mathcal{W}^{-\infty}(\mathbb{R}^d) \langle x \rangle^{-\alpha} \otimes B(\mathbb{C}^2).$$

*It follows that  $[W_{\text{out/in}}^{\text{ad}}, \pi^+]$  is a compact operator on  $\mathcal{H}^m$  for  $m \in \mathbb{R}$ .*

To prove Prop. 6.2, we will need the following lemma; its proof is given in Appendix A.5.

**Lemma 6.3.** *Assume conditions (std) for  $\delta > 0$ . Then for all  $m, k \in \mathbb{R}_+$ :*

$$\sup_{t \geq 0} \|\langle D_x \rangle^m \langle x \rangle^k \mathcal{U}^{\text{ad}}(0, t) (\langle x \rangle + \langle t \rangle)^{-k} \langle D_x \rangle^{-m}\|_{B(\mathcal{H}^0)} < \infty.$$

**Proof of Prop. 6.2.** Recall that we have set  $W_{\text{out/in}}^{\text{ad}}(t) = \mathcal{U}^{\text{ad}}(0, t) \mathcal{U}_{\text{out/in}}^{\text{ad}}(t, 0)$ . We have for  $m \in \mathbb{N}$ ,  $\alpha > 0$ :

$$(6.15) \quad \begin{aligned} & \langle D_x \rangle^m \langle x \rangle^\alpha \partial_t (W_{\text{out/in}}^{\text{ad}}(t) \pi^+ (W_{\text{out/in}}^{\text{ad}}(t))^{-1}) \langle x \rangle^\alpha \langle D_x \rangle^m \\ &= \langle D_x \rangle^m \langle x \rangle^\alpha \mathcal{U}^{\text{ad}}(0, t) [R_{-\infty}(t), \pi^+] \mathcal{U}^{\text{ad}}(t, 0) \langle x \rangle^\alpha \langle D_x \rangle^m \\ &= \langle D_x \rangle^m \langle x \rangle^\alpha \mathcal{U}^{\text{ad}}(0, t) (\langle x \rangle + \langle t \rangle)^{-\alpha} \langle D_x \rangle^{-m} \\ & \quad \times \langle D_x \rangle^m (\langle x \rangle + \langle t \rangle)^\alpha [R_{-\infty}(t), \pi^+] (\langle x \rangle + \langle t \rangle)^\alpha \langle D_x \rangle^m \\ & \quad \times \langle D_x \rangle^{-m} (\langle x \rangle + \langle t \rangle)^{-\alpha} \mathcal{U}^{\text{ad}}(t, 0) \langle x \rangle^\alpha \langle D_x \rangle^m \\ &=: R_{m,\alpha}(t) \times M_{m,\alpha}(t) \times R_{m,\alpha}(t)^\dagger. \end{aligned}$$

Since  $R_{-\infty}(t) \in \Psi_{\text{std}}^{-\infty, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2)$  we know that

$$\|M_{m,\alpha}(t)\|_{B(\mathcal{H}^m)} \in O(\langle t \rangle^{-1-\delta+2\alpha}).$$

From Lemma 6.3 we know that  $\|R_{m,\alpha}(t)\|_{B(\mathcal{H}^m)} \in O(1)$ , which implies the same bound for  $R_{m,\alpha}(t)^\dagger$ . Thus from (6.15) we obtain that

$$\langle D_x \rangle^m \langle x \rangle^\alpha \partial_t (W_{\text{out/in}}^{\text{ad}}(t) \pi^+ (W_{\text{out/in}}^{\text{ad}}(t)^{-1}) \langle x \rangle^\alpha \langle D_x \rangle^m) \in O(\langle t \rangle^{-1-\delta+2\alpha}).$$

This is integrable for  $\alpha < \delta/2$ . By integrating from  $t = 0$  to  $t = \pm\infty$ , since  $m$  is arbitrary this implies that:

$$\lim_{t \rightarrow \pm\infty} W_{\text{out/in}}^{\text{ad}}(t) \pi^+ W_{\text{out/in}}^{\text{ad}}(t)^{-1} - \pi^+ \in \langle x \rangle^{-\alpha} \mathcal{W}^{-\infty}(\Sigma) \langle x \rangle^{-\alpha}.$$

Since  $W_{\text{out/in}}^{\text{ad}} = \lim_{t \rightarrow \pm\infty} W_{\text{out/in}}^{\text{ad}}(t)$  this proves the proposition.  $\square$

**6.5. Inhomogeneous Cauchy problem.** Fixing  $\gamma$  with  $\frac{1}{2} < \gamma < \frac{1}{2} + \delta$ , we set:

$$\mathcal{Y}^m := \langle t \rangle^{-\gamma} L^2(\mathbb{R}; H^m), \quad \mathcal{Y}^{\text{ad},m} := \langle t \rangle^{-\gamma} L^2(\mathbb{R}; \mathcal{H}^m).$$

The exponent  $\gamma$  is chosen so that  $\mathcal{Y}^m \subset L^1(\mathbb{R}; \mathcal{E}^m)$ ,  $\mathcal{Y}^{\text{ad},m} \subset L^1(\mathbb{R}; \mathcal{H}^m)$ . The benefit of working with  $\mathcal{Y}^{(\text{ad}),m}$  is that these are Hilbert spaces; this will be needed in Subsect. 7.6.

**Definition 6.4.** We denote by  $\mathcal{X}^m$  the space of  $u \in C^0(\mathbb{R}; H^{m+1}) \cap C^1(\mathbb{R}; H^m)$  such that  $Pu \in \mathcal{Y}^m$ , and similarly by  $\mathcal{X}^{\text{ad},m}$  the space of  $u^{\text{ad}} \in C^0(\mathbb{R}; \mathcal{H}^m)$  such that  $P^{\text{ad}}u^{\text{ad}} \in \mathcal{Y}^{\text{ad},m}$ . We equip  $\mathcal{X}^{(\text{ad}),m}$  with the Hilbert norms:

$$(6.16) \quad \begin{aligned} \|u^{\text{ad}}\|_m^2 &:= \|\varrho_0^{\text{ad}} u^{\text{ad}}\|_{\mathcal{H}^m}^2 + \|P^{\text{ad}}u^{\text{ad}}\|_{\mathcal{Y}^{\text{ad},m}}^2, \\ \|u\|_m^2 &:= \|\varrho_0 u\|_{\mathcal{E}^m}^2 + \|Pu\|_{\mathcal{Y}^m}^2. \end{aligned}$$

The existence and uniqueness of the Cauchy problem for  $P$  and  $P^{\text{ad}}$  implies that  $\mathcal{X}^{(\text{ad}),m}$  are Hilbert spaces, as stated implicitly in the following lemma.

**Lemma 6.5.** *The map*

$$(6.17) \quad \begin{aligned} \varrho_0 \oplus P : \mathcal{X}^m &\rightarrow \mathcal{E}^m \oplus \mathcal{Y}^m \\ u &\mapsto (\varrho_0 u, Pu) \end{aligned}$$

is boundedly invertible with inverse given by:

$$(6.18) \quad (\varrho_0 \oplus P)^{-1}(v, f) = \pi_0 \mathcal{U}(t, 0)v - i\pi_0 \int_0^t \mathcal{U}(t, s) \pi_1^* f(s) ds.$$

Similarly, the map

$$(6.19) \quad \begin{aligned} \varrho_0^{\text{ad}} \oplus P^{\text{ad}} : \mathcal{X}^{\text{ad},m} &\rightarrow \mathcal{H}^m \oplus \mathcal{Y}^{\text{ad},m} \\ u^{\text{ad}} &\mapsto (\varrho_0^{\text{ad}} u^{\text{ad}}, P^{\text{ad}}u^{\text{ad}}) \end{aligned}$$

is boundedly invertible with inverse given by:

$$(6.20) \quad (\varrho_0^{\text{ad}} \oplus P^{\text{ad}})^{-1}(v^{\text{ad}}, f^{\text{ad}}) = \mathcal{U}^{\text{ad}}(t, 0)v^{\text{ad}} + i \int_0^t \mathcal{U}^{\text{ad}}(t, s) f^{\text{ad}}(s) ds.$$

It follows that

$$(6.21) \quad \begin{aligned} \mathcal{X}^m &\hookrightarrow C^k(\mathbb{R}; H^{m+1-k}), \\ \mathcal{X}^{\text{ad},m} &\hookrightarrow C^k(\mathbb{R}; \mathcal{H}^{m-k}), \end{aligned}$$

continuously for  $m \in \mathbb{R}$ ,  $k \in \mathbb{N}$ .

The following facts are easy computations that make use of (6.3):

$$(6.22) \quad \begin{aligned} T^{-1} \varrho &\in B(\mathcal{X}^m, \mathcal{X}^{\text{ad},m+\frac{1}{2}}), \quad -T^{-1} \pi_1^* \in B(\mathcal{Y}^m, \mathcal{Y}^{\text{ad},m+\frac{1}{2}}), \\ \pi_0 T &\in B(\mathcal{X}^{\text{ad},m+\frac{1}{2}}, \mathcal{X}^m), \quad -\pi_1 T \in B(\mathcal{Y}^{\text{ad},m+\frac{1}{2}}, \mathcal{Y}^m). \end{aligned}$$

In the sequel we will also need the auxiliary identities

$$\begin{aligned}
 \text{Ran } T^{-1}\varrho &= \text{Ker}(\varrho\pi_0 - \mathbf{1})T, \\
 (T^{-1}\varrho)^{-1} &= \pi_0 T \text{ on } \text{Ran } T^{-1}\varrho, \\
 \text{Ran } T^{-1}\pi_1^* &= \text{Ker } \pi_0 T, \\
 (T^{-1}\pi_1^*)^{-1} &= \pi_1 T \text{ on } \text{Ran } T^{-1}\pi_1^*.
 \end{aligned}
 \tag{6.23}$$

**6.6. Retarded and advanced propagators.** The retarded/advanced propagators for  $P^{\text{ad}}$  are defined as follows:

$$(G_+^{\text{ad}} f^{\text{ad}})(t) := i \int_{-\infty}^t \mathcal{U}^{\text{ad}}(t, s) f^{\text{ad}}(s) ds, \quad (G_-^{\text{ad}} f)(t) := -i \int_t^{+\infty} \mathcal{U}^{\text{ad}}(t, s) f^{\text{ad}}(s) ds,
 \tag{6.24}$$

for  $f^{\text{ad}} \in L^1(\mathbb{R}; \mathcal{H}^m)$ . Using (6.9) one obtains:

$$\begin{aligned}
 G_{\pm}^{\text{ad}} &\in B(L^1(\mathbb{R}; \mathcal{H}^m), C^0(\mathbb{R}; \mathcal{H}^m)), \\
 (G_{\pm}^{\text{ad}})^{\dagger} &= G_{\mp}^{\text{ad}} \text{ on } L^1(\mathbb{R}; \mathcal{H}^m), \quad P^{\text{ad}} G_{\pm}^{\text{ad}} = \mathbf{1} \text{ on } L^1(\mathbb{R}; \mathcal{H}^m).
 \end{aligned}$$

The analogous propagators for  $P$  are:

$$(G_+ f)(t) = -i\pi_0 \int_{-\infty}^t \mathcal{U}(t, s) \pi_1^* f ds, \quad (G_- f)(t) = i\pi_0 \int_t^{+\infty} \mathcal{U}(t, s) \pi_1^* f(s) ds,
 \tag{6.25}$$

for  $f \in L^1(\mathbb{R}; H^m)$ . One has:

$$\begin{aligned}
 G_{\pm} &\in B(L^1(\mathbb{R}; H^m), C^0(\mathbb{R}; H^{m+1}) \cap C^1(\mathbb{R}; H^m)), \\
 G_{\pm}^* &= G_{\mp} \text{ on } L^1(\mathbb{R}; H^m), \quad P G_{\pm} = \mathbf{1} \text{ on } L^1(\mathbb{R}; H^m).
 \end{aligned}$$

Using (6.4) we have the relation:

$$G_{\pm} = -\pi_0 T G_{\pm}^{\text{ad}} T^{-1} \pi_1^*.
 \tag{6.26}$$

**6.7. Fredholm problems from scattering data.** We now want to define the maps that assign to an element of  $\mathcal{X}^{(\text{ad}),m}$  its scattering data in the standard sense, as well as its Feynman and anti-Feynman data. By *Feynman data* we mean positive-frequency data of a solution at  $+\infty$  and negative-frequency data at  $-\infty$ , and by *anti-Feynman* the reverse.

**Proposition 6.6.** *The limits*

$$s\text{-}\lim_{t \rightarrow \pm\infty} \mathcal{W}_{\text{out/in}}^{\text{ad}}(0, t) \varrho_t^{\text{ad}}, \quad \text{resp. } s\text{-}\lim_{t \rightarrow \pm\infty} \mathcal{W}_{\text{out/in}}(0, t) \varrho_t,$$

exist in  $B(\mathcal{X}^{\text{ad},m}, \mathcal{H}^m)$ , resp. in  $B(\mathcal{X}^m, \mathcal{E}^m)$ , and equal  $(W_{\text{out/in}}^{\text{ad}})^{-1}$  on  $\text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}}$ , resp.  $(W_{\text{out/in}})^{-1}$  on  $\text{Ker } P|_{\mathcal{X}^m}$ .

**Proof.** Let  $u^{\text{ad}} \in \mathcal{X}^{\text{ad},m}$ . By Lemma 6.5 we have

$$\mathcal{W}_{\text{out}}^{\text{ad}}(0, t) \varrho_t^{\text{ad}} u^{\text{ad}} = \mathcal{W}_{\text{out}}^{\text{ad}}(0, t) \mathcal{U}^{\text{ad}}(t, 0) v^{\text{ad}} + i \int_0^t \mathcal{W}_{\text{out}}^{\text{ad}}(0, t) \mathcal{U}^{\text{ad}}(t, 0) \mathcal{U}^{\text{ad}}(0, s) f^{\text{ad}}(s) ds$$

which by dominated convergence tends to  $(W_{\text{out}}^{\text{ad}})^{-1}(v^{\text{ad}} - \varrho_0^{\text{ad}} G_-^{\text{ad}} f^{\text{ad}})$  as  $t \rightarrow +\infty$ . Similarly we obtain that  $\mathcal{W}_{\text{in}}^{\text{ad}}(0, t) \varrho_t^{\text{ad}} u^{\text{ad}}$  converges to  $(W_{\text{in}}^{\text{ad}})^{-1}(v^{\text{ad}} - \varrho_0^{\text{ad}} G_+^{\text{ad}} f^{\text{ad}})$  as  $t \rightarrow -\infty$ . The proof in the scalar case is similar.  $\square$

We can now introduce four scattering data maps  $\varrho_I^{(\text{ad})} : \mathcal{X}^{(\text{ad}),m} \rightarrow \mathcal{H}^m$ . Note the presence of the operators  $T_{\text{out/in}}^{-1}$  below; this simplifies some considerations later on.

**Definition 6.7.** *We set:*

$$\begin{aligned}\varrho_{\text{out/in}}^{\text{ad}} &:= \text{s-}\lim_{t \rightarrow \pm\infty} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \varrho_t^{\text{ad}}, \\ \varrho_{\text{out/in}} &:= \text{s-}\lim_{t \rightarrow \pm\infty} T_{\text{out/in}}^{-1} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \varrho_t, \\ \varrho_{\text{F}}^{(\text{ad})} &:= \pi^+ \varrho_{\text{out}}^{(\text{ad})} + \pi^- \varrho_{\text{in}}^{(\text{ad})}, \\ \varrho_{\overline{\text{F}}}^{(\text{ad})} &:= \pi^- \varrho_{\text{out}}^{(\text{ad})} + \pi^+ \varrho_{\text{in}}^{(\text{ad})}.\end{aligned}$$

**Lemma 6.8.** *For  $I \in \{\text{in}, \text{out}, \text{F}, \overline{\text{F}}\}$  we have:*

$$(6.27) \quad \varrho_I = \varrho_I^{\text{ad}} T^{-1} \varrho,$$

$$(6.28) \quad \varrho_I^{\text{ad}} = W_I^{\text{ad}\dagger} \circ \varrho_0^{\text{ad}} \text{ on } \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad}, m}},$$

$$\varrho_I = W_I^{\text{ad}\dagger} T^{-1}(0) \varrho_0 \text{ on } \text{Ker } P|_{\mathcal{X}^m},$$

for  $I \in \{\text{in}, \text{out}, \text{F}, \overline{\text{F}}\}$ , where

$$(6.29) \quad W_{\text{F}}^{\text{ad}\dagger} := \pi^+ W_{\text{out}}^{\text{ad}\dagger} + \pi^- W_{\text{in}}^{\text{ad}\dagger}, \quad W_{\overline{\text{F}}}^{\text{ad}\dagger} := \pi^- W_{\text{out}}^{\text{ad}\dagger} + \pi^+ W_{\text{in}}^{\text{ad}\dagger}.$$

**Proof.** To prove (6.27) we write:

$$\begin{aligned}\varrho_{\text{out/in}} &= T_{\text{out/in}}^{-1} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \varrho_t + o(1) = \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) T_{\text{out/in}}^{-1} \varrho_t + o(1) \\ &= \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) T^{-1}(t) \varrho_t + o(1) = \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \varrho_t^{\text{ad}} T^{-1} \varrho + o(1).\end{aligned}$$

This implies (6.27) for  $I = \text{out/in}$  and then for  $I = \text{F}/\overline{\text{F}}$ . The first statement of (6.28) follows then from the fact that  $\varrho_{\text{out/in}}^{\text{ad}} = W_{\text{out/in}}^{\text{ad}\dagger}$  on  $\text{Ker } P^{\text{ad}}$ , the second from (6.27) and the fact that  $T^{-1} \varrho : \text{Ker } P \rightarrow \text{Ker } P^{\text{ad}}$ .  $\square$

**Lemma 6.9.** *Let  $I \in \{\text{F}, \overline{\text{F}}\}$ . Then  $W_I^{\text{ad}} W_I^{\text{ad}\dagger} - \mathbf{1}$  and  $W_I^{\text{ad}\dagger} W_I^{\text{ad}} - \mathbf{1}$  are compact on  $\mathcal{H}^m$  and hence  $W_I^{\text{ad}}, W_I^{\text{ad}\dagger}$  are Fredholm. Moreover:*

$$\text{Ker } W_I^{\text{ad}(\dagger)}|_{\mathcal{H}^m} = \text{Ker } W_I^{\text{ad}(\dagger)}|_{\mathcal{E}^{\text{ad}, \infty}}, \quad \text{coKer } W_I^{\text{ad}(\dagger)}|_{\mathcal{H}^m} = \text{coKer } W_I^{\text{ad}(\dagger)}|_{\mathcal{E}^{\text{ad}, -\infty}},$$

and hence  $\text{ind}(W_I^{\text{ad}(\dagger)})|_{\mathcal{H}^m}$  is independent on  $m$ .

**Proof.** We consider only the F case. We have

$$W_{\text{F}}^{\text{ad}} W_{\text{F}}^{\text{ad}\dagger} = \mathbf{1} + K_1, \quad K_1 = W_{\text{out}}^{\text{ad}} \pi^+ (W_{\text{out}}^{\text{ad}})^{-1} - \pi^+ + W_{\text{in}}^{\text{ad}} \pi^- (W_{\text{in}}^{\text{ad}})^{-1} - \pi^-,$$

$$W_{\text{F}}^{\text{ad}\dagger} W_{\text{F}}^{\text{ad}} = \mathbf{1} + K_2, \quad K_2 = \pi^+ (W_{\text{out}}^{\text{ad}})^{-1} W_{\text{in}}^{\text{ad}} \pi^- + \pi^- (W_{\text{in}}^{\text{ad}})^{-1} W_{\text{out}}^{\text{ad}} \pi^+.$$

By Prop. 6.2 we see that  $K_1, K_2$  are compact on  $\mathcal{H}^m$  and moreover map  $\mathcal{H}^m$  to  $\mathcal{H}^\infty$ . Therefore  $\text{Ker } W_{\text{F}}^{\text{ad}\dagger}|_{\mathcal{H}^m} \subset \text{Ker}(\mathbf{1} + K_1)|_{\mathcal{H}^m} \subset \mathcal{H}^\infty$  hence  $\text{Ker } W_{\text{F}}^{\text{ad}\dagger}|_{\mathcal{H}^m} = \text{Ker } W_{\text{F}}^{\text{ad}\dagger}|_{\mathcal{H}^\infty}$ . Similarly, identifying  $(\mathcal{H}^m)^*$  with  $\mathcal{H}^{-m}$  and  $\text{coKer } A$  with  $\text{Ker } A^*$  we have  $\text{coKer } W_{\text{F}}^{\text{ad}\dagger}|_{\mathcal{H}^m} \subset \text{Ker}(\mathbf{1} + K_2^*)|_{\mathcal{H}^m} \subset \mathcal{H}^\infty$ , hence  $\text{coKer } W_{\text{F}}^{\text{ad}\dagger}|_{\mathcal{H}^m} = \text{coKer } W_{\text{F}}^{\text{ad}\dagger}|_{\mathcal{H}^{-\infty}}$ .  $\square$

We will need the following lemma, see [BB, Prop. A.1] for its proof. The next few results are simple applications of it, following the strategy in [BS1] in the case of the Dirac equation on a compact cylinder.

**Lemma 6.10.** *Let  $\mathcal{K}$  be a Hilbert space and  $\mathcal{E}, \mathcal{F}$  Banach spaces. Let  $K : \mathcal{K} \rightarrow \mathcal{E}, Q : \mathcal{K} \rightarrow \mathcal{F}$  be bounded and assume that  $Q$  is surjective. Then  $K : \text{Ker } Q \rightarrow \mathcal{E}$  is Fredholm (of index  $l$ ) iff  $K \oplus Q : \mathcal{K} \rightarrow \mathcal{E} \oplus \mathcal{F}$  is Fredholm (of index  $l$ ).*

**Lemma 6.11.** *For  $I \in \{\text{in}, \text{out}, \text{F}, \overline{\text{F}}\}$ , the operator*

$$\varrho_I^{(\text{ad})} : \{u^{(\text{ad})} \in \mathcal{X}^{(\text{ad}), m} : P^{(\text{ad})} u^{(\text{ad})} = 0\} \rightarrow \mathcal{H}^m$$

is Fredholm of index equal  $\text{ind } W_I^{\text{ad}\dagger}$  and is invertible for  $I \in \{\text{in}, \text{out}\}$ .

**Proof.** We apply (6.28) and the fact that  $\varrho_0^{\text{ad}} : \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}} \rightarrow \mathcal{H}^m$  and  $T^{-1}(0)\varrho_0 : \text{Ker } P|_{\mathcal{X}^m} \rightarrow \mathcal{H}^{m+\frac{1}{2}}$  are bijections, by Lemma 6.5.  $\square$

**Lemma 6.12.** *The maps*

$$\begin{aligned}\varrho_I^{\text{ad}} \oplus P^{\text{ad}} &: \mathcal{X}^{\text{ad},m} \rightarrow \mathcal{H}^m \oplus \mathcal{Y}^{\text{ad},m}, \\ \varrho_I \oplus P &: \mathcal{X}^m \rightarrow \mathcal{H}^{m+\frac{1}{2}} \oplus \mathcal{Y}^m,\end{aligned}$$

are Fredholm of index  $\text{ind } W_I^{\text{ad}\dagger}$ .

**Proof.** We use Lemma 6.10 with  $\mathcal{K} = \mathcal{X}^{\text{ad},m}$  resp.  $\mathcal{X}^m$ ,  $\mathcal{E} = \mathcal{H}^m$  resp.  $\mathcal{H}^{m+\frac{1}{2}}$ ,  $\mathcal{F} = \mathcal{Y}^{\text{ad},m}$  resp.  $\mathcal{Y}^m$ ,  $K = \varrho_I^{\text{ad}}$  resp.  $\varrho_I$ ,  $Q = P^{\text{ad}}$  resp.  $P$ . The assumptions of Lemma 6.10 are satisfied in view of Lemma 6.11 and Lemma 6.5 which gives surjectivity of  $P^{\text{ad}}$  resp.  $P$ .  $\square$

Let us introduce the following notation: if  $I = \text{in/out}$  then  $I^c := \text{out/in}$  and if  $I = \text{F}/\overline{\text{F}}$  then  $I^c := \overline{\text{F}}/\text{F}$ .

**Theorem 6.13.** *Let  $\mathcal{X}_I^{(\text{ad}),m} := \{u \in \mathcal{X}^{(\text{ad}),m} : \varrho_{I^c}^{(\text{ad})}u = 0\}$ , equipped with the topology of  $\mathcal{X}^{(\text{ad}),m}$ . Then*

$$\begin{aligned}P^{\text{ad}} &: \mathcal{X}_I^{\text{ad},m} \rightarrow \mathcal{Y}^{\text{ad},m}, \\ P &: \mathcal{X}_I^m \rightarrow \mathcal{Y}^m\end{aligned}$$

are Fredholm of index  $\text{ind } W_{I^c}^{\text{ad}\dagger}$ .

**Proof.** It suffices to check the assumptions of Lemma 6.10 for  $\mathcal{K} = \mathcal{X}^{\text{ad},m}$  resp.  $\mathcal{X}^m$ ,  $\mathcal{E} = \mathcal{Y}^{\text{ad},m}$  resp.  $\mathcal{Y}^m$ ,  $\mathcal{F} = \mathcal{H}^m$  resp.  $\mathcal{H}^{m+\frac{1}{2}}$ ,  $K = P^{\text{ad}}$  resp.  $P$ , and  $Q = \varrho_{I^c}^{\text{ad}}$  resp.  $\varrho_{I^c}$ . The Fredholm property of  $K \oplus Q$  follows from Lemma 6.12, so it remains to check that  $\varrho_{I^c}^{\text{ad}} : \mathcal{X}^{\text{ad},m} \rightarrow \mathcal{H}^m$  and  $\varrho_{I^c} : \mathcal{X}^m \rightarrow \mathcal{H}^{m+\frac{1}{2}}$  are surjective. This is obvious if  $I = \text{out/in}$  using (6.28) and Lemma 6.5. Let us now consider the case  $I = \text{F}$ .

Let  $\eta_{\text{out/in}} \in C^\infty(\mathbb{R})$  with  $\eta_{\text{in}}(t) + \eta_{\text{out}}(t) = 1$  and  $\eta_{\text{out/in}}(t) = 1$  for large  $\pm t$ . Then

$$\varrho_{\text{out/in}}^{(\text{ad})} \circ \eta_{\text{out/in}} = \varrho_{\text{out/in}}^{(\text{ad})}, \quad \varrho_{\text{in/out}}^{(\text{ad})} \circ \eta_{\text{out/in}} = 0.$$

Furthermore  $\eta_{\text{out/in}} \text{Ker } P^{(\text{ad})}|_{\mathcal{X}^{(\text{ad}),m}} \subset \mathcal{X}^{(\text{ad}),m}$ . It follows that

$$\begin{aligned}\varrho_{\text{F}}^{\text{ad}} \mathcal{X}^{\text{ad},m} &\supset \varrho_{\text{F}}^{\text{ad}}(\eta_{\text{in}} \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}} + \eta_{\text{out}} \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}}) \\ &= (\pi^+ \varrho_{\text{out}}^{\text{ad}} + \pi^- \varrho_{\text{in}}^{\text{ad}})(\eta_{\text{in}} \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}} + \eta_{\text{out}} \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}}) \\ &= \pi^+ \varrho_{\text{out}}^{\text{ad}} \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}} + \pi^- \varrho_{\text{in}}^{\text{ad}} \text{Ker } P^{\text{ad}}|_{\mathcal{X}^{\text{ad},m}} = \pi^+ \mathcal{H}^m + \pi^- \mathcal{H}^m = \mathcal{H}^m.\end{aligned}$$

This proves  $\varrho_{\text{F}}^{\text{ad}} : \mathcal{X}^{\text{ad},m} \rightarrow \mathcal{H}^m$  is surjective. The same argument shows that  $\varrho_{\text{F}} : \mathcal{X}^m \rightarrow \mathcal{H}^{m+\frac{1}{2}}$  is surjective. In the analogous way we obtain surjectivity of  $\varrho_{\overline{\text{F}}}^{(\text{ad})}$ .  $\square$

**6.8. Retarded/advanced propagators.** We now show that as anticipated, the retarded/advanced propagators  $G_{\pm}^{\text{ad}}$  are the inverses of  $P^{\text{ad}} : \mathcal{X}_{\text{out/in}}^{\text{ad},m} \rightarrow \mathcal{Y}^{\text{ad},m}$ , and a similar statement holds true in the scalar case.

**Proposition 6.14.**  *$P^{(\text{ad})} : \mathcal{X}_{\text{out/in}}^{(\text{ad}),m} \rightarrow \mathcal{Y}^{(\text{ad}),m}$  are boundedly invertible with inverse equal to  $G_{\pm}^{(\text{ad})}$ .*

**Proof.** We only treat the case of  $G_+^{(\text{ad})}$ . We have seen in Subsect. 6.6 that

$$G_+^{\text{ad}} \in B(L^1(\mathbb{R}; \mathcal{H}^m), C^0(\mathbb{R}; \mathcal{H}^m))$$

and  $P^{\text{ad}}G_+^{\text{ad}} = \mathbf{1}$  on  $L^1(\mathbb{R}; \mathcal{H}^m)$ , hence  $G_+^{\text{ad}} \in B(\mathcal{Y}^{\text{ad},m}, \mathcal{X}^{\text{ad},m})$  and  $P^{\text{ad}}G_+^{\text{ad}} = \mathbf{1}$  on  $\mathcal{Y}^{\text{ad},m}$ . Since  $\lim_{t \rightarrow -\infty} \varrho_t^{\text{ad}} G_+^{\text{ad}} f^{\text{ad}} = 0$ , we have  $G_+^{\text{ad}} \mathcal{Y}^{\text{ad},m} \subset \mathcal{X}_{\text{out}}^{\text{ad},m}$ . It remains to show that  $G_+^{\text{ad}} P^{\text{ad}} = \mathbf{1}$  on  $\mathcal{X}_{\text{out}}^{\text{ad},m}$ . If  $u^{\text{ad}} \in \mathcal{X}_{\text{out}}^{\text{ad},m}$  we have:

$$\begin{aligned} (G_+^{\text{ad}} P^{\text{ad}} u^{\text{ad}})(t) &= \int_{-\infty}^t \mathcal{W}^{\text{ad}}(t, s) (\bar{\partial}_s - iH^{\text{ad}}(s)) u^{\text{ad}} ds \\ &= \lim_{t_+ \rightarrow -\infty} \int_{-\infty}^t \mathcal{W}^{\text{ad}}(t, s) (\bar{\partial}_s - iH^{\text{ad}}(s)) u^{\text{ad}} ds \\ &= \lim_{t_+ \rightarrow -\infty} [\mathcal{W}^{\text{ad}}(t, s) u(s)]_{t_+}^t - \lim_{t_+ \rightarrow -\infty} \int_{t_+}^t (-\bar{\partial}_s + iH^{\text{ad}}(s)) \mathcal{W}^{\text{ad}}(t, s) u^{\text{ad}}(s) ds \\ &= u^{\text{ad}}(t), \end{aligned}$$

since  $\lim_{t_+ \rightarrow -\infty} u^{\text{ad}}(t_+) = 0$  in view of  $u^{\text{ad}} \in \mathcal{X}_{\text{out}}^{\text{ad},m}$ . In the scalar case we obtain from (6.3) that  $(D_t - H(t)) T G_+^{\text{ad}} T^{-1} = \mathbf{1}$  hence  $(\varrho \pi_0 - \mathbf{1}) T G_+^{\text{ad}} T^{-1} \pi_1^* = 0$  which implies that  $P G_+ = \mathbf{1}$  on  $\mathcal{Y}^m$ . Conversely, by (6.22), (6.27) we know that  $T^{-1} \varrho : \mathcal{X}_{\text{out}}^m \rightarrow \mathcal{X}_{\text{out}}^{\text{ad},m+\frac{1}{2}}$ . Since  $G_+^{\text{ad}} P^{\text{ad}} = \mathbf{1}$  on  $\mathcal{X}^{\text{ad},m+\frac{1}{2}}$  this yields

$$T G_+^{\text{ad}} T^{-1} (D_t - H(t)) \varrho = T G_+^{\text{ad}} P^{\text{ad}} T^{-1} \varrho = \varrho \text{ on } \mathcal{X}_{\text{out}}^m,$$

hence  $G_+ P = \mathbf{1}$  on  $\mathcal{X}_{\text{out}}^m$  using  $(D_t - H(t)) \varrho = \pi_1^* \pi_1 (D_t - H(t))$ . This completes the proof.  $\square$

**6.9. The Fredholm inverses for  $P^{(\text{ad})}$  on  $\mathcal{X}_{\text{F}}^{(\text{ad}),m}$ .** From Thm. 6.13 we know that  $P^{(\text{ad})} : \mathcal{X}_{\text{F}}^{(\text{ad}),m} \rightarrow \mathcal{Y}^{(\text{ad}),m}$  are Fredholm. We will now construct explicit approximate inverses  $G_{\text{F}}^{(\text{ad})}$  of  $P^{(\text{ad})} : \mathcal{X}_{\text{F}}^{(\text{ad}),m} \rightarrow \mathcal{Y}^m$ , which requires some special care because of the requirement  $\varrho_{\text{F}}^{(\text{ad})} \circ G_{\text{F}}^{(\text{ad})} = 0$  that follows from the definition of  $\mathcal{X}_{\text{F}}^{(\text{ad}),m}$  (in fact, for instance the time-ordered Feynman propagators associated to the *in* or *out* state<sup>11</sup> fail to satisfy this condition in general). We will then show that  $G_{\text{F}}$  has Feynman-type wavefront set.

**6.9.1. Auxiliary diagonal Hamiltonian.** We denote by  $H^{\text{d}}(t)$  the diagonal part of  $H^{\text{ad}}(t)$ , see Subsect. 4.3. We recall that:

$$(6.30) \quad \begin{aligned} V_{-\infty}^{\text{ad}}(t) &= H^{\text{d}}(t) - H^{\text{ad}}(t) \in \Psi_{\text{std}}^{-\infty, -1-\delta}(\mathbb{R}; \mathbb{R}^d) \otimes \mathbb{C}^2, \\ H^{\text{d}}(t) &= \begin{pmatrix} \epsilon^+(t) & 0 \\ 0 & \epsilon^-(t) \end{pmatrix}, \text{ where} \\ \epsilon^{\pm}(t) &= \epsilon^{\pm}(t)^*, \quad \epsilon^{\pm}(t) \mp \epsilon(t) \in \Psi_{\text{std}}^{0, -1-\delta}(\mathbb{R}; \mathbb{R}^d). \end{aligned}$$

Let  $\mathcal{W}^{\text{d}}(t, s)$  be the evolution generated by the Hamiltonian  $H^{\text{d}}(t)$  defined in (6.6). Using (6.30) we see that  $\mathcal{W}^{\text{d}}(t, s)$  is well defined and moreover  $\sup_{t, s \in \mathbb{R}} \|\mathcal{W}^{\text{d}}(t, s)\|_{B(\mathcal{H}^m)} < \infty$  using the same argument as for  $\mathcal{W}(t, s)$ . Since  $H^{\text{d}}(t) = H^{\text{d}\dagger}(t)$  we also have

$$(6.31) \quad \mathcal{W}^{\text{d}}(t, s)^\dagger = \mathcal{W}^{\text{d}}(s, t).$$

We set correspondingly

$$P^{\text{d}} := D_t - H^{\text{d}}(t) = P^{\text{ad}} - V_{-\infty}^{\text{ad}}(t).$$

Note that since  $\|V_{-\infty}^{\text{ad}}(t)\|_{B(\mathcal{H}^m)} = O(\langle t \rangle^{-1-\delta})$  and we have assumed that  $\gamma < \frac{1}{2} + \delta$ , we see that for  $u \in C^0(\mathbb{R}; \mathcal{H}^m)$  we have  $P^{\text{ad}} u \in \mathcal{Y}^{\text{ad},m}$  if and only if  $P^{\text{d}} u \in \mathcal{Y}^{\text{ad},m}$  and the two norms in (6.16) on  $\mathcal{X}^{\text{ad},m}$  defined with  $P^{\text{ad}}$  and  $P^{\text{d}}$  are equivalent.

Finally we define the operator  $\mathcal{W}^{\text{d}} : \mathcal{H}^m \rightarrow \mathcal{X}^m$  by:

$$(6.32) \quad \mathcal{W}^{\text{d}} v^{\text{ad}}(t) := \mathcal{W}^{\text{d}}(t, 0) v^{\text{ad}}, \quad v^{\text{ad}} \in \mathcal{H}^m.$$

<sup>11</sup>These are analysed for instance by Isozaki in [Is].

By the remark above,  $\mathcal{U}^d \in B(\mathcal{H}^m, \mathcal{X}^{\text{ad},m})$ .

6.9.2. *Fredholm inverse for  $P^{\text{ad}}$  on  $\mathcal{X}_F^{\text{ad},m}$ .*

**Definition 6.15.** We set for  $f^{\text{ad}} \in \mathcal{Y}^{\text{ad},m}$ :

$$G_F^{\text{ad}} f^{\text{ad}}(t) := i \int_{-\infty}^t \mathcal{U}^d(t,0) \pi^+ \mathcal{U}^d(0,s) f^{\text{ad}}(s) ds - i \int_t^{+\infty} \mathcal{U}^d(t,0) \pi^- \mathcal{U}^d(0,s) f^{\text{ad}}(s) ds.$$

Using the ‘time-kernel notation’  $A(t,s) := \varrho_t \circ A \circ \varrho_s^*$  we can write:

$$\begin{aligned} G_F^{\text{ad}}(t,s) &= i\theta(t-s) \mathcal{U}^d(t,0) \pi^+ \mathcal{U}^d(0,s) - i\theta(s-t) \mathcal{U}^d(t,0) \pi^- \mathcal{U}^d(0,s) \\ &= i\mathcal{U}^d(t,0) \pi^+ \mathcal{U}^d(0,s) - i\theta(s-t) \mathcal{U}^d(t,s), \end{aligned}$$

where  $\theta$  is the Heaviside step function. Let us also observe that since  $[\mathcal{U}^d(t,s), \pi^\pm] = 0$ , we have

$$(6.33) \quad G_F^{\text{ad}} = G_+^d \pi^+ + G_-^d \pi^-,$$

where  $G_\pm^d$  are the retarded/advanced propagators for  $H^d(t)$ , defined in analogy to  $G_\pm^{\text{ad}}$ .

**Theorem 6.16.** Let  $m \in \mathbb{R}$ . We have:

- i)  $G_F^{\text{ad}} \in B(\mathcal{Y}^{\text{ad},m}, \mathcal{X}_F^{\text{ad},m})$ ,  $P^{\text{ad}} G_F^{\text{ad}} = \mathbf{1}_{\mathcal{Y}^{\text{ad},m}} + K_{\mathcal{Y}^{\text{ad},m}}$ , where  $K_{\mathcal{Y}^{\text{ad},m}}$  is compact on  $\mathcal{Y}^{\text{ad},m}$ ,
- ii)  $G_F^{\text{ad}} P^{\text{ad}} = \mathbf{1}_{\mathcal{X}_F^{\text{ad},m}} + K_{\mathcal{X}_F^{\text{ad},m}}$ , where  $K_{\mathcal{X}_F^{\text{ad},m}}$  is compact on  $\mathcal{X}_F^{\text{ad},m}$ ,
- iii)  $i^{-1} q^{\text{ad}}(G_F^{\text{ad}} - (G_F^{\text{ad}})^\dagger) \geq 0$  on  $\mathcal{Y}^{\text{ad},m}$ , for  $m \geq 0$ .

To prove Thm. 6.16 we will need the following lemma.

**Lemma 6.17.**  $V_{-\infty}^{\text{ad}} : \mathcal{X}^{\text{ad},m} \rightarrow \mathcal{Y}^{\text{ad},m}$  is compact.

**Proof.** From (6.21) we first obtain that the injection  $\mathcal{X}^{\text{ad},m} \hookrightarrow C^k(\mathbb{R}; \mathcal{H}^{m-k})$  is bounded for any  $k \in \mathbb{N}$ ,  $m \in \mathbb{R}$ . We pick  $\varepsilon > 0$  such that  $\gamma < \frac{1}{2} + \delta - \varepsilon$  and write  $V_{-\infty}^{\text{ad}}(t)$  as  $\langle t \rangle^{-1-\delta+\varepsilon} \langle x \rangle^{-\varepsilon} Y^{\text{ad}}(t)$ , where  $Y^{\text{ad}}(t) \in C^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\mathbb{R}^d) \otimes B(\mathbb{C}^2))$ . It follows that  $Y^{\text{ad}} : C^k(\mathbb{R}; \mathcal{H}^m) \rightarrow C^k(\mathbb{R}; \mathcal{H}^{m'})$  is bounded for any  $m, m' \in \mathbb{R}$ ,

$$(6.34) \quad V_{-\infty}^{\text{ad}} : \mathcal{X}^m \rightarrow \langle t \rangle^{-1-\delta+\varepsilon} C^k(\mathbb{R}; \mathcal{H}^{m'}) \text{ is compact for any } k \in \mathbb{N}, m, m' \in \mathbb{R}.$$

We use (6.34) for  $k = 0, s' = s$ , and the fact that the injection  $\langle t \rangle^{-1-\delta+\varepsilon} C^0(\mathbb{R}; \mathcal{H}^m) \hookrightarrow \langle t \rangle^{-\gamma} L^2(\mathbb{R}; \mathcal{H}^m) = \mathcal{Y}^{\text{ad},m}$  is bounded since  $\gamma < \frac{1}{2} + \delta - \varepsilon$ . It follows that  $V_{-\infty}^{\text{ad}} : \mathcal{X}^{\text{ad},m} \rightarrow \mathcal{Y}^{\text{ad},m}$  is compact.  $\square$

**Proof of Thm. 6.16** *Proof of i):* note first that  $G_F^{\text{ad}} = G_+^d \pi^+ + G_-^d \pi^- \in B(\mathcal{Y}^{\text{ad},m}, \mathcal{X}^{\text{ad},m})$  since  $G_\pm^d \in B(\mathcal{Y}^{\text{ad},m}, \mathcal{X}^{\text{ad},m})$ . We then have:

$$\begin{aligned} P^{\text{ad}} G_F^{\text{ad}} &= P^{\text{d}} G_F^{\text{ad}} + V_{-\infty}^{\text{ad}} G_F^{\text{ad}} \\ &= P^{\text{d}} G_+^d \pi^+ + P^{\text{d}} G_-^d \pi^- + V_{-\infty}^{\text{ad}} G_F^{\text{ad}} \\ &= \mathbf{1}_{\mathcal{Y}^{\text{ad},m}} + V_{-\infty}^{\text{ad}} G_F^{\text{ad}}, \end{aligned}$$

by Prop. 6.14 applied to  $P^{\text{d}}$ . By Lemma 6.17,  $V_{-\infty}^{\text{ad}} G_F^{\text{ad}}$  is compact on  $\mathcal{Y}^{\text{ad},m}$ .

It remains to check that  $G_F^{\text{ad}} : \mathcal{Y}^{\text{ad},m} \rightarrow \mathcal{X}_F^{\text{ad},m}$ , i.e.  $\pi^+ \varrho_{\text{in}}^{\text{ad}} G_F^{\text{ad}} = \pi^- \varrho_{\text{out}}^{\text{ad}} G_F^{\text{ad}} = 0$ . We have:

$$\pi^+ \varrho_{\text{in}}^{\text{ad}} G_F^{\text{ad}} = \varrho_{\text{in}}^{\text{ad}} \pi^+ (G_+^d \pi^+ + G_-^d \pi^-) = \varrho_{\text{in}}^{\text{ad}} G_+^d \pi^+ = 0,$$

since  $[G_\pm^d, \pi^\pm] = 0$  and  $\varrho_{\text{in}}^{\text{ad}} G_+^d = 0$ . Similarly we obtain that  $\pi^- \varrho_{\text{out}}^{\text{ad}} G_F^{\text{ad}} = 0$ , which completes the proof of i).

*Proof of ii):* we have by (6.33):

$$G_{\mathbb{F}}^{\text{ad}} P^{\text{ad}} = G_{\mathbb{F}}^{\text{ad}} P^{\text{d}} + G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}} = G_{+}^{\text{d}} P^{\text{d}} \pi^{+} + G_{-}^{\text{d}} P^{\text{d}} \pi^{-} + G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}}.$$

If  $u \in \mathcal{X}_{\mathbb{F}}^{\text{ad},m}$  we have  $\pi^{+} \varrho_{\text{in}}^{\text{ad}} u = \varrho_{\text{in}}^{\text{ad}} \pi^{+} u = 0$  and  $\pi^{-} \varrho_{\text{out}}^{\text{ad}} u = \varrho_{\text{out}}^{\text{ad}} \pi^{-} u = 0$ . By Prop. 6.14 applied to  $P^{\text{d}}$  we have  $G_{+}^{\text{d}} P^{\text{d}} \pi^{+} u = \pi^{+} u$ ,  $G_{-}^{\text{d}} P^{\text{d}} \pi^{-} u = \pi^{-} u$ , hence

$$G_{\mathbb{F}}^{\text{ad}} P^{\text{ad}} = \mathbf{1}_{\mathcal{X}_{\mathbb{F}}^{\text{ad},m}} + G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}}.$$

Again, by Lemma 6.17  $G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}}$  is compact on  $\mathcal{X}^{\text{ad},m}$ .

*Proof of iii):* using the time-kernel notation we have by (6.31)

$$\begin{aligned} (G_{\mathbb{F}}^{\text{ad}})^{\dagger}(t, s) &= G_{\mathbb{F}}^{\text{ad}}(s, t)^{\dagger} \\ &= i\theta(t-s)\mathcal{W}^{\text{d}}(t, 0)\pi^{-}\mathcal{W}^{\text{d}}(0, s) - i\theta(s-t)\mathcal{W}^{\text{d}}(t, 0)\pi^{+}\mathcal{W}^{\text{d}}(0, s), \end{aligned}$$

hence

$$i^{-1}(G_{\mathbb{F}}^{\text{ad}} - (G_{\mathbb{F}}^{\text{ad}})^{\dagger})(t, s) = \mathcal{W}^{\text{d}}(t, 0)(\pi^{+} - \pi^{-})\mathcal{W}^{\text{d}}(0, s) =: \mathcal{W}^{\text{d}}(t)q^{\text{ad}}(\mathcal{W}^{\text{d}})^{\dagger}(s),$$

where  $\mathcal{W}^{\text{d}}$  is defined in (6.32). It follows that

$$i^{-1}(f^{\text{ad}}|q^{\text{ad}}(G_{\mathbb{F}}^{\text{ad}} - (G_{\mathbb{F}}^{\text{ad}})^{\dagger})f^{\text{ad}})_{\mathcal{H}^0} = ((\mathcal{W}^{\text{d}})^{\dagger}f^{\text{ad}}|(q^{\text{ad}})^2(\mathcal{W}^{\text{d}})^{\dagger}f^{\text{ad}})_{\mathcal{H}^0} \geq 0,$$

hence  $i^{-1}q^{\text{ad}}(G_{\mathbb{F}}^{\text{ad}} - (G_{\mathbb{F}}^{\text{ad}})^{\dagger}) \geq 0$  on  $\mathcal{H}^0$  hence on  $\mathcal{H}^m$  for  $m \geq 0$ .  $\square$

### 6.9.3. Fredholm inverse for $P$ on $\mathcal{X}_{\mathbb{F}}^m$ .

**Theorem 6.18.** *Assume (std). Let*

$$(6.35) \quad G_{\mathbb{F}} := -\pi_0 T G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^*.$$

*We have:*

- i)  $G_{\mathbb{F}} \in B(\mathcal{Y}^m, \mathcal{X}_{\mathbb{F}}^m)$ ,  $P G_{\mathbb{F}} = \mathbf{1}_{\mathcal{Y}^m} + K_{\mathcal{Y}^m}$ , where  $K_{\mathcal{Y}^m}$  is compact on  $\mathcal{Y}^m$ ,
- ii)  $G_{\mathbb{F}} P = \mathbf{1}_{\mathcal{X}_{\mathbb{F}}^m} + K_{\mathcal{X}_{\mathbb{F}}^m}$ , where  $K_{\mathcal{X}_{\mathbb{F}}^m}$  is compact on  $\mathcal{X}_{\mathbb{F}}^m$ ,
- iii)  $i^{-1}(G_{\mathbb{F}} - G_{\mathbb{F}}^*) \geq 0$  on  $\mathcal{Y}^m$ , for  $m \geq 0$ ,
- iv)  $P G_{\mathbb{F}} - \mathbf{1}$ ,  $G_{\mathbb{F}} P - \mathbf{1}$  are smoothing operators,
- v)  $\text{WF}(G_{\mathbb{F}})' = (\text{diag}_{T^*M}) \cup \bigcup_{t \leq 0} (\Phi_t(\text{diag}_{T^*M}) \cap \pi^{-1}\mathcal{N})$ .

*In particular  $G_{\mathbb{F}}$  is a Feynman parametrix of  $P$  in the sense of [DH].*

**Proof.** *Proof of i):* from (6.22) and Thm. 6.16 we see that  $G_{\mathbb{F}} \in B(\mathcal{Y}^m, \mathcal{X}^m)$ . Let us show that  $G_{\mathbb{F}}$  maps  $\mathcal{Y}^m$  into  $\mathcal{X}_{\mathbb{F}}^m$ . For  $V_{-\infty}^{\text{ad}}$  the operator introduced in (6.30) we have:

$$P^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} = \mathbf{1} + V_{-\infty}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} \Rightarrow T P^{\text{ad}} T^{-1} T G_{\mathbb{F}}^{\text{ad}} T^{-1} = \mathbf{1} + T V_{-\infty}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1}.$$

Using (6.3) this implies that:

$$(6.36) \quad (D_t - H(t)) T G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* = \pi_1^* + T V_{-\infty}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* =: \pi_1^* + R_1,$$

where  $R_1 \in B(\mathcal{Y}^m, \langle t \rangle^{-1-\delta} C^0(\mathbb{R}; \mathcal{E}^m))$ , using that  $V_{-\infty}^{\text{ad}} \in \Psi_{\text{std}}^{-\infty, -1-\delta}(\mathbb{R}; \mathbb{R}^d) \otimes B(\mathbb{C}^2)$ . This implies that

$$\varrho \pi_0 T G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* = T G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* + R_2,$$



where  $R_2 \in B(\mathcal{Y}^m, \langle t \rangle^{-1-\delta} C^0(\mathbb{R}; \mathcal{E}^m))$ . We now have:

$$\begin{aligned}
\mathcal{U}_{\text{out/in}}(0, t) \varrho_t G_{\mathbb{F}} f &= -\mathcal{U}_{\text{out/in}}(0, t) \varrho_t \pi_0 T G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* f \\
&= -\mathcal{U}_{\text{out/in}}(0, t) T(t) \varrho_t^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* f + o(1) \\
&= -T_{\text{out/in}} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) T_{\text{out/in}}^{-1} T(t) \varrho_t^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* f + o(1) \\
&= -T_{\text{out/in}} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \varrho_t^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* f + o(1) \\
&= -T_{\text{out/in}} \varrho_{\text{out/in}}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* f + o(1),
\end{aligned}$$

hence

$$(6.37) \quad \varrho_{\text{out/in}} G_{\mathbb{F}} = -\varrho_{\text{out/in}}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^*.$$

By Thm. 6.16 we have  $\varrho_{\mathbb{F}}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} = 0$ , i.e.  $\pi^- \varrho_{\text{out}}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} = \pi^+ \varrho_{\text{in}}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}} = 0$ , which by (6.37) gives  $\varrho_{\mathbb{F}} G_{\mathbb{F}} = 0$ . It follows that  $G_{\mathbb{F}}$  maps  $\mathcal{Y}^m$  to  $\mathcal{X}_{\mathbb{F}}^m$  as claimed.

From (6.36), we obtain by an easy computation:

$$(6.38) \quad P G_{\mathbb{F}} = \mathbf{1} - \pi_1 R_1 - D_t \pi_0 R_1 + i r \pi_0 R_1.$$

Using (6.34) we obtain that  $R_1 : \mathcal{Y}^m \rightarrow \langle t \rangle^{-1-\delta+\varepsilon} C^k(\mathbb{R}; \mathcal{E}^{m'})$  is compact for any  $m, m', k$ , hence  $P G_{\mathbb{F}} - \mathbf{1}$  is compact on  $\mathcal{Y}^m$ .

*Proof of ii):* by Thm. 6.16 and (6.3) we know that:

$$G_{\mathbb{F}}^{\text{ad}} T^{-1} (D_t - H(t)) T = G_{\mathbb{F}}^{\text{ad}} P^{\text{ad}} = \mathbf{1} + G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}} \text{ on } \mathcal{X}_{\mathbb{F}}^{\text{ad}, m+\frac{1}{2}},$$

hence

$$T G_{\mathbb{F}}^{\text{ad}} T^{-1} (D_t - H(t)) T = T + T G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}} \text{ on } \mathcal{X}_{\mathbb{F}}^{\text{ad}, m+\frac{1}{2}}.$$

By (6.22), (6.27) we know that  $T^{-1} \varrho : \mathcal{X}_{\mathbb{F}}^m \rightarrow \mathcal{X}_{\mathbb{F}}^{\text{ad}, m+\frac{1}{2}}$ . It follows that

$$T G_{\mathbb{F}}^{\text{ad}} T^{-1} (D_t - H(t)) \varrho = \varrho + T G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}} T^{-1} \varrho, \text{ on } \mathcal{X}_{\mathbb{F}}^m.$$

Since  $(D_t - H(t)) \varrho = \pi_1^* \pi_1 (D_t - H(t))$ , we obtain that

$$\begin{aligned}
(6.39) \quad G_{\mathbb{F}} P &= \pi_0 T G_{\mathbb{F}}^{\text{ad}} T^{-1} \pi_1^* \pi_1 (D_t - H(t)) \varrho \\
&= \pi_0 \varrho + \pi_0 T G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}} T^{-1} \varrho \\
&= \mathbf{1} + \pi_0 T G_{\mathbb{F}}^{\text{ad}} V_{-\infty}^{\text{ad}} T^{-1} \varrho \text{ on } \mathcal{X}_{\mathbb{F}}^m.
\end{aligned}$$

Using (6.22) and Lemma 6.17 we obtain that  $G_{\mathbb{F}} P - \mathbf{1}$  is compact on  $\mathcal{X}_{\mathbb{F}}^m$ , which proves *ii)*.

*Proof of iii):* we note that for any operator  $A^{\text{ad}}$  one has

$$\pi_0 A^{\text{ad}} \pi_1^* = \pi_1 q A^{\text{ad}} \pi_1^*, \text{ hence } (\pi_0 A^{\text{ad}} \pi_1^*)^* = \pi_1 q A^{\text{ad}\dagger} \pi_1^*.$$

This gives

$$i(G_{\mathbb{F}} - G_{\mathbb{F}}^*) = i^{-1} \pi_1 q T (G_{\mathbb{F}}^{\text{ad}} - G_{\mathbb{F}}^{\text{ad}\dagger}) T^{-1} \pi_1^* = i^{-1} (\pi_1 T) q^{\text{ad}} (G_{\mathbb{F}}^{\text{ad}} - G_{\mathbb{F}}^{\text{ad}\dagger}) (\pi_1 T)^* \geq 0,$$

by Thm. 6.16 *iii)*.

*Proof of iv):* we first see using  $\mathcal{U}^{\text{d}}(t, s)(D_s - H^{\text{d}}(s)) = 0$  and integration by parts that  $G_{\mathbb{F}}^{\text{ad}}$  maps compactly supported elements of  $H^{-p}(\mathbb{R}; \mathcal{H}^{-k})$  into  $H^p(\mathbb{R}; \mathcal{H}^{-k-2p})$  for  $k, p \in \mathbb{N}$ , hence  $V_{-\infty}^{\text{ad}} G_{\mathbb{F}}^{\text{ad}}$  maps compactly supported elements of  $H^{-p}(\mathbb{R}; \mathcal{H}^k)$  into  $H^p(\mathbb{R}, \mathcal{H}^k)$ . The same argument shows that  $G_{\mathbb{F}}^{\text{ad}}$  maps also compactly supported elements  $H^{-p}(\mathbb{R}; \mathcal{H}^k)$  into  $H^p(\mathbb{R}, \mathcal{H}^k)$ . By (6.36), (6.38), (6.39) this implies *iv)*.

*Proof of v):* let  $\omega_{\text{ref}}$  be the Hadamard state given by the projections  $c_{\text{ref}}^{\pm}(0)$ , see Subsect. 4.4. If  $\Lambda_{\text{ref}}^{\pm}$  are its two-point functions (see Subsect. 2.4), then as shown in [GOW],  $G_{\text{F,ref}} = i\Lambda_{\text{ref}}^+ + G_+$  is a Feynman inverse for  $P$ , i.e.  $PG_{\text{F,ref}} = G_{\text{F,ref}}P = \mathbf{1}$  on  $C_c^\infty(\mathbb{R}^{1+d})$  and

$$\text{WF}'(G_{\text{F,ref}}) = (\text{diag}_{T^*M}) \cup \bigcup_{t \leq 0} (\Phi_t(\text{diag}_{T^*M}) \cap \pi^{-1}\mathcal{N}).$$

Moreover we know (see e.g. [GOW, Thm. 7.10, Prop. 7.11]) that  $G_{\text{F,ref}}$  is given by the analog of (6.35) with  $\mathcal{U}^d$  replaced by  $\mathcal{U}^{\text{ad}}$  in the definition of  $G_{\text{F}}^{\text{ad}}$ . From (4.22) we obtain that  $\mathcal{U}^d(t, s) - \mathcal{U}^{\text{ad}}(t, s) \in C^\infty(\mathbb{R}^2; \mathcal{W}^{-\infty}(\mathbb{R}^d))$ , which implies that  $G_{\text{F}} - G_{\text{F,ref}}$  is smoothing and completes the proof of *v)*.  $\square$

## 7. ASYMPTOTICALLY MINKOWSKI SPACETIMES

**7.1. Assumptions.** In this final section we consider asymptotically Minkowski spacetimes and prove analogues of the results from Sect. 6 by using the reduction procedure from Sect. 5.

We work on  $M = \mathbb{R}^{1+d}$ , whose elements are denoted by  $y = (t, y)$ .

For  $\delta \in \mathbb{R}$  we denote by  $S_{\text{std}}^\delta(\mathbb{R}^{1+d})$  the class of smooth functions such that

$$\partial_y^\alpha f \in O(\langle y \rangle^{\delta - |\alpha|}), \quad \alpha \in \mathbb{N}^{1+d}.$$

The analogous spaces on  $\mathbb{R}^d$  will be denoted by  $S_{\text{sd}}^\delta(\mathbb{R}^d)$ .

We denote by  $\eta_{\mu\nu}$  the Minkowski metric on  $\mathbb{R}^{1+d}$ , fix a Lorentzian metric  $g$  on  $\mathbb{R}^{1+d}$  and consider the Klein-Gordon operator

$$(7.1) \quad P = -\square_g + V(y),$$

where  $V$  is again a smooth real function. We assume that  $(M, g)$  is asymptotically Minkowski and  $V$  is asymptotically constant in the following sense:

- i)*  $g_{\mu\nu}(y) - \eta_{\mu\nu} \in S_{\text{std}}^{-\delta}(\mathbb{R}^{1+d})$ ,  $\delta > 1$ ,
- ii)*  $V(y) - m^2 \in S_{\text{std}}^{-\delta}(\mathbb{R}^{1+d})$ ,  $m > 0$ ,  $\delta > 1$ ,
- (aM) *iii)*  $(\mathbb{R}^{1+d}, g)$  is globally hyperbolic,
- iv)*  $(\mathbb{R}^{1+d}, g)$  has a time function  $\tilde{t}$  with  $\tilde{t} - t \in S_{\text{std}}^{1-\epsilon}(\mathbb{R}^{1+d})$  for  $\epsilon > 0$ .

**Remark 7.1.** We conjecture that (aM) *iv)* follows from (aM) *i)*, *iii)*.

**7.2. Global hyperbolicity and non-trapping condition.** The null geodesics of  $g$  coincide modulo reparametrization with the projections on the base of null bicharacteristics of  $m(x, \xi) = |\xi|^{-1}\xi \cdot g^{-1}(x)\xi$ . We recall that  $\Phi_s$  is the flow of the Hamiltonian vector field  $H_p$ ,  $p(y, \xi) = \xi \cdot g^{-1}y\xi$ , which acts naturally on  $S^*\mathbb{R}^{1+d} = T^*\mathbb{R}^{1+d} \cap \{|\xi| = 1\}$ . Null bicharacteristics stay in one of the two connected components  $\mathcal{N}^\pm$  of  $\mathcal{N}$ . We set

$$\Gamma_{\text{in/out}}^\pm = \{X \in S^\pm : \phi_s(X) \not\rightarrow \infty \text{ as } s \rightarrow \pm\infty\}.$$

The familiar *non-trapping condition* is:

$$(nt) \text{ there are no trapped null geodesics of } g, \text{ i.e. } \Gamma_{\text{in}}^\pm = \Gamma_{\text{out}}^\pm = \emptyset.$$

By a well-known argument, this actually implies that  $\Gamma_{\text{in/out}}^\pm = \emptyset$ , see Lemma 7.2 below, hence any null geodesic escapes to infinity both when the affine parameter  $s$  tends to  $+\infty$  and to  $-\infty$ .

**Lemma 7.2.** *If (nt) holds then  $\Gamma_{\text{in}}^\pm = \Gamma_{\text{out}}^\pm = \emptyset$ .*

**Proof.** We drop the  $\pm$  superscript. We claim that  $\Gamma_{\text{in}} \neq \emptyset$  or  $\Gamma_{\text{out}} \neq \emptyset$  implies  $\Gamma \neq \emptyset$ . In fact let  $X_0 \in \Gamma_{\text{in}}$ ,  $K_1$  a compact set such that  $\{\Phi_s(X_0) : s \geq 0\} \subset K_1$ . Let  $s_j \rightarrow +\infty$  a sequence such that  $X_j = \Phi_{s_j}(X_0) \rightarrow X_\infty \in K_1$ . Clearly  $\Phi_s(X_j) = \Phi_{s+s_j}(X_0) \rightarrow \Phi_s(X_\infty)$  for any  $s \in \mathbb{R}$ .

For  $j$  large enough we have  $\Phi_{s+s_j}(X_0) \in K_1$  hence  $\Phi_s(X_\infty) \in K_1$  for any  $s \in \mathbb{R}$ , which means that  $X_\infty \in \Gamma$ .  $\square$

**Proposition 7.3.** *Assume (aM) i). Then*

- (1)  $(\mathbb{R}^{1+d}, g)$  is globally hyperbolic iff (nt) holds,
- (2) if (aM), iii) and iv) hold then there exists a Cauchy time function  $\tilde{t}$  such that  $\tilde{t} - t \in C_c^\infty(\mathbb{R}^{1+d})$ .

In the sequel we will work with the Cauchy time function  $\tilde{t}$  obtain in Prop. 7.3 (2).

**Proof.** First let us prove (1). By (aM) i) we have

$$\{p, t\} = \partial_\tau(|\xi|^{-1}(\tau^2 - k^2)) + O(\langle x \rangle^{-\delta}|\xi|^{-1}) \geq \tau|\xi|^{-1} + O(\langle x \rangle^{-\delta}|\xi|^{-1}).$$

It follows that there exist  $c_0 > 0$  and compact sets  $K^\pm \subset \mathcal{N}^\pm$  such that

$$(7.2) \quad \pm\{m, t\} \geq c_0 \text{ on } \mathcal{N}^\pm \setminus K^\pm$$

This implies that if  $X \in \mathcal{N}^+$  and  $\phi_s(X) \rightarrow \infty$  when  $s \rightarrow \pm\infty$  then  $t \circ \phi_s(X) \rightarrow \pm\infty$  when  $s \rightarrow \pm\infty$ . Of course a similar statement is true for  $X \in \mathcal{N}^-$  with the reversed sign.

Let us set  $\Sigma_s = t^{-1}(s)$ . Using (7.2) we obtain that there exists  $T_0 > 0$  such that any null geodesic intersects  $\Sigma_{\pm T}$  transversally for  $T \geq T_0$  and hence enters  $I^\pm(\Sigma_{\pm T})$ . Moreover  $\Sigma_{\pm T}$  is achronal for  $T$  large enough, since  $\partial_t$  is a future directed time-like vector field in  $\{\pm t \geq \pm T\}$  for  $T$  large enough. We can apply then the Geroch-Sánchez theorem (see for instance [Wa2, Thm. 8.3.7] for its basic version), which implies that  $\Sigma_{\pm T}$  are Cauchy hypersurfaces for  $T$  large enough, which completes the proof of (1)  $\Leftarrow$ .

Assume now that  $(\mathbb{R}^{1+d}, g)$  is globally hyperbolic and (nt) is violated. Let  $\gamma = \{x(s) : s \in \mathbb{R}\}$  be an (affine parametrized) null geodesic which is past and future trapped, ie  $\gamma \subset K$  for some compact set  $K$ . Since  $(\mathbb{R}^{1+d}, g)$  is strongly causal, for each  $x \in K$  there exists an open neighborhood  $V(x)$  of  $x$  such that  $\gamma$  enters  $V(x)$  only once, ie  $\{s \in \mathbb{R} : x(s) \in V(x)\} =: I(x)$  is a bounded open interval. By compactness of  $K$  we have  $x(s) \notin K$  for  $s \notin \cup_1^n I(x_i)$ , which is a contradiction. This completes the proof of (1)  $\Rightarrow$ .

Now let us prove (2). Let  $\tilde{t}$  be the time function in (aM) iii). First of all, we note that it follows from (aM) that  $-C^{-1} \leq d\tilde{t} \cdot g^{-1}d\tilde{t} \leq -C$  for some  $C > 0$ . We fix a cutoff function  $\chi \in C_c^\infty(\mathbb{R}^{1+d})$  with  $0 \leq \chi \leq 1$ ,  $\chi = 1$  near 0 and set  $\chi_R(y) = \chi(R^{-1}y)$ ,  $\hat{t}_R = \chi_R\tilde{t} + (1 - \chi_R)t$ . We have:

$$d\hat{t}_R = \chi_R d\tilde{t} + (1 - \chi_R)dt + (\tilde{t} - t)d\chi_R.$$

The covector  $\alpha_R = \chi_R d\tilde{t} + (1 - \chi_R)dt$  is a convex combination of future directed timelike covectors, which using (aM) i) implies that there exists  $C > 0$  such that  $-C^{-1} \leq \alpha_R \cdot g^{-1}\alpha_R \leq -C$ , uniformly for  $R \geq 1$ . The error term  $(\tilde{t} - t)d\chi_R$  is of norm  $O(R^{-\epsilon})$ , which shows that  $\hat{t}_R$  is a time function for  $R$  large enough. Let us fix such an  $R$  and denote  $\hat{t}_R$  by  $\hat{t}$ . Clearly  $\hat{t} - t \in C_c^\infty(\mathbb{R}^{1+d})$ . It remains to check that  $\hat{t}$  is a Cauchy time function. First using that  $\hat{t} = t + C_c^\infty(\mathbb{R}^{1+d})$  we obtain that

$$(7.3) \quad \limsup_{T \rightarrow +\infty} \hat{t}|_{\Sigma_{-T}} = -\infty, \quad \liminf_{T \rightarrow +\infty} \hat{t}|_{\Sigma_T} = +\infty.$$

Let now  $\gamma$  be an inextendible future directed continuous causal curve and  $s \in \mathbb{R}$ . Since  $\hat{t}$  is a time function,  $\gamma$  intersects  $\hat{t}^{-1}(s)$  at most once. By global hyperbolicity,  $\gamma$  intersects the Cauchy hypersurfaces  $\Sigma_{\pm T}$  for  $T$  large enough. By (7.3) this implies choosing  $T$  very large that  $\gamma$  intersects  $\hat{t}^{-1}(s^\pm)$  for some  $s_- < s < s_+$  hence also  $\hat{t}^{-1}(s)$ . Therefore  $\hat{t}^{-1}(s)$  is a Cauchy hypersurface for each  $s$  and  $\hat{t}$  is a Cauchy time function.  $\square$

**7.3. Reduction to the model case.** We now repeat the constructions in Subsect. 5.2, taking into account the additional space-time decay of  $g$  and  $V$ .

After possibly redefining  $\tilde{t}$  by adding a constant, we can assume that  $\Sigma := \tilde{t}^{-1}(\{0\}) = \{0\} \times \mathbb{R}^d$ , so that  $\Sigma$  is a Cauchy hypersurface both for  $g$  and  $\eta$ .

We set  $v = \frac{g^{-1}d\tilde{t}}{d\tilde{t} \cdot g^{-1}d\tilde{t}}$ , so that  $v = \partial_{\tilde{t}}$  outside a compact set. If  $\phi_t$  is the flow of  $v$ , we set as before:

$$\chi : \mathbb{R} \times \Sigma \in (t, \mathbf{x}) \mapsto \phi_t(0, \mathbf{x}) \in \mathbb{R}^{1+d},$$

so that  $\tilde{t}(\chi(t, \mathbf{x})) = t$ . Due to the additional space decay properties, the diffeomorphism  $\chi$  has better properties than the ones stated in Lemma 5.1.

**Lemma 7.4.** *Assume (aM). Then*

$$\chi^*g = -\hat{c}^2(t, \mathbf{x})dt^2 + \hat{h}(t, \mathbf{x})d\mathbf{x}^2, \quad \chi^*V = \hat{V},$$

where:

$$\hat{h}, \hat{h}^{-1}, \hat{c}, \hat{c}^{-1}, \hat{V} \in S_{\text{std}}^0(\mathbb{R}^{1+d}).$$

Moreover there exist diffeomorphisms  $y_{\text{out/in}}$  of  $\Sigma$  with

$$y_{\text{out/in}}(\mathbf{x}) - \mathbf{x} \in S_{\text{sd}}^{1-\delta}(\mathbb{R}^d)$$

such that if

$$\hat{h}_{\text{out/in}} := y_{\text{out/in}}^* \delta,$$

where  $\delta$  is the flat Riemannian metric on  $\mathbb{R}^d$ , we have:

$$\hat{h} - \hat{h}_{\text{out/in}}, \hat{c} - 1, \hat{V} - m^2 \in S_{\text{std}}^{-\delta}(\mathbb{R}_{\pm} \times \mathbb{R}^d).$$

**Proof.** We have  $v = \partial_t + S_{\text{std}}^{-\delta}$ , which also implies that

$$(7.4) \quad \langle \phi_s(0, \mathbf{x}) \rangle \geq C(\langle s \rangle + \langle \mathbf{x} \rangle), \quad C > 0.$$

Setting  $w := \pi_y v$ , we have  $\pi_y \chi(t, \mathbf{x}) = \pi_y \mathbf{x} + \int_0^t w(\phi_s(\mathbf{x})) ds$ . Using that  $w \in S_{\text{std}}^{-\delta}(\mathbb{R}^{1+d})$ , we obtain that

$$y_{\text{out/in}}(\mathbf{x}) := \lim_{t \rightarrow \pm\infty} \pi_y \chi(t, \mathbf{x})$$

exist and:

$$(7.5) \quad \pi_y \chi(t, \mathbf{x}) - y_{\text{out/in}}(\mathbf{x}) \in S_{\text{std}}^{1-\delta}(\mathbb{R}_{\pm} \times \mathbb{R}^d), \quad y_{\text{out/in}}(\mathbf{x}) - \mathbf{x} \in S_{\text{sd}}^{1-\delta}(\mathbb{R}^d).$$

By (aM), *iii*), we also have  $\chi(t, \mathbf{x}) = (t, \pi_y \chi(t, \mathbf{x}))$  for  $|t| + |\mathbf{x}| \geq C$ , hence

$$D\chi(t, \mathbf{x}) = \begin{pmatrix} 1 & 0 \\ 0 & Dy_{\text{out/in}}(\mathbf{x}) \end{pmatrix} + S_{\text{std}}^{-\delta}(\mathbb{R}_{\pm} \times \mathbb{R}^d).$$

This estimate and (7.4) imply the assertion.  $\square$

As in Subsect. 5.2, we set  $\hat{P} = \chi^*P$ ,  $\tilde{P} = \hat{c}^{1-n/2} \hat{P} \hat{c}^{1+n/2}$ . In a similar vein we obtain that:

$$(7.6) \quad \tilde{P} = \bar{\partial}_t^2 + r(t, \mathbf{x})\bar{\partial}_t + a(t, \mathbf{x}, \bar{\partial}_x),$$

where now by Lemma 7.4,  $r, a$  satisfy (std) for  $\delta > 1$  with

$$(7.7) \quad a_{\text{out/in}}(\mathbf{x}, \bar{\partial}_x) := -\Delta_{\hat{h}_{\text{out/in}}} + m^2 = \chi_{\text{out/in}}^*(-\Delta_x + m^2).$$

There are several inconveniences related to the possibility that  $a_{\text{out}} \neq a_{\text{in}}$ . It turns out, however, that they can be circumvented by considering the dynamics associated to the free Laplace operator  $-\Delta_x + m^2$  instead of  $\mathcal{U}_{\text{out/in}}(t, s)$ .

**7.4. Wave operators.** We use the same notation as in Sect. 6. Let  $\Sigma_s := \tilde{t}^{-1}(\{s\})$  for  $m \in \mathbb{R}$ . Using the diffeomorphism  $\chi$  we identify  $\Sigma_s$  with  $\mathbb{R}^d$  to define the Sobolev spaces  $H^m(\Sigma_s)$ . We introduce the energy spaces:

$$\mathcal{E}^m(s) := H^{1+m}(\Sigma_s) \oplus H^m(\Sigma_s), \quad m \in \mathbb{R}.$$

Of course under  $\chi$  all spaces  $\mathcal{E}^m(s)$  equal  $\mathcal{E}^m(\mathbb{R}^d)$  with uniformly equivalent norms. We denote by  $\mathcal{U}(t, s) : \mathcal{E}^m(s) \rightarrow \mathcal{E}^m(t)$  the Cauchy evolution associated to  $P$ . We recall that:

$$(7.8) \quad \mathcal{U}(t, s) = Z(t)\mathcal{U}^{\text{ad}}(t, s)Z^{-1}(s),$$

where  $Z(t) : \mathcal{E}^m(t) \rightarrow \mathcal{H}^{m+\frac{1}{2}}$  was defined in Lemma 5.3. We set

$$P_{\text{free}} := \bar{\partial}_t^2 - \Delta_x + m^2,$$

and

$$Z_{\text{out/in}} := (\chi_{\text{out/in}}^*)^{-1}T_{\text{out/in}}, \quad \chi_{\text{out/in}}(t, \mathbf{x}) := (t, y_{\text{out/in}}(\mathbf{x})).$$

Denoting by  $\mathcal{U}_{\text{free}}(t, s)$  the usual Cauchy evolution for  $P_{\text{free}}$  we have by (7.7):

$$\mathcal{U}_{\text{free}}(t, s) = Z_{\text{out/in}}\mathcal{U}_{\text{out/in}}^{\text{ad}}(t, s)Z_{\text{out/in}}^{-1}.$$

**Proposition 7.5.** *The limits*

$$(7.9) \quad W_{\text{out/in}} := \lim_{t \rightarrow \pm\infty} \mathcal{U}(0, t)\mathcal{U}_{\text{free}}(t, 0)$$

*exist in  $B(\mathcal{E}^m(0))$  with inverses*

$$(7.10) \quad W_{\text{out/in}}^{-1} = W_{\text{out/in}}^\dagger = \lim_{t \rightarrow \pm\infty} \mathcal{U}_{\text{free}}(0, t)\mathcal{U}(t, 0).$$

*Moreover one has:*

$$(7.11) \quad W_{\text{out/in}} = Z(0)W_{\text{out/in}}^{\text{ad}}Z_{\text{out/in}}^{-1},$$

*where we recall that  $W_{\text{out/in}}^{\text{ad}} = \lim_{t \rightarrow \pm\infty} \mathcal{U}^{\text{ad}}(0, t)\mathcal{U}_{\text{out/in}}^{\text{ad}}(t, 0)$ .*

**Proof.** The existence of the limits (7.9), (7.10) follows from the Cook argument, using the short range condition  $\delta > 1$ . The identity (7.11) follows from

$$\lim_{t \rightarrow \pm\infty} Z(t)Z_{\text{out/in}} - \mathbf{1} = 0 \text{ in } B(\mathcal{H}^m),$$

by Lemma 5.4.  $\square$

**7.5. The out/in Hadamard states.** We now consider the *out/in* Hadamard states  $\omega_{\text{out/in}}$  constructed in Thm. 5.5, whose covariances are denoted by  $c_{\text{out/in}}^\pm$ . We denote by  $c_{\text{free}}^{\pm, \text{vac}}$  the covariance of the free vacuum state associated to  $P_{\text{free}}$ . An easy computation shows that

$$(7.12) \quad c_{\text{free}}^{\pm, \text{vac}} = Z_{\text{out}}\pi^\pm Z_{\text{out}}^{-1} = Z_{\text{in}}\pi^\pm Z_{\text{in}}^{-1}.$$

**Proposition 7.6.** *We have*

$$c_{\text{out/in}}^\pm = W_{\text{out/in}}c_{\text{free}}^{\pm, \text{vac}}W_{\text{out/in}}^{-1} = \text{w-} \lim_{t \rightarrow \pm\infty} \mathcal{U}(0, t)c_{\text{free}}^{\pm, \text{vac}}\mathcal{U}(t, 0) \text{ in } \mathcal{E}^m.$$

**Proof.** We have

$$\begin{aligned}
 & \mathcal{U}(0, t) \mathcal{U}_{\text{free}}(t, 0) c_{\text{free}}^{\pm, \text{vac}} \mathcal{U}_{\text{free}}(0, t) \mathcal{U}(t, 0) \\
 &= Z(0) \mathcal{U}^{\text{ad}}(0, t) Z(t)^{-1} Z_{\text{out/in}} \mathcal{U}_{\text{out/in}}^{\text{ad}}(t, 0) Z_{\text{out/in}}^{-1} c_{\text{free}}^{\pm, \text{vac}} Z_{\text{out/in}} \\
 & \quad \times \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) Z_{\text{out/in}}^{-1} Z(t) \mathcal{U}^{\text{ad}}(t, 0) Z(0)^{-1} \\
 &= Z(0) \mathcal{U}^{\text{ad}}(0, t) \mathcal{U}_{\text{out/in}}^{\text{ad}}(t, 0) Z_{\text{out/in}}^{-1} c_{\text{free}}^{\pm, \text{vac}} Z_{\text{out/in}} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \mathcal{U}^{\text{ad}}(t, 0) Z(0)^{-1} + o(1) \\
 &= Z(0) \mathcal{U}^{\text{ad}}(0, t) \mathcal{U}_{\text{out/in}}^{\text{ad}}(t, 0) \pi^{\pm} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \mathcal{U}^{\text{ad}}(t, 0) Z(0)^{-1} + o(1) \\
 &= Z(0) \mathcal{U}^{\text{ad}}(0, t) \pi^{\pm} \mathcal{U}_{\text{out/in}}^{\text{ad}}(0, t) \mathcal{U}^{\text{ad}}(t, 0) Z(0)^{-1} + o(1) = c_{\text{out/in}}^{\pm} + o(1),
 \end{aligned}$$

using Thm. 5.5. Letting  $t \rightarrow \pm\infty$  we obtain the proposition.  $\square$

**7.6. Fredholm problems and Feynman pseudo-inverse.** Following the notation in (7.6), the objects introduced in Sect. 6 will be denoted with tildes, like  $\tilde{\mathcal{X}}^m, \tilde{\mathcal{Y}}^m$ , etc. We define the spaces

$$\begin{aligned}
 (7.13) \quad & \mathcal{Y}^m := (\chi^{-1})^* \tilde{\mathcal{Y}}^m = (\chi^{-1})^* ((t)^{-\gamma} L^2(\mathbb{R}; H^m)), \\
 & \mathcal{X}^m := (\chi^{-1})^* \tilde{\mathcal{X}}^m = (\chi^{-1})^* \{ \tilde{u} \in (C^1(\mathbb{R}; H^{m+1}) \cap C^0(\mathbb{R}; H^m)) : \tilde{P}u \in \tilde{\mathcal{Y}}^m \}.
 \end{aligned}$$

In particular  $\mathcal{X}^m$  is the space of  $u \in \mathcal{D}'(\mathbb{R}^{1+d})$  such that  $u \circ \chi \in C^1(\mathbb{R}; H^{m+1}) \cap C^0(\mathbb{R}; H^m)$  and  $Pu \in \mathcal{Y}^m$ . We equip  $\mathcal{Y}^m$  and  $\mathcal{X}^m$  with the norms obtained from  $\tilde{\mathcal{Y}}^m$  and  $\tilde{\mathcal{X}}^m$ .

**Definition 7.7.** We set  $\varrho_{\text{out/in}} := s\text{-}\lim_{t \rightarrow \pm\infty} \mathcal{U}_{\text{free}}(0, t) \varrho_t$  and

$$\begin{aligned}
 \varrho_{\text{F}} &:= c_{\text{free}}^{+, \text{vac}} \varrho_{\text{out}} + c_{\text{free}}^{-, \text{vac}} \varrho_{\text{in}}, & W_{\text{F}}^{\dagger} &:= c_{\text{free}}^{+, \text{vac}} W_{\text{out}}^{\dagger} + c_{\text{free}}^{-, \text{vac}} W_{\text{in}}^{\dagger}, \\
 \varrho_{\bar{\text{F}}} &:= c_{\text{free}}^{-, \text{vac}} \varrho_{\text{out}} + c_{\text{free}}^{+, \text{vac}} \varrho_{\text{in}}, & W_{\bar{\text{F}}}^{\dagger} &:= c_{\text{free}}^{-, \text{vac}} W_{\text{out}}^{\dagger} + c_{\text{free}}^{+, \text{vac}} W_{\text{in}}^{\dagger},
 \end{aligned}$$

and for  $I \in \{\text{in}, \text{out}, \text{F}, \bar{\text{F}}\}$ :

$$\mathcal{X}_I^m := \{u \in \mathcal{X}^m : \varrho_I u = 0\}.$$

**Theorem 7.8.** Assume (aM) and let  $P, \mathcal{X}_I^m$  be as defined in (7.1) and Def. 7.7 for  $m \in \mathbb{R}$  and  $I \in \{\text{in}, \text{out}, \text{F}, \bar{\text{F}}\}$ . Then:

- (1)  $P : \mathcal{X}_I^m \rightarrow \mathcal{Y}^m$  is Fredholm of index  $\text{ind } W_{I^c}^{\dagger}$ , and invertible with inverse  $G_{\pm}$  if  $I = \text{out/in}$ . Furthermore,  $\text{Ker } P|_{\mathcal{X}_I^m} \subset C^{\infty}(M)$  and the index does not depend on the Sobolev order  $m$ .
- (2) Let

$$G_{\text{F}} := (\chi^{-1})^* (\hat{c}^{1+n/2} \tilde{G}_{\text{F}} \hat{c}^{1-n/2}),$$

where  $\tilde{G}_{\text{F}}$  is the operator defined in (6.35) and  $\hat{c}, \chi$  are defined in Subsect. 7.3. Then:

- i)  $G_{\text{F}} \in B(\mathcal{Y}^m, \mathcal{X}_{\text{F}}^m)$ ,  $P G_{\text{F}} = \mathbf{1}_{\mathcal{Y}^m} + K_{\mathcal{Y}^m}$ , where  $K_{\mathcal{Y}^m}$  is compact on  $\mathcal{Y}^m$ ,
- ii)  $G_{\text{F}} P = \mathbf{1}_{\mathcal{X}_{\text{F}}^m} + K_{\mathcal{X}_{\text{F}}^m}$ , where  $K_{\mathcal{X}_{\text{F}}^m}$  is compact on  $\mathcal{X}_{\text{F}}^m$ ,
- iii)  $i^{-1}(G_{\text{F}} - G_{\text{F}}^*) \geq 0$  on  $\mathcal{Y}^m$ , for  $m \geq 0$ ,
- iv)  $P G_{\text{F}} - \mathbf{1}, G_{\text{F}} P - \mathbf{1}$  are smoothing operators,
- v)  $\text{WF}(G_{\text{F}})' = (\text{diag}_{T^*M}) \cup \bigcup_{t \leq 0} (\Phi_t(\text{diag}_{T^*M}) \cap \pi^{-1}\mathcal{N})$ .

In particular,  $G_{\text{F}}$  is a Feynman parametrix of  $P$  in the sense of [DH].

**Proof.** The maps

$$\begin{aligned}\mathcal{Y}^m \ni f &\mapsto \tilde{f} := \hat{c}^{1-n/2} f \circ \chi \in \tilde{\mathcal{Y}}^m, \\ \mathcal{X}^m \ni u &\mapsto \tilde{u} := \hat{c}^{1+n/2} u \circ \chi \in \tilde{\mathcal{Y}}^m,\end{aligned}$$

are boundedly invertible and furthermore,  $Pu = f$  iff  $\tilde{P}\tilde{u} = \tilde{f}$ . Moreover by the computations in Subject. 5.3 we obtain that  $Z^{-1}\varrho u = T^{-1}\tilde{\varrho}\tilde{u}$  and hence  $u \in \mathcal{X}_I^m$  iff  $\tilde{u} \in \tilde{\mathcal{X}}_I^m$ . The theorem follows hence from Thm. 6.18 provided we check that

$$(7.14) \quad \text{ind } W_I^\dagger = \text{ind } W_I^{\text{ad}\dagger}.$$

This is obvious for  $I = \text{out/in}$  since the operators are then bijective. Let us check (7.14) for  $I = \bar{\mathbb{F}}$  for example. We denote by  $Z_{\text{free}}$  the analog of  $Z_{\text{out/in}}$  with  $\epsilon_{\text{out/in}}$  replaced by  $\epsilon_{\text{free}} = (-\Delta_x + m^2)^{\frac{1}{2}}$  and  $\chi_{\text{out/in}}$  replaced by  $\mathbf{1}$ . Using (7.11) and (7.12) we obtain that

$$Z_{\text{free}}^{-1} W_{\bar{\mathbb{F}}}^\dagger = (Z_{\text{free}}^{-1} Z_{\text{out}} \pi^- W_{\text{out}}^{\text{ad}\dagger} + Z_{\text{free}}^{-1} Z_{\text{in}} \pi^+ W_{\text{in}}^{\text{ad}\dagger}) Z(0)^{-1} = S \circ Z_{\bar{\mathbb{F}}}^{\text{ad}\dagger} \circ Z(0)^{-1},$$

for  $S = Z_{\text{free}}^{-1} Z_{\text{out}} \pi^- + Z_{\text{free}}^{-1} Z_{\text{in}} \pi^+$ . But since  $c_{\text{free}}^{\pm, \text{vac}} = Z_{\text{free}} \pi^\pm Z_{\text{free}}^{-1}$ ,  $Z_{\text{free}}^{-1} Z_{\text{out/in}}$  commutes with  $\pi^+$  and  $\pi^-$ , using again (7.12). Therefore  $S = \pi^- Z_{\text{free}}^{-1} Z_{\text{out}} \pi^- + \pi^+ Z_{\text{free}}^{-1} Z_{\text{in}} \pi^+$  is invertible and hence  $\text{ind } W_{\bar{\mathbb{F}}}^\dagger = \text{ind } W_{\bar{\mathbb{F}}}^{\text{ad}\dagger}$ .  $\square$

## APPENDIX A

**A.1. Proof of Prop. 3.11.** To prove Prop. 3.11 we first need an auxiliary lemma about parameter-dependent pseudodifferential calculus.

We start by introducing parameter dependent versions of the spaces  $\Psi^m(\Sigma)$ ,  $S^0(\mathbb{R}; \Psi^m(\Sigma))$  and  $\Psi_{\text{std}}^{m,0}(\mathbb{R}; \mathbb{R}^d)$ .

We define the symbol classes  $\tilde{S}^m(T^*\Sigma)$  for  $m \in \mathbb{R}$  as the space of functions  $c(x, k, \lambda) \in C^\infty(T^*\Sigma \times \mathbb{R})$  such that:

$$\partial_\lambda^\gamma \partial_x^\alpha \partial_k^\beta c(x, k, \lambda) \in O(\langle k \rangle + \langle \lambda \rangle)^{m-|\beta|-\gamma}, \quad \alpha, \beta \in \mathbb{N}^d, \quad \gamma \in \mathbb{N},$$

as usual understood after fixing a good chart cover and good chart diffeomorphisms, with uniformity of the constants with respect to the element of the cover. The standard example of such a symbol is  $c(x, k, \lambda) = (a(x, k) + \langle \lambda \rangle^m)$ , for  $a \in S^m(T^*\Sigma)$  elliptic and positive.

The subspaces of symbols poly-homogeneous in  $(k, \lambda)$  are denoted by  $\tilde{S}_{\text{ph}}^m(T^*\Sigma)$ . We define  $\tilde{\mathcal{W}}^{-\infty}(\Sigma)$  as the set of smooth maps  $\mathbb{R} \ni \lambda \mapsto a(\lambda) \in \mathcal{W}^{-\infty}(\Sigma)$  such that:

$$\|\partial_\lambda^\gamma a(\lambda)\|_{B(H^{-p}(\Sigma), H^p(\Sigma))} \in O(\langle \lambda \rangle^{-n}), \quad \forall m, n, \gamma \in \mathbb{N},$$

and we set

$$\tilde{\Psi}^m(\Sigma) := \text{Op}(\tilde{S}_{\text{ph}}^m(T^*\Sigma)) + \tilde{\mathcal{W}}^{-\infty}(\Sigma).$$

We also define the time-dependent versions:

$$S^0(\mathbb{R}; \tilde{S}_{\text{ph}}^m(T^*\Sigma)), \quad S^0(\mathbb{R}; \tilde{\mathcal{W}}^{-\infty}(\Sigma)), \quad S^0(\mathbb{R}; \tilde{\Psi}^m(\Sigma)),$$

in analogy with Subject. 3.3. For example  $c(t, x, k, \lambda) \in S^0(\mathbb{R}; \tilde{S}^m(T^*\Sigma))$  if

$$\partial_t^n \partial_\lambda^\gamma \partial_x^\alpha \partial_k^\beta c(t, x, k, \lambda) \in O(\langle t \rangle^{-n} (\langle k \rangle + \langle \lambda \rangle)^{m-|\beta|-\gamma}), \quad \alpha, \beta \in \mathbb{N}^d, \quad \gamma, n \in \mathbb{N}.$$

If  $\Sigma = \mathbb{R}^d$  we define similarly  $\tilde{S}_{\text{std}}^{m,0}(\mathbb{R}; T^*\mathbb{R}^d)$  to be the space of functions  $c(t, x, k, \lambda)$  such that:

$$\partial_t^n \partial_\lambda^\gamma \partial_x^\alpha \partial_k^\beta c(t, x, k, \lambda) \in O(\langle t \rangle^{-n} (\langle x \rangle + \langle t \rangle)^{-n} (\langle k \rangle + \langle \lambda \rangle)^{m-|\beta|-\gamma}), \quad \alpha, \beta \in \mathbb{N}^d, \quad \gamma, n \in \mathbb{N}.$$

We define  $\widetilde{\mathcal{W}}_{\text{std}}^{-\infty}(\mathbb{R}; \mathbb{R}^d)$  as the set of smooth maps  $\mathbb{R} \ni \lambda \mapsto a(\lambda) \in \mathcal{W}_{\text{std}}^{-\infty}(\mathbb{R}; \mathbb{R}^d)$  such that:

$$\|\partial_t^n \partial_\lambda^\gamma (D_x^2 + x^2)^m a(t, \lambda) (D_x^2 + x^2)^m\|_{B(L^2(\mathbb{R}^d))} \in O(\langle t \rangle^{-n} \langle \lambda \rangle^{-n}), \quad \forall n \in \mathbb{N},$$

and we set

$$\widetilde{\Psi}_{\text{std}}^{m,0}(\mathbb{R}; \mathbb{R}^d) = \text{Op}^w(\widetilde{S}_{\text{std,ph}}^{m,0}(\mathbb{R}; T^*\mathbb{R}^d)) + \widetilde{\mathcal{W}}_{\text{std}}^{-\infty}(\mathbb{R}; \mathbb{R}^d).$$

**Lemma A.1.** *Let  $a(t) \in S^0(\mathbb{R}; \Psi^2(\Sigma))$  resp.  $\Psi_{\text{std}}^{2,0}(\mathbb{R}; \mathbb{R}^d)$  such that  $a(t)$  is elliptic, selfadjoint on  $L^2(\Sigma)$  with  $a(t) \geq c_0 \mathbf{1}$ ,  $c_0 > 0$ . Then  $(a(t) + \lambda^2)^{-1} \in S^0(\mathbb{R}; \widetilde{\Psi}^{-2}(\Sigma))$  resp.  $\widetilde{\Psi}_{\text{std}}^{2,0}(\mathbb{R}; \mathbb{R}^d)$ .*

**Proof.** The proof is based on a reduction to the situation without the parameter  $\lambda$ . We first present the argument in the time-independent case.

Let us denote by  $l \in \mathbb{R}$  the dual variable to  $\lambda$ . We consider the manifold of bounded geometry  $\Sigma_x \times \mathbb{R}_l$  equipped with the metric  $h_{ij}(x) dx^i dx^j + dl^2$ . As good chart covering we can take  $\widetilde{U}_i = U_i \times \mathbb{R}$ ,  $\widetilde{\psi}_i(x, l) = (\psi_i(x), l)$  where  $\{U_i, \psi_i\}_{i \in \mathbb{N}}$  is a good chart covering for  $(\Sigma, h)$ . A subordinate good partition of unity is  $\widetilde{\chi}_i(x, l) = \chi_i(x)$ .

The classes  $S_{\text{ph}}^m(T^*(\Sigma \times \mathbb{R}))$  are then defined as in Subsect. 3.3 and one sets as in Subsect. 3.4:

$$\mathcal{W}^{-\infty}(\Sigma \times \mathbb{R}) = \bigcap_{m \in \mathbb{N}} B(H^{-m}(\Sigma \times \mathbb{R}), H^m(\Sigma \times \mathbb{R})),$$

and  $\widetilde{\Psi}^m(\Sigma \times \mathbb{R}) = \text{Op}(S_{\text{ph}}^m(T^*(\Sigma \times \mathbb{R}))) + \mathcal{W}^{-\infty}(\Sigma \times \mathbb{R})$ , where  $\widetilde{\text{Op}}$  is defined as in Subsect. 3.5 with  $\Sigma$  replaced by  $\Sigma \times \mathbb{R}$ . Note that because of our choice of the chart covering  $\widetilde{\text{Op}}$  is the usual Weyl quantization w.r.t. the  $(l, \lambda)$  variables. We note that

$$\widetilde{S}^m(T^*\Sigma) = \{c \in S_{\text{ph}}^m(T^*(\Sigma \times \mathbb{R})) : \partial_l c = 0\},$$

and denoting by  $T_l$  the group of translations in  $l$  we have

$$[T_l, \widetilde{\text{Op}}(c)] = 0, \forall l \in \mathbb{R} \Leftrightarrow c \in \widetilde{S}^m(T^*\Sigma).$$

Equivalently, if  $\mathcal{F}$  is the Fourier transform in  $l$  we have

$$(A.1) \quad \begin{aligned} c &\in S_{\text{ph}}^m(T^*(\Sigma \times \mathbb{R})), [T_l, \widetilde{\text{Op}}(c)] = 0 \\ &\Leftrightarrow \mathcal{F} \widetilde{\text{Op}}(c) \mathcal{F}^{-1} = \int_{\mathbb{R}}^{\oplus} \text{Op}(c(\lambda)) d\lambda, \text{ for } c(\lambda) \in \widetilde{S}^m(T^*\Sigma). \end{aligned}$$

Let now  $w \in \mathcal{W}^{-\infty}(\Sigma \times \mathbb{R})$  with  $[w, T_l] = 0$ . We have:

$$(A.2) \quad \mathcal{F} w \mathcal{F}^{-1} = \int_{\mathbb{R}}^{\oplus} w(\lambda) d\lambda.$$

Since  $w \in \bigcap_{m \in \mathbb{N}} B(H^{-m}(\Sigma \times \mathbb{R}), H^m(\Sigma \times \mathbb{R}))$  we obtain that:

$$\int_{\mathbb{R}} \langle \lambda \rangle^n \|w(\lambda) u(\lambda)\|_{H^p(\Sigma)}^2 d\lambda \leq C_{n,p} \int_{\mathbb{R}} \langle \lambda \rangle^{-n} \|u(\lambda)\|_{H^{-p}(\Sigma)}^2 d\lambda, \quad \forall n, p \in \mathbb{N},$$

or equivalently

$$\int_{\mathbb{R}}^{\oplus} \langle \lambda \rangle^n (-\Delta_h + 1)^{p/2} w(\lambda) (-\Delta_h + 1)^{p/2} d\lambda \in B(L^2(\Sigma \times \mathbb{R})).$$

This implies that

$$\|w(\lambda)\|_{B(H^{-p/2}(\Sigma), H^{p/2}(\Sigma))} \in O(\langle \lambda \rangle^{-n})$$

The same estimates hold for  $\partial_\gamma w(\lambda)$ , which shows that

$$w(\lambda) \in \widetilde{\mathcal{W}}^{-\infty}(\Sigma).$$



Conversely, if  $w(\lambda) \in \widetilde{\mathcal{W}}^{-\infty}(\Sigma)$  it is immediate that  $w$  defined by (A.2) belongs to  $\mathcal{W}^{-\infty}(\Sigma \times \mathbb{R})$ . Hence we have shown

$$(A.3) \quad \begin{aligned} w &\in \mathcal{W}^{-\infty}(\Sigma \times \mathbb{R}), \quad [w, T_l] = 0 \\ \Leftrightarrow \mathcal{F}w\mathcal{F}^{-1} &= \int_{\mathbb{R}}^{\oplus} w(\lambda)d\lambda, \quad \text{for } w(\lambda) \in \widetilde{\mathcal{W}}^{-\infty}(\Sigma). \end{aligned}$$

Let us now consider the time-dependent situation. If we define the time-dependent classes  $C_b^\infty(\mathbb{R}; \widetilde{S}^m(T^*\Sigma))$ ,  $C_b^\infty(\mathbb{R}; \widetilde{\mathcal{W}}^{-\infty}(\Sigma))$  and  $C_b^\infty(\mathbb{R}; \widetilde{\Psi}^m(\Sigma))$  in the obvious way, then

$$(A.4) \quad \begin{aligned} c &\in C_b^\infty(\mathbb{R}; S_{\text{ph}}^m(T^*(\Sigma \times \mathbb{R}))), \quad [T_l, \widetilde{\text{Op}}(c)(t)] = 0 \\ \Leftrightarrow \mathcal{F}\widetilde{\text{Op}}(c)(t)\mathcal{F}^{-1} &= \int_{\mathbb{R}}^{\oplus} \text{Op}(c(t, \lambda))d\lambda, \quad c(t, \lambda) \in C_b^\infty(\mathbb{R}; \widetilde{S}^m(T^*\Sigma)), \\ w &\in C_b^\infty(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma \times \mathbb{R})), \quad [w(t), T_l] = 0 \\ \Leftrightarrow \mathcal{F}w(t)\mathcal{F}^{-1} &= \int_{\mathbb{R}}^{\oplus} w(t, \lambda)d\lambda, \quad w(t, \lambda) \in C_b^\infty(\mathbb{R}; \widetilde{\mathcal{W}}^{-\infty}(\Sigma)). \end{aligned}$$

The same results hold also if we replace  $C_b^\infty(\mathbb{R}; A)$  by  $S^\delta(\mathbb{R}; A)$  for  $A = S_{\text{ph}}^m(T^*(\Sigma \times \mathbb{R}))$ ,  $\widetilde{S}^m(T^*\Sigma)$  etc. In fact it suffices to note that  $c(t) \in S^\delta(\mathbb{R}; A)$  iff  $\langle t \rangle^{-\delta+n} \partial_t^n c(t) \in C_b^\infty(\mathbb{R}; A)$  for all  $n \in \mathbb{N}$ .

Let now  $a(t) \in S^0(\mathbb{R}; \Psi^2(\Sigma))$  be as in the lemma and let  $A(t) = a(t) + D_l^2$  acting on  $L^2(\Sigma \times \mathbb{R})$ . The operator  $A(t)$  is elliptic in  $S^0(\mathbb{R}; \Psi^2(\Sigma \times \mathbb{R}))$ , selfadjoint on  $H^2(\Sigma \times \mathbb{R})$  with  $A(t) \geq c_0 \mathbf{1}$  for  $c_0$  as in the lemma. Applying Thm. 3.7 in the special case  $\alpha = -1$  we obtain that  $A(t)^{-1} \in S^0(\mathbb{R}; \Psi^{-m}(\Sigma \times \mathbb{R}))$ . We have

$$\mathcal{F}A(t)^{-1}\mathcal{F}^{-1} = \int_{\mathbb{R}}^{\oplus} (a(t) + \lambda^2)^{-1}d\lambda,$$

which by (A.4) implies that  $(a(t) + \lambda^2)^{-1} \in S^0(\mathbb{R}; \widetilde{\Psi}^{-2}(\Sigma))$ .

If  $a(t) \in \Psi_{\text{std}}^{2,0}(\mathbb{R}; \mathbb{R}^d)$  we consider the operator  $A(t) = a(t) + D_l^2$  again. One introduces analogous classes of time-dependent pseudodifferential operators acting on  $\mathbb{R}_x^d \times \mathbb{R}_l$ . For example the symbol classes are defined by the conditions

$$\partial_t^n \partial_x^\alpha \partial_k^\beta \partial_l^\gamma a(t, x, k, l, \lambda) \in O(\langle x \rangle^{|\alpha|-n} \langle t \rangle^{|\alpha|-n} \langle k \rangle^{m-|\beta|-\gamma}), \quad \alpha, \beta \in \mathbb{N}^d, \quad n, p, \gamma \in \mathbb{N}.$$

To obtain a pdo calculus which is stable under composition one has to add an ideal included in  $S^0(\mathbb{R}; \mathcal{W}^{-\infty}(\mathbb{R}_x^d \times \mathbb{R}_l))$ , consisting of operator-valued functions  $\mathbb{R} \ni t \mapsto a(t)$  such that

$$\|\partial_t^n (D_l^2 + D_x^2 + x^2)^n a(t) (D_l^2 + D_x^2 + x^2)^n\|_{B(L^2(\mathbb{R}_x^d \times \mathbb{R}_l))} \in O(\langle t \rangle^{-n}) \quad \forall n \in \mathbb{N}.$$

Again Seeley's theorem and the analog of (A.4) are valid for this class of pseudodifferential operators. The proof can be completed by exactly the same arguments.  $\square$

**Proof of Prop. 3.11.** In view of the identity

$$a_1^{1+\alpha} - a_2^{1+\alpha} = (a_1 - a_2)a_1^\alpha + a_2(a_1^\alpha - a_2^\alpha),$$

we see that it suffices to prove the proposition for  $0 < \alpha < 1$ . We will use the following formula, valid for example if  $a$  is a selfadjoint operator on a Hilbert space  $\mathcal{H}$  with  $a \geq c\mathbf{1}$ ,  $c > 0$ :

$$(A.5) \quad a^\alpha = C_\alpha \int_0^{+\infty} (a+s)^{-1} s^\alpha ds = C_\alpha \int_{\mathbb{R}} (a+\lambda^2)^{-1} \lambda^{2\alpha+1} d\lambda, \quad \alpha \in \mathbb{R},$$

where the integrals are norm convergent in say,  $B(\text{Dom } a^m, \mathcal{H})$  for  $m$  large enough.

We will detail the proof in the first case of Prop. 3.11, i.e.  $a_i \in S^0(\mathbb{R}; \Psi^2(\Sigma))$ . The second case can be handled similarly.

We have for  $r(t) = a_1(t) - a_2(t)$ :

$$\begin{aligned} (a_1(t) + \lambda^2)^{-1} &= (a_2(t) + \lambda^2)^{-1} (\mathbf{1} + (a_2(t) + \lambda^2)r(t)(a_1(t) + \lambda^2)^{-1}) \\ &= (a_2(t) + \lambda^2)^{-1} + (a_2(t) + \lambda^2)^{-2} (a_2(t) + \lambda^2)r(t)(a_1(t) + \lambda^2)^{-1} \\ &= (a_2(t) + \lambda^2)^{-1} + (a_2(t) + \lambda^2)^{-2} a_2^{k/2}(t) c_1(t, \lambda) \\ &= (a_2(t) + \lambda^2)^{-1} + a_2(t) c_2(t, \lambda), \end{aligned}$$

where using Lemma A.1,  $c_1(t, \lambda) \in S^{-\delta}(\mathbb{R}; \tilde{\Psi}^0(\Sigma))$  and  $c_2(t, \lambda) \in S^{-\delta}(\mathbb{R}; \tilde{\Psi}^{-4}(\Sigma))$ . From (A.5) we obtain that:

$$(A.6) \quad a_1^\alpha(t) - a_2^\alpha(t) = C_\alpha a_2^{k/2}(t) \int_{\mathbb{R}} r_2(t, \lambda) \lambda^{2\alpha+1} d\lambda.$$

We now write  $r_2(t, \lambda)$  as  $\text{Op}(d_2(t, \lambda)) + w_2(t, \lambda)$ , for  $d_2 \in S^{-\delta}(\mathbb{R}; \tilde{S}_{\text{ph}}^{-4}(T^*\Sigma))$  and  $w_2(t, \lambda) \in S^{-\delta}(\mathbb{R}; \tilde{\mathcal{W}}^{-\infty}(\Sigma))$ . Using that

$$\int_{\mathbb{R}} (\langle \xi \rangle + \langle \lambda \rangle)^{-4-k} \lambda^{2\alpha+1} d\lambda \sim \langle \xi \rangle^{2\alpha-2-k},$$

we first obtain that

$$\int_{\mathbb{R}} d_2(t, \lambda) \lambda^{2\alpha+1} d\lambda \in S^{-\delta}(\mathbb{R}; S_{\text{ph}}^{2\alpha-2}(\Sigma)).$$

Similarly we obtain that  $\int_{\mathbb{R}} w_2(t, \lambda) \lambda^{2\alpha+1} d\lambda \in S^{-\delta}(\mathbb{R}; \mathcal{W}^{-\infty}(\Sigma))$ . Using (A.6) this implies that  $a_1^\alpha(t) - a_2^\alpha(t) \in S^{-\delta}(\mathbb{R}; \Psi^{2\alpha}(\Sigma))$ , as claimed.

**A.2. Proof of Prop. 4.5.** We follow the proof in [GW1]. The out and in cases are treated similarly. We set  $a_0 = \frac{1}{2}(\epsilon^{-1}\partial_t\epsilon + \epsilon^{-1}r\epsilon)$ ,

$$F(c) := \frac{1}{2}\epsilon^{-1}(\partial_t c + [\epsilon, c] + irc - c^2) = G(c) - \frac{1}{2}\epsilon^{-1}c^2.$$

and look for  $b(t)$  as  $\epsilon(t) + b_0$ , where  $b_0 = a_0 + F(b_0)$ . Let us start by studying some properties of the map  $F$ . First if  $c \in \Psi_{(*)}^{0, -\mu}$  then:

$$\begin{aligned} G(c) &\in \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{0,-1-\mu} + \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{0,-\mu} + \Psi_{(*)}^{-1,0} \Psi_{(*)}^{0,-1-\delta} \times \Psi_{(*)}^{0,-\mu}, \\ \epsilon^{-1}c^2 &\in \Psi_{(*)}^{-1,-2\mu}, \end{aligned}$$

hence

$$(A.7) \quad c \in \Psi_{(*)}^{0,-\mu} \Rightarrow F(c) \in \Psi_{(*)}^{-1,-\mu}.$$

Secondly, if  $c_1, c_2 \in \Psi_{(*)}^{0,-\mu}$  and  $c_1 - c_2 \in \Psi_{(*)}^{-j,-\mu}$  then:

$$\begin{aligned} G(c_1) - G(c_2) &= G(c_1 - c_2) \\ &\in \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{-j,-1-\mu} + \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{-j,-\mu} + \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{0,-1-\delta} \times \Psi_{(*)}^{-j,-\mu}, \\ \epsilon^{-1}(c_1^2 - c_2^2) &= \epsilon^{-1}c_1(c_1 - c_2) + \epsilon^{-1}(c_1 - c_2)c_2 \\ &\in \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{0,-\mu} \times \Psi_{(*)}^{-j,-\mu} + \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{-j,-\mu} \times \Psi_{(*)}^{0,-\mu}, \end{aligned}$$

hence

$$(A.8) \quad c_1, c_2 \in \Psi_{(*)}^{0,-\mu}, \quad c_1 - c_2 \in \Psi_{(*)}^{-j,-\mu} \Rightarrow F(c_1) - F(c_2) \in \Psi_{(*)}^{-j-1,-\mu}.$$

We also have

$$\begin{aligned} a_0 &= \frac{i}{2}(\epsilon^{-1}\partial_t\epsilon + \epsilon^{-1}r\epsilon) \\ &\in \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{1,-1-\delta} + \Psi_{(*)}^{-1,0} \times \Psi_{(*)}^{0,-1-\delta} \times \Psi_{(*)}^{1,0} \in \Psi_{(*)}^{0,-1-\delta}. \end{aligned}$$

We now follow the proof in [GW1, Lemma A.1], setting  $b_0 = a_0$ ,  $b_n = a_0 + F(b_{n-1})$ , and obtain by induction that  $b_n - b_{n-1} \in \Psi_{(*)}^{-n,-1-\delta}$ . We set

$$b_0 \sim a_0 + \sum_{n=1}^{\infty} b_n - b_{n-1} \in \Psi_{(*)}^{0,-1-\delta}$$

by Lemma 3.12. We obtain that

$$i\partial_t b - b^2 + a + irb \in \Psi_{(*)}^{-\infty,-1-\delta}.$$

By construction we have  $b(t) = \epsilon(t) + \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma)$ . Applying Prop. 3.11 we get

$$\epsilon(t) = \epsilon_{\text{out/in}} + \Psi_{(*)}^{1,-\delta}(\mathbb{R}_{\pm}; \Sigma) \text{ in } \mathbb{R}_{\pm} \times \Sigma.$$

□

**A.3. Proof of Prop. 4.6.** From Prop. 4.5 we first obtain that  $b^+ - b^- = (b + b^*) = 2\epsilon + \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma)$ . It follows first that  $(b^+ - b^-)^2 = 4a + \Psi_{(*)}^{1,-1-\delta}(\mathbb{R}; \Sigma)$  and then by Prop. 4.5 that

$$(b^+ - b^-)^{\alpha} = ((b^+ - b^-)^2)^{\alpha/2} = \begin{cases} (2\epsilon)^{\frac{1}{2}} + \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma), & \alpha = \frac{1}{2} \\ (2\epsilon)^{-\frac{1}{2}} + \Psi_{(*)}^{-3/2,-1-\delta}(\mathbb{R}; \Sigma), & \alpha = -\frac{1}{2}. \end{cases}$$

We obtain again by Prop. 4.5 that:

$$\begin{aligned} [(b^+ - b^-)^{-\frac{1}{2}}, b^{\pm}] &= [(2\epsilon)^{-\frac{1}{2}} + \Psi_{(*)}^{-3/2,-1-\delta}(\mathbb{R}; \Sigma), \pm\epsilon + \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma)] \in \Psi_{(*)}^{-3/2,-1-\delta}(\mathbb{R}; \Sigma), \\ \partial_t(b^+ - b^-)^{-\frac{1}{2}}(b^+ - b^-)^{\frac{1}{2}} &= (\partial_t(2\epsilon)^{-\frac{1}{2}} + \Psi_{(*)}^{-3/2,-2-\delta}(\mathbb{R}; \Sigma)) \times \Psi_{(*)}^{\frac{1}{2},0}(\mathbb{R}; \Sigma) \\ &= \partial_t(2\epsilon)^{-\frac{1}{2}} \times \Psi_{(*)}^{\frac{1}{2},0}(\mathbb{R}; \Sigma) + \Psi_{(*)}^{-1,-2-\delta}(\mathbb{R}; \Sigma). \end{aligned}$$

Since by Prop. 3.11  $(2\epsilon)^{-\frac{1}{2}} = (2\epsilon_{\text{out/in}})^{-\frac{1}{2}} + \Psi_{(*)}^{-3/2,-\delta}(\mathbb{R}_{\pm}; \Sigma)$ , we have

$$\partial_t(2\epsilon)^{-\frac{1}{2}} \in \Psi_{(*)}^{-3/2,-1-\delta}(\mathbb{R}; \Sigma) \Rightarrow \partial_t(b^+ - b^-)^{-\frac{1}{2}}(b^+ - b^-)^{\frac{1}{2}} \in \Psi_{(*)}^{-1,-1-\delta}(\mathbb{R}; \Sigma).$$

Since by hypothesis  $(H^*)$ ,  $r \in \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma)$ , we obtain that  $r_b^{\pm} \in \Psi_{(*)}^{0,-1-\delta}(\mathbb{R}; \Sigma)$ . Finally we obtain immediately from Prop. 4.5 that  $r_{-\infty}^{\pm} = i\partial_t b^{\pm} - (b^{\pm})^2 + a + irb^{\pm} \in \Psi_{(*)}^{-\infty,-1-\delta}(\mathbb{R}; \Sigma)$ . □

**A.4. Proof of Lemma 5.1.** Let us fix two good chart coverings  $\{U_i, \psi_i\}_{i \in \mathbb{N}}$  and  $\{\tilde{U}_i, \tilde{\psi}_i\}_{i \in \mathbb{N}}$  with  $U_i \Subset \tilde{U}_i$ . Since  $b \in C_b^{\infty}(\mathbb{R}; \text{BT}_0^1(\Sigma, k))$ , we obtain easily by transporting  $b$  to  $B_n(0, 1)$  using  $\psi_i$  that there exists  $t_{+, \epsilon} > 0$  such that  $y(t, s, \cdot)$  is a bounded diffeomorphism of  $(\Sigma, k)$ , uniformly for  $|t - s| \leq t_{+, \epsilon}$ . By the group property of the flow we can replace  $t_{+, \epsilon}$  by any  $t_+ > 0$ , keeping the above uniformity property.

Moreover if  $b_i := (\psi_i^{-1})^* b$  we obtain from (ast) that  $b_i \in S^{-\delta}(\mathbb{R}; \text{BT}_0^1(B_n(0, 1)))$ , uniformly in  $i \in \mathbb{N}$ . If  $y_i(t, s, \cdot)$  denotes the flow of  $b_i$  we obtain that:

$$y_i(t, s, x) = x + \int_s^t b_i(\sigma, y_i(\sigma, s, x)) d\sigma.$$

From this we obtain that there exists  $t_+ \gg 1$  such that  $y_i(\pm t, \pm t_+, \cdot) : B_n(0, \frac{1}{2}) \rightarrow B_n(0, 1)$  for all  $t \geq t_+$  and moreover

$$\lim_{t \rightarrow \pm\infty} y_i(t, \pm t_+, y) = \int_{\pm t_+}^{\pm\infty} b_i(\sigma, y_i(\sigma, \pm t_+, x)) ds =: y_i(\pm\infty, t_+, x).$$

We can also choose  $t_+$  large enough so that if we set

$$(A.9) \quad y(\pm\infty, \pm t_+, x) := \psi_i^{-1} \circ y_i(\pm\infty, \pm t_+, \cdot) \circ \psi_i(y), \quad x \in U_i$$

then  $y(\pm\infty, \pm t_+, \cdot)$  is well defined, and is a bounded diffeomorphism of  $(\Sigma, k)$ . We now set:

$$y_{\text{out/in}} := y(\pm\infty, \pm t_+, \cdot) \circ y(\pm t_+, 0, \cdot),$$

which is also a bounded diffeomorphism of  $(\Sigma, k)$ . We also obtain from (A.10) and the previous estimates on  $y(t, s, \cdot)$  for  $|t - s| \leq t_+$  that  $\{y(t, 0, \cdot)\}_{t \in \mathbb{R}}$  is a bounded family of bounded diffeomorphisms of  $(\Sigma, k)$ . Moreover from (A.9) we obtain that

$$(A.10) \quad y_i(t, 0, x) - y_{i, \text{out/in}}(x) \in S^{1-\delta'}(\mathbb{R}; C_b^\infty(B_n(0, 1))), \quad \text{uniformly in } i \in \mathbb{N}.$$

Let us now consider the metric  $\chi^* g$ .

Since  $v \cdot dt = 0$ ,  $\chi^* g = {}^t D\chi(g \circ \chi) D\chi = -\hat{c}^2(t, x) dt^2 + \hat{h}(t, x) dx^2$ . Using (A.10) we obtain that

$$\begin{aligned} \hat{c}(t, x) &= c(t, y(t, x)) + S^{-2\delta'}(\mathbb{R}; \text{BT}_0^0(\Sigma)) \\ &= c_{\text{out/in}}(y(t, x)) + S^{-\min(2\delta', \delta)}(\mathbb{R}_\pm; \text{BT}_0^0(\Sigma)) \\ &= c_{\text{out/in}}(y_{\text{out/in}}(x)) + S^{-\min(1-\delta', \delta)}(\mathbb{R}_\pm; \text{BT}_0^0(\Sigma)). \end{aligned}$$

Similarly,

$$\begin{aligned} \hat{h}(t, x) &= {}^t Dy(t, x) h(t, y(t, x)) Dy(t, x) \\ &= {}^t Dy(t, x) h_{\text{out/in}}(y(t, x)) Dy(t, x) + S^{-\delta}(\mathbb{R}_\pm; \text{BT}_2^0(\Sigma)) \\ &= {}^t Dy_{\text{out/in}}(x) h_{\text{out/in}}(y_{\text{out/in}}(x)) Dy_{\text{out/in}}(x) + S^{-\min(1-\delta', \delta)}(\mathbb{R}_\pm; \text{BT}_2^0(\Sigma)), \\ \chi^* V &= r(t, y(t, x)) = r_{\text{out/in}}(y(t, x)) + S^{-\delta}(\mathbb{R}_\pm; \text{BT}_0^0(\Sigma)) \\ &= V_{\text{out/in}}(y_{\text{out/in}}(x)) + S^{-\min(1-\delta', \delta)}(\mathbb{R}_\pm; \text{BT}_0^0(\Sigma)). \end{aligned}$$

Since by definition

$$\hat{h}_{\text{out/in}} = y_{\text{out/in}}^* h_{\text{out/in}}, \quad \hat{c}_{\text{out/in}} = y_{\text{out/in}}^* c_{\text{out/in}}, \quad \hat{V}_{\text{out/in}} = y_{\text{out/in}}^* V_{\text{out/in}},$$

we obtain the assertion.  $\square$

**A.5. Proof of Lemma 6.3.** By interpolation, it suffices to prove the lemma for  $m, k \in \mathbb{N}$ . Let us set

$$\begin{aligned} T_{m,k}(t) &= \langle \epsilon(0) \rangle^m \langle x \rangle^k \mathcal{U}^{\text{ad}}(0, t) (\langle x \rangle + \langle t \rangle)^{-k} \langle \epsilon(0) \rangle^{-m}, \\ R_{m,k}(t, s) &= \mathcal{U}^{\text{ad}}(t, s) \langle \epsilon(s) \rangle^m \langle x \rangle^k \mathcal{U}^{\text{ad}}(s, t) (\langle x \rangle + \langle t \rangle)^{-k} \langle \epsilon(0) \rangle^{-m}. \end{aligned}$$

Using the uniform ellipticity of  $\epsilon(t)$  it suffices to prove that

$$(A.11) \quad \sup_{t \geq 0} \|T_{m,k}(t)\|_{B(\mathcal{H}^0)} < \infty.$$

We claim that

$$(A.12) \quad \sup_{0 \leq s \leq t} \|R_{m,k}(t, s)\|_{B(\mathcal{H}^0)} < \infty,$$

This of course implies (A.11) by taking  $s = 0$  and using that  $\mathcal{U}^{\text{ad}}(t, s)$  is uniformly bounded in  $B(\mathcal{H}^0)$  by Prop. 5.6. To prove (A.12) we compute

$$(A.13) \quad \begin{aligned} & \partial_s R_{m,k}(t, s) \\ &= \mathcal{U}^{\text{ad}}(t, s) (\partial_s \langle \epsilon(s) \rangle^m + [H^{\text{ad}}(s), -i \langle \epsilon(s) \rangle^m]) \langle x \rangle^k \mathcal{U}^{\text{ad}}(s, t) (\langle x \rangle + \langle t \rangle)^{-k} \langle \epsilon(0) \rangle^{-m} \\ & \quad + \mathcal{U}^{\text{ad}}(t, s) \langle \epsilon(s) \rangle^m [H^{\text{ad}}(s), -i \langle x \rangle^k] \mathcal{U}^{\text{ad}}(s, t) (\langle x \rangle + \langle t \rangle)^{-k} \langle \epsilon(0) \rangle^m. \end{aligned}$$

Recall that as in (5.13):

$$H^{\text{ad}}(t) = \begin{pmatrix} \epsilon(t) & 0 \\ 0 & -\epsilon(t) \end{pmatrix} + \Psi_{\text{std}}^{0, -1-\delta} \otimes B(\mathbb{C}^2)$$

by Prop. 4.5, 4.6. Hence:

$$(\partial_s \langle \epsilon(s) \rangle^m + [H^{\text{ad}}(s), -i \langle \epsilon(s) \rangle^m]) \in \Psi_{\text{std}}^{m, -1-\delta}(\mathbb{R}; \Sigma) \otimes B(\mathbb{C}^2),$$

and we can write:

$$(A.14) \quad (\partial_s \langle \epsilon(s) \rangle^m + [H^{\text{ad}}(s), -i \langle \epsilon(s) \rangle^m]) = A_m(s) \langle \epsilon(s) \rangle^m \langle x \rangle^{-1},$$

where

$$(A.15) \quad \|A_m(s)\|_{B(\mathcal{H})} \in O(1),$$

since  $(\langle x \rangle + \langle t \rangle)^{-1-\delta} \leq \langle x \rangle^{-1}$ .

Similarly we have

$$(A.16) \quad \langle \epsilon(s) \rangle^m [H^{\text{ad}}(s), i \langle x \rangle^k] = C_{m,k}(s) \langle \epsilon(s) \rangle^m \langle x \rangle^{k-1},$$

where

$$(A.17) \quad \|C_{m,k}(s)\|_{B(\mathcal{H}^0)} \in O(1).$$

We also set

$$B_{m,k}(t) = (\langle x \rangle + \langle t \rangle)^{-k+1} \langle \epsilon(0) \rangle^{-m} (\langle x \rangle + \langle t \rangle)^{k-1} \langle \epsilon(0) \rangle^m,$$

and we have by pseudodifferential calculus

$$(A.18) \quad \|B_{m,k}(t)\|_{B(\mathcal{H}^0)} \in O(1).$$

Hence we can rewrite (A.13) as

$$(A.19) \quad \begin{aligned} & \partial_s R_{m,k}(t, s) \\ &= \mathcal{U}^{\text{ad}}(t, s) D_{m,k}(s) \mathcal{U}^{\text{ad}}(s, t) \times R_{m,k-1}(t, s) \times B_{m,k}(t) \times (\langle x \rangle + \langle t \rangle)^{-1}, \end{aligned}$$

where

$$(A.20) \quad D_{m,k}(s) = A_m(s) + C_{m,k}(s), \quad \|D_{m,k}(s)\|_{B(\mathcal{H}^0)} \in O(1).$$

We can prove now (A.12) by induction for  $k$ . First, note that by Prop. 5.6, 1), (A.12) holds for  $k = 0$ . Assume that (A.12) holds for  $k - 1$ . Integrating (A.19) from  $t$  to  $s$  we obtain:

$$\|R_{m,k}(t, s) - R_{m,k}(t, t)\| \leq \int_0^t \|R_{m,k-1}(t, \sigma)\| \langle t \rangle^{-1} dt \in O(1), \text{ for } 0 \leq s \leq t$$

by the induction hypothesis. We conclude the proof of (A.12) using that

$$\|R_{m,k}(t, t)\| = \|\langle \epsilon(t) \rangle^m \langle x \rangle^k (\langle x \rangle + \langle t \rangle)^{-k} \langle \epsilon(0) \rangle^m\| \in O(1).$$

This completes the proof of the lemma.  $\square$

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