ON THE POSITIVITY OF PROPAGATOR DIFFERENCES

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Abstract. We discuss positivity properties of 'distinguished propagators', i.e. distinguished *inverses* of operators that frequently occur in scattering theory and wave propagation. We relate this to the work of Duistermaat and Hörmander on distinguished *parametrices* (approximate inverses), which has played a major role in quantum field theory on curved spacetimes recently.

1. Introduction and main results

In this short paper we discuss positivity properties of the differences of 'propagators', i.e. inverses of operators of the kind that frequently occur in scattering theory and wave propagation. Concretely, we discuss various settings in which there are function spaces, corresponding to the 'distinguished parametrices' of Duistermaat and Hörmander [6], on which these operators are Fredholm; in the case of actual invertibility one has inverses and one can ask about the positivity properties of their differences. As we recall below, Duistermaat and Hörmander analyzed possibilities for choices of *parametrices* (approximate inverses modulo smoothing) possessing such positivity properties; here we show that certain of the *actual inverses* possess these properties, and we give a new proof of the Duistermaat-Hörmander theorem when our Fredholm setup is applicable. Such a result is relevant to quantum field theory on curved spacetimes, with work in this direction, relying on the Duistermaat-Hörmander framework, initiated by Radzikowski [25]; see the work of Brunetti, Fredenhagen and Köhler [2, 3], of Dappiaggi, Moretti and Pinamonti [4, 24, 5] and of Gérard and Wrochna [10, 11] for more recent developments. It turns out that the positivity properties are closely connected to the positivity of spectral measure for the Laplacian in scattering theory.

As background, we first recall that in elliptic settings, or microlocally (in $T^*X \setminus o$) where a pseudodifferential operator P on a manifold X is elliptic, there are no choices to make: parametrices (as well as inverses when one has a globally well-behaved 'fully elliptic' problem and these exist) are essentially unique; here for parametrices uniqueness is up to smoothing terms. On the other hand, if P is scalar with real principal symbol p (with a homogeneous representative), or simply has real scalar principal symbol, then Hörmander's theorem [20] states that singularities of solutions to $Pu = f$ propagate along bicharacteristics (integral curves of the Hamilton vector field H_p) in the characteristic set Σ, in the sense that $\mathrm{WF}^s(u) \setminus \mathrm{WF}^{s-m+1}(Pu) \subset \Sigma$ is invariant under the Hamilton flow; here m is the order of P.

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In terms of estimates, the propagation theorem states that one can estimate u in H^s microlocally at a point $\alpha \in T^*X \setminus o$ if one has an a priori estimate for u in H^s at $\gamma_\alpha(t)$ for some $t > 0$, where γ_α is the bicharacteristic through α, and if one has an a priori estimate for Pu in H^{s-m+1} microlocally along $\gamma_\alpha|_{[0,t]}$; the analogous statement for $t < 0$ also holds.

Such a propagation statement is empty where H_p is radial, i.e. is a multiple of the radial vector field in $T^*X \setminus o$, with the latter being the infinitesimal generator of dilations in the fibers of $T^*X \setminus o$. However, these radial points also have been analyzed, starting with the work of Guillemin and Schaeffer [12] in the case of isolated radial points, further explored by Hassell, Melrose and Vasy [14, 15] inspired by the work of Herbst [17] and Herbst and Skibsted [18] on a scattering problem, by Melrose [22] for Lagrangian submanifolds of normal sources/sinks in scattering theory, and by Vasy [31] in a very general situation (more general than radial points), with a more detailed analysis by Haber and Vasy in [13]; see also the work of Dyatlov and Zworski [7] for their role in dynamical systems. (In a more complicated direction, in N-body scattering these correspond to the propagation set of Sigal and Soffer [26]; see [9] for a discussion that is microlocal in the radial variable and see [28] for a fully microlocal discussion.)

In order to make the picture very clear, consider the Hamilton flow on $S^*X = (T^*X \setminus o)/\mathbb{R}^+$ rather than on $T^*X \setminus o$. This is possible if $m = 1$ since the Hamilton vector field then is homogeneous of degree 0 and thus can be thought of as a vector field on S^*X. For general m one can reduce to this case by multiplying by a positive elliptic factor; the choice of the elliptic factor changes the Hamilton vector field but within Σ only by a positive factor; in particular the bicharacteristics only get reparameterized. Thus a radial point is a critical point for the Hamilton vector field on S^*X (i.e. where the vector field vanishes); in the cases discussed here it is a non-degenerate source or sink.

In fact, it is better to think of S^*X as 'fiber infinity' $\partial\overline{T^*}X$ on the fiber compactification of T^*X. Here recall that if V is a k-dimensional vector space, it has a natural compactification $\overline{V}$ obtained by gluing a sphere, namely $(V \setminus 0)/\mathbb{R}^+$ to infinity. Explicitly this can be done e.g. by putting a (positive definite) inner product on V, so $V \setminus 0$ is identified with $\mathbb{R}^+_r \times \mathbb{S}^{k-1}$, with r the distance from 0, and using 'reciprocal polar coordinates' $(\rho, \omega) \in (0, \infty) \times \mathbb{S}^{k-1}$, $\rho = r^{-1}$, to glue in the sphere at $\rho = 0$, so that the resulting manifold is covered with the two (generalized) coordinate charts V and $[0, \infty)_\rho \times \mathbb{S}^{k-1}$ with overlap $V \setminus 0$, resp. $(0, \infty)_\rho \times \mathbb{S}^{k-1}$, identified as above. This process gives a smooth structure independent of choices, and correspondingly it can be applied to compactify the fibers of T^*X. For standard microlocal analysis the relevant location is fiber infinity, so one may instead simply work with $S^*X \times [0, \epsilon)_\rho$, if one so desires, with the choice of a homogeneous degree -1 function ρ on $T^*X \setminus o$ giving the identification.

The advantage for this point of view is that the Hamilton vector field in fact induces a vector field $\mathsf{H}_p = \rho^{m-1} H_p$ on $\overline{T^*}X$, tangent to $\partial\overline{T^*}X$, whose linearization at radial points in $\partial\overline{T^*}X$ is well defined. This includes the normal to the fiber boundary behavior, i.e. that on homogeneous degree -1 functions on $T^*X \setminus o$, via components $\rho\partial_\rho$ of the vector field; this disappears in the quotient picture. We are then interested in critical points that are sources/sinks within Σ even in this extended sense, so $H_p\rho = \rho^{-m+2}\beta_0$, where ρ is a boundary defining function, e.g. a positive homogeneous degree -1 function on $T^*X \setminus o$ near $\partial\overline{T^*}X$, and where $\beta_0 > 0$

at sources, $\beta_0 < 0$ at sinks. Such behavior is automatic for Lagrangian submanifolds of radial points (these are the maximal dimensional sets of non-degenerate radial points). The typical basic result is that there is a threshold regularity s_0 such that for $s < s_0$ one has a propagation of singularities type result: if a punctured neighborhood $U \setminus \Lambda$ of a source/sink type radial set Λ is disjoint from $\mathrm{WF}^s(u)$ and the corresponding neighborhood U is disjoint from $\mathrm{WF}^{s-m+1}(Pu)$, then $\Lambda \cap \mathrm{WF}^s(u) = \emptyset$, i.e. one can propagate estimates into Λ, while if $s > s_1 > s_0$, and $\mathrm{WF}^{s_1}(u) \cap \Lambda = \emptyset$ then one can gets *'for free'* H^s regularity at Λ, i.e. $\mathrm{WF}^s(u) \cap \Lambda = \emptyset$.

Here we emphasize that all of the results below hold in the more general setting discussed in [31, Section 2.2], where Λ are 'normal sources/sinks', but need not consist of actual radial points, i.e. there may be a non-trivial Hamilton flow within Λ — this is the case for instance in problems related to Kerr-de Sitter spaces. Furthermore, the setup is also stable under general pseudodifferential (small!) perturbations of order m (with real principal symbol), even though the dynamics can change under these; this is due to the stability of the estimates (and the corresponding stability of the normal dynamics in a generalized sense) see [31, Section 2.7].

Now, the estimates given by the propagation theorem let one estimate u somewhere in terms of *Pu provided one has an estimate for u somewhere else.* But where can such an estimate come from? A typical situation for hyperbolic equations is Cauchy data, which is somewhat awkward from the microlocal analysis perspective and indeed is very ill-suited to Feynman type propagators. A more natural place is from radial sets: if one is in a sufficiently regular (above the threshold) Sobolev space, one gets regularity for free there in terms of a weaker (but stronger than the threshold) Sobolev norm. (This weaker norm is relatively compact in the settings of interest, and thus is irrelevant for Fredholm theory.) This can then be propagated along bicharacteristics, and indeed can be propagated into another radial set provided that we use Sobolev spaces which are weaker than the threshold regularity there. This typically requires the use of variable order Sobolev spaces, but as the propagation of singularities still applies for these, provided the Sobolev order is monotone decreasing in the direction in which we propagate our estimates (see [1, Appendix]), this is not a problem. Note that in order to obtain Fredholm estimates eventually we need analogous estimates for the adjoint (relative to L^2) P^* on dual (relative to L^2) spaces; since the dual of above, resp. below threshold regularity is regularity below, resp. above threshold regularity, for the adjoint one will need to propagate estimates in the *opposite direction.* Notice that *within each connected component* one has to have the same direction of propagation relative to the Hamilton flow, but of course one can make different choices in different connected components. This general framework was introduced by the author in [31], further developed with Baskin and Wunsch in [1], with Hintz in [19] and with Gell-Redman and Haber in [8].

Returning to the main theme of the paper, we recall that in their influential paper [6] Duistermaat and Hörmander used the Fourier integral operators they just developed to construct distinguished parametrices for real principal type equations: for each component of the characteristic set, one chooses the direction in which estimates, or equivalently singularities of forcing (i.e. of f for u being the parametrix applied to f) propagate along the Hamilton flow in the sense discussed above. Here the direction is most conveniently measured relative to the Hamilton flow in the characteristic set. Thus, with k components of the characteristic set, there are 2^k distinguished parametrices. Notice that there are two special choices for the distinguished parametrices: the one propagating estimates forward everywhere along the H_p-flow, and the one propagating estimates backward everywhere along the H_p-flow; these are the Feynman and anti-Feynman parametrices (defined up to smoothing operators). Duistermaat and Hörmander showed that, if the operator P is formally self-adjoint, one can choose these parametrices (which are defined modulo smoothing operators a priori) so that they are all formally skew-adjoint, and further such that $\imath$ times the difference between any of these parametrices and the Feynman, i.e. the H_p-forward, parametrix is positive. They also stated that they do not see a way of fixing the smoothing ambiguity, though the paper suggests that this would be important in view of the relationship to quantum field theory, as suggested to the authors by Wightmann.

The purpose of this paper is to show how, under a natural additional assumption on the global dynamics, the ambiguity can be fixed for all propagators, and exact positivity can be shown for the extreme difference of propagators. A byproduct is a simple proof of the positivity for a suitable choice of distinguished parametrices (not just the extreme difference), giving a different proof of the Duistermaat-Hörmander result. However, one cannot expect in general that the differences other than the extreme difference are actually positive; thus, if positivity is desired, the *only* natural choice is that of the Feynman propagators.

In order to achieve this, in the simplest setting of compact manifolds without boundary, X, we require a non-trapping dynamics for the formally self-adjoint operator P of order m. Here non-trapping is understood in the sense that the characteristic set Σ of P has connected components Σ_j, $j = 1, \ldots, k$, in each of which one is given smooth conic submanifolds $\Lambda_{j,\pm}$ (with $\Lambda_\pm = \cup_j \Lambda_{j,\pm}$) which act as normal sources $(-)$ or sinks $(+)$ for the bicharacteristic flow within Σ_j in a precise sense described above, and all bicharacteristics in Σ_j except those in $\Lambda_{j,\pm}$, tend to $\Lambda_{j,+}$ in the forward and to $\Lambda_{j,-}$ in the backward direction (relative to the flow parameter) along the bicharacteristic flow, see Figure 1. (As recalled above, this setup can be generalized further, for instance it is stable under general perturbations in $\Psi^m(X)$ even though the details of the dynamics are not such in general.) In this case, on variable order weighted Sobolev spaces H^s, with s monotone increasing/decreasing in each component of the characteristic set along the Hamilton flow, and satisfying threshold inequalities at $\Lambda_{j,\pm}$, $P : \mathcal{X} \to \mathcal{Y}$ is Fredholm, where

$$\mathcal{X} = \{u \in H^s : \ Pu \in H^{s-m+1}\}, \ \mathcal{Y} = H^{s-m+1}. \tag{1}$$

Here the Fredholm estimates take the form

$$\begin{aligned} \|u\|_{H^s} &\leq C(\|Pu\|_{H^{s-m+1}} + \|u\|_{H^r}), \\ \|v\|_{H^{s'}} &\leq C(\|P^*v\|_{H^{s'-m+1}} + \|v\|_{H^{r'}}), \end{aligned} \tag{2}$$

for appropriate r, r' with compact inclusion $H^s \to H^r, H^{s'} \to H^{r'}$, where we take $s' = -s + m - 1$, so $s' - m + 1 = -s$. Note that with this choice of s' the space on the left hand side, resp. in the first term on the right hand side, of the first inequality is the dual (relative to L^2) of the first space of the right hand side, resp. the left hand side of the second inequality, as required for the functional analytic setup. Here (2) is an estimate in terms of Sobolev spaces (which $\mathcal{Y}$ is, but $\mathcal{X}$ is not), but it implies the Fredholm property (1); see [31, Section 2.6].

If $P = P^*$, then the threshold regularity is $(m-1)/2$, i.e. s can be almost constant, but it has to be slightly below $(m-1)/2$ at one end of each bicharacteristic, and slightly above $(m-1)/2$ at the other. *Assuming that these problems are invertible*, the inverse is independent of the choice of s in a natural sense, as long as the increasing/decreasing direction of s is kept unchanged along each component of the characteristic set (see [31, Remark 2.9]). Note that in the case of invertibility, the compact term of (2) can be dropped, and one concludes that $P^{-1} : H^{s-m+1} \to H^s$, $(P^*)^{-1} : H^{-s} \to H^{-s+m-1}$ are bounded maps, with $(P^*)^{-1} = (P^{-1})^*$. (Here invertibility is not a serious issue for our purposes; see Remark 3.) Letting $I \subset \{1, \ldots, k\} = J_k$ be the subset on which s is increasing (i.e. where estimates are propagated *backwards*), we denote by

$$P_I^{-1} : \mathcal{Y}_I \to \mathcal{X}_I$$

the corresponding inverse; here $\mathcal{X}_I, \mathcal{Y}_I$ stand for the spaces $\mathcal{X}, \mathcal{Y}$ above for any choice of s compatible with I. Thus, $P_\emptyset^{-1}$ is the Feynman, or forward propagator, i.e. it propagates estimates H_p-forward along the bicharacteristics, so for $\phi \in \mathcal{C}^\infty(X)$, $\mathrm{WF}(P_\emptyset^{-1}\phi) \subset \cup_j \Lambda_{j,+}$, while $P_{J_k}^{-1}$ is the backward, or anti-Feynman, propagator. For general $\phi \in H^{s-m+1}$, $\mathrm{WF}(P_\emptyset^{-1}\phi)$ is contained in the union of the image of $\mathrm{WF}(\phi)$ under the forward Hamilton flow (interpreted so that the image of the sources under the forward flow is all bicharacteristics emanating from them) with the sinks $\cup_j \Lambda_{j,+}$; the analogous statement for the backward flow holds for $\mathrm{WF}(P_{J_k}^{-1}\phi)$. Such a setup is explained in detail in [31, Section 2].

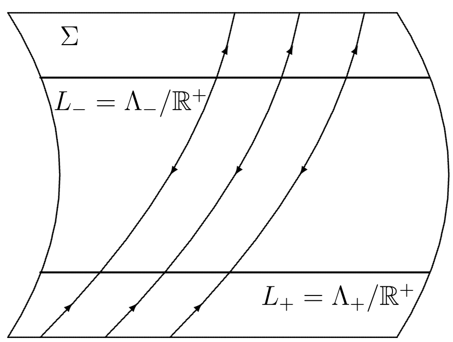

FIGURE 1. The characteristic set Σ (here connected) and the Hamilton dynamics for a problem satisfying our assumptions. Here Σ is a torus, with the left and right, as well as the top and bottom, edges identified. An example is the multiplication operator by a real valued function on a compact manifold with non-degenerate zeros. This is closely related to the Fourier transform of the basic Euclidean scattering problem, $\Delta - \lambda$, $\lambda > 0$, which is multiplication by $|\xi|^2 - \lambda$. The dynamics is exactly as shown above when the zero set is a circle.

We recall an example, which will also be used below, from [31], given in this form in [33]. If one considers the Minkowski wave operator $\Box_g$ on $\mathbb{R}^{n+1}_{z,t}$, or more conveniently $x^{-(n-2)/2-2}\Box_g x^{(n-2)/2}$, with $x = (|z|^2 + t^2)^{-1/2}$, then the Mellin transform of this operator in the radial variable on $\mathbb{R}^{n+1}$, or its reciprocal x, is a family of operators on the sphere $\mathbb{S}^n$; here $\mathbb{S}^n$ arises as a smooth transversal to the dilation orbits on $\mathbb{R}^{n+1}\setminus o$. This family P_σ, depending on the Mellin dual parameter σ, is an example of this setup with $X=\mathbb{S}^n$. As explained in [33], in fact P_σ is elliptic/hyperbolic in the region of $\mathbb{S}^n$ interior/exterior of the Minkowski light cone; it turns out to be related to the spectral family of the Laplacian on hyperbolic space, resp. the d'Alembertian on de Sitter space. This example, and natural generalizations, such as the spectral family of Laplacian and the Klein-Gordon operator on *even asymptotically hyperbolic and de Sitter spaces* (even on differential forms), respectively, discussed in [30] and [29], will arise again later in this paper.

The basic idea of such a compact dynamical setup first appeared in Melrose's work on scattering [22], where $P=\Delta-\lambda$, Δ is the Laplacian of a scattering metric (large end of a cone), $\lambda>0$. In that case there are only two propagators, whose difference is essentially the spectral measure, so the positivity statement is that of the spectral measure for Δ. In some sense then, while one should not think of P as a self-adjoint operator in our general setting (though it is formally self-adjoint), since the adjoint propagates estimates always the opposite way (corresponding to having to work in dual function spaces), one still has a positivity property analogous to these spectral measures. Indeed, from a certain perspective, the proof given below is inspired by an analogous proof in scattering theory, related to Melrose's 'boundary pairing' [22, Section 13], though in that setting there are more standard proofs as well. We refer to the discussion around Theorem 8 for more detail.

The main result is the following.

Theorem 1. *Suppose $P=P^*\in\Psi(X)$ is as above (i.e. X is compact, the principal symbol p is real, the Hamilton dynamics is non-trapping), possibly acting on a vector bundle with scalar principal symbol. If $P_{J_k}^{-1}$, $P_\emptyset^{-1}$ exist (rather than P being merely Fredholm between the appropriate spaces) then the operator $\imath(P_{J_k}^{-1}-P_\emptyset^{-1})$ is positive, i.e. it is symmetric*

$$\langle \imath(P_{J_k}^{-1}-P_\emptyset^{-1})\phi,\psi\rangle=\langle\phi,\imath(P_{J_k}^{-1}-P_\emptyset^{-1})\psi\rangle,\qquad \phi,\psi\in\mathcal{C}^\infty(X),\tag{3}$$

and for all $\phi\in\mathcal{C}^\infty(X)$,

$$\langle \imath(P_{J_k}^{-1}-P_\emptyset^{-1})\phi,\phi\rangle\geq 0.\tag{4}$$

Remark 2. Note that this is the same formula (in particular the sign matches) as in the work of Duistermaat and Hörmander [6, Theorem 6.6.2] (taking into account that we have inverses, while they had parametrices) when $S_{\tilde n}$ of [6, Theorem 6.6.2] is replaced by $E^+_{\tilde N}-E^+_\emptyset$. Indeed, the statement obtained by replacing $S_{\tilde n}$ of [6, Theorem 6.6.2] by $E^+_{\tilde N}-E^+_\emptyset$ is an immediate consequence of the theorem in view of [6, Equation (6.6.4)]; for the signs we need to keep in mind that in that paper $S_{\tilde n}$ is 'relative to' the backward, anti-Feynman, propagator (parametrix), denoted by $E^+_\emptyset$ there, i.e. it is $E^+_{(\tilde n)}-E^+_\emptyset$.

Note also that the proof given below also shows the symmetry of $\imath(P_{I^c}^{-1}-P_I^{-1})$ for any $I\subset J_k$, assuming these inverses exist (rather than P being just Fredholm between the corresponding spaces) although positivity properties are lost. However, see Corollary 4 for a parametrix statement, and Remark 3 regarding invertibility.

Remark 3. As the following proof shows, only minor changes are needed if P is merely Fredholm between the appropriate spaces. Namely for each I let $\mathcal{W}_I$ be a complementary subspace to the finite dimensional subspace $\mathrm{Ker}_I P = \mathrm{Ker} P$ of $\mathcal{X}_I$. Then for $\phi \in \mathrm{Ran}_I P = \mathrm{Ran}\, P \subset \mathcal{Y}_I$ there exists a unique $u \in \mathcal{W}_I$ such that $Pu = \phi$; we may define $P_I^{-1}\phi = u$. Then (3) holds if we require in addition $\phi, \psi \in \mathrm{Ran}_\emptyset P \cap \mathrm{Ran}_{J_k} P$ and (4) holds if we require $\phi \in \mathrm{Ran}_\emptyset P \cap \mathrm{Ran}_{J_k} P$, as follows immediately from the proof we give below. (These are finite codimension conditions!) Note that different choices of $\mathcal{W}_I$ do not affect either of the inner products (3)-(4) since P_I^{-1} applied to an element ϕ of $\mathrm{Ran}_I P$ is being paired with an element of $\mathrm{Ran}_{I^c} P$, and the latter annihilates (i.e. is orthogonal with respect to the L^2 pairing) $\mathrm{Ker}_I P$, i.e. changing $P_I^{-1}\phi$ by an element of $\mathrm{Ker}_I P$ leaves the inner product unchanged.

We now discuss what happens under an additional hypothesis, $\mathrm{Ker}_\emptyset P, \mathrm{Ker}_{J_k} P \subset \mathcal{C}^\infty(X)$. In this case, $\mathrm{Ker}_\emptyset P = \mathrm{Ker}_{J_k} P$ (since elements of both are simply elements of $\mathcal{C}^\infty(X)$ which are mapped to 0 by P); denote this finite dimensional space by $\mathcal{F}$. In this case one can use the L^2-orthocomplements of $\mathcal{F}$ to define $\mathcal{W}_\emptyset$ and $\mathcal{W}_{J_k}$ in $\mathcal{X}_\emptyset$, resp. $\mathcal{X}_{J_k}$. That is, $\mathcal{W}_\emptyset$, resp. $\mathcal{W}_{J_k}$ are the subspaces of $\mathcal{X}_\emptyset$, resp. $\mathcal{X}_{J_k}$, consisting of distributions L^2-orthogonal to $\mathcal{F}$ (which is a subset of both of these spaces!); this makes sense since $\mathcal{F}$ is a subspace of $\mathcal{C}^\infty(X)$. Similarly, $\mathcal{F}$ gives orthocomplements to $\mathrm{Ran}_\emptyset P$ and $\mathrm{Ran}_{J_k} P$ in $\mathcal{Y}_\emptyset$, resp, $\mathcal{Y}_{J_k}$. Thus, one can define $P_I^{-1}\phi$, $\phi \in \mathcal{Y}_I$, $I = \emptyset, J_k$, by defining it to be $P_I^{-1}\phi_1$, $\phi = \phi_1 + \phi_2 \in \mathrm{Ran}_I P + \mathcal{F}$, where P_I^{-1} takes values in $\mathcal{W}_I$. In this case, the inner products (3)-(4) are unaffected by the second component of the function in both slots, and thus they remain true for all $\phi, \psi \in \mathcal{C}^\infty(X)$.

While the assumption $\mathrm{Ker}_\emptyset P, \mathrm{Ker}_{J_k} P \subset \mathcal{C}^\infty(X)$ may seem unnatural, one expects it to hold in analogy with scattering theory: there incoming or outgoing elements of the tempered distributional nullspace of the operator necessarily vanish, giving that any such element is necessarily Schwartz. This can in fact be proved in the present setting as well using the functional calculus for an elliptic operator; since this is a bit involved we defer this to another paper, and we choose to discuss this here only in the setting of Theorem 8 for differential operators, where this is straightforward since the role of the elliptic operator is played by the weight x.

Proof. The symmetry statement is standard; one can arrange the function spaces so that $P_{J_k}^{-1}$ is exactly the inverse of $P^* = P$ on (essentially) the duals of the spaces (in reversed role) on which $P_\emptyset^{-1}$ inverts P, so $P_{J_k}^{-1} = (P_\emptyset^{-1})^*$, see [31, Section 2] and (2) above. Here 'essentially' refers to the fact that the Fredholm estimates (2), with the compact terms dropped as remarked above, due to invertibility, give bounded maps $P^{-1} : H^{s-m+1} \to H^s$, $(P^*)^{-1} : H^{-s} \to H^{-s+m-1}$, with $(P^*)^{-1} = (P^{-1})^*$. Correspondingly, the symmetry actually holds for any $\phi, \psi \in H^{-s} \cap H^{s-m+1}$, s satisfying the requirements for the $\emptyset$-inverse.

We turn to the proof of positivity, with $I = J_k$ to minimize double subscripts. Let $\mathcal{J}_r$, $r \in (0,1)$ be a family of (finitely) smoothing operators, converging to $\mathcal{J}_0 = \mathrm{Id}$ as $r \to 0$ in the usual manner, so $\mathcal{J}_r \in \Psi^{-N}(X)$, $N > 1$ for $r \in (0,1)$, $\mathcal{J}_r$, $r \in (0,1)$ is uniformly bounded in $\Psi^0(X)$, converging to Id in $\Psi^\epsilon(X)$ for all $\epsilon > 0$. Concretely, with ρ a defining function of $S^*X = \partial\overline{T}^* X$ (e.g. homogeneous of degree -1 away from the zero section), we can let the principal symbol j_r of $\mathcal{J}_r$ be $(1 + r\rho^{-1})^{-N}$, $N > 1$. Let $u_I = P_I^{-1}\phi$, $u_\emptyset = P_\emptyset^{-1}\phi$. Then for $\phi \in \mathcal{C}^\infty(X)$, as

$Pu_I = \phi = Pu_\emptyset$,

$$\begin{aligned}\langle \imath(P_I^{-1} - P_\emptyset^{-1})\phi, \phi\rangle &= \langle \imath(u_I - u_\emptyset), Pu_\emptyset\rangle \\ &= \lim_{r\to 0}\langle \imath\mathcal{J}_r(u_I - u_\emptyset), Pu_\emptyset\rangle = \lim_{r\to 0}\langle \imath[P,\mathcal{J}_r](u_I - u_\emptyset), u_\emptyset\rangle.\end{aligned}$$

Now note that $[P,\mathcal{J}_r]$ is uniformly bounded in $\Psi^{m-1}(X)$, converging to $[P,\mathrm{Id}] = 0$ in $\Psi^{m-1+\epsilon}(X)$, $\epsilon > 0$, so $[P,\mathcal{J}_r] \to 0$ strongly as a bounded operator $H^\sigma \to H^{\sigma-m+1}$. By a standard microlocal argument about distributions with disjoint wave front set, using also the above statements on $[P,\mathcal{J}_r]$, we have

$$\lim_{r\to 0}\langle \imath[P,\mathcal{J}_r]u_I, u_\emptyset\rangle = 0. \tag{5}$$

To see this claim, let $\Lambda_\pm = \cup_j \Lambda_{\pm,j}$, $Q_+ \in \Psi^0(X)$ be such that $\mathrm{WF}'(\mathrm{Id} - Q_+)\cap\Lambda_+ = \emptyset$, $\mathrm{WF}'(Q_+)\cap\Lambda_- = \emptyset$, i.e. Q_+ is microlocally the identity at Λ_+, microlocally 0 at Λ_-, we have (as $I = J_k$) $Q_+u_I \in \mathcal{C}^\infty(X)$, $(\mathrm{Id} - Q_+)u_\emptyset \in \mathcal{C}^\infty(X)$ since $\mathrm{WF}(u_\emptyset) \subset \Lambda_+$, $\mathrm{WF}(u_I) \subset \Lambda_-$. Define Q_- similarly, with $\Lambda_\pm$ interchanged, and such that $\mathrm{WF}'(\mathrm{Id} - Q_+)\cap\mathrm{WF}'(\mathrm{Id} - Q_-) = \emptyset$ (so at each point at least one of $Q_\pm$ is microlocally the identity); then $Q_-u_\emptyset \in \mathcal{C}^\infty(X)$ and $(\mathrm{Id} - Q_-)u_I \in \mathcal{C}^\infty(X)$. Thus,

$$\begin{aligned}\langle \imath[P,\mathcal{J}_r]u_I, u_\emptyset\rangle =& \langle \imath[P,\mathcal{J}_r]Q_+u_I, u_\emptyset\rangle + \langle Q_-^*[P,\mathcal{J}_r](\mathrm{Id} - Q_+)u_I, u_\emptyset\rangle \\ &+ \langle (\mathrm{Id} - Q_-^*)[P,\mathcal{J}_r](\mathrm{Id} - Q_+)u_I, u_\emptyset\rangle.\end{aligned}$$

Now the first term goes to 0 as $r \to 0$ since $Q_+u_I \in \mathcal{C}^\infty(X)$ in view of the stated strong convergence of the commutator to 0, while the second term goes to 0 similarly due to $Q_-u_\emptyset \in \mathcal{C}^\infty(X)$ and the stated strong convergence of the commutator to 0. Finally, in view of the disjoint wave front set of $\mathrm{Id} - Q_+$ and $\mathrm{Id} - Q_-$, thus $\mathrm{Id} - Q_+$ and $\mathrm{Id} - Q_-^*$, $(\mathrm{Id} - Q_-^*)[P,\mathcal{J}_r](\mathrm{Id} - Q_+)$ is in fact uniformly bounded in $\Psi^{-k}(X)$ for any k, and indeed converges to 0 in $\Psi^{-k}(X)$, so the third term also goes to 0. This proves (5).

So it remains to consider $-\langle \imath[P,\mathcal{J}_r]u_\emptyset, u_\emptyset\rangle$. But the principal symbol of $\imath[P,\mathcal{J}_r]$ is

$$H_p j_r = Nr\rho^{-2}(1 + r\rho^{-1})^{-1}(H_p\rho)j_r$$

which takes the form $c_r^2 j_r$ at the sources (as $H_p\rho = \rho^{-m+2}\beta_0$ with β_0 positive there), and $-c_r^2 j_r$ at the sinks. In our case, the wave front set of $u_\emptyset$ is at the sinks Λ_+, so are concerned about the second region. Let c_r be a symbol with square $-Nr\rho^{-2}(1+r\rho^{-1})^{-1}(H_p\rho)\chi_+^2$, where χ_+ is a cutoff function, identically 1 near Λ_+, supported close to Λ_+, and letting C_r be a quantization of this with the quantization arranged using local coordinates and a partition of unity; these are being specified so that C_r is uniformly bounded in $\Psi^{(m-1)/2}(X)$, and *still tends to* 0 *in* $\Psi^{(m-1)/2+\epsilon}(X)$ *for* $\epsilon > 0$. Similarly, let E_r be a quantization of $Nr\rho^{-2}(1+r\rho^{-1})^{-1}(H_p\rho)(1-\chi_+^2)$. Then we have

$$\imath[P,\mathcal{J}_r] = -C_r^*\tilde{\mathcal{J}}_r^*\tilde{\mathcal{J}}_r C_r + E_r + F_r,$$

where the principal symbol of $\tilde{\mathcal{J}}_r$ is the square root of that of $\mathcal{J}_r$, where the family E_r is uniformly bounded in $\Psi^{m-1}(X)$, has (uniform!) wave front set disjoint from Λ_+, while F_r is uniformly bounded in $\Psi^{m-2}(X)$, and further both E_r and F_r tend to 0 in higher order pseudodifferential operators. The disjointness of the uniform wave front set of E_r from Λ_+, thus from the wave front set of $u_\emptyset$, and further that it tends to 0 as $r \to 0$ in the relevant sense, shows by an argument similar to the proof of (5) that

$$\lim_{r\to 0}\langle E_r u_\emptyset, u_\emptyset\rangle = 0.$$

On the other hand, as $u_\emptyset$ is in $H^{(m-1)/2-\epsilon}$ for all $\epsilon > 0$, the fact that $F_r \to 0$ in $\Psi^{m-2+\epsilon}$, $\epsilon > 0$, and thus $F_r \to 0$ strongly as a family of operators $H^{(m-1)/2-\epsilon} \to H^{-(m-1)/2+\epsilon}$, $\epsilon < 1/2$, yields that

$$\lim_{r\to 0}\langle F_r u_\emptyset, u_\emptyset\rangle = 0.$$

Finally,

$$\langle C_r^* \tilde{\mathcal{J}}_r^* \tilde{\mathcal{J}}_r C_r u_\emptyset, u_\emptyset\rangle \geq 0$$

for all r, so

$$\begin{aligned}\langle \imath(P_I^{-1} - P_\emptyset^{-1})\phi, \phi\rangle &= \lim_{r\to 0}\langle \imath[P, \mathcal{J}_r](u_I - u_\emptyset), u_\emptyset\rangle \\ &= \lim_{r\to 0}\langle C_r^* \tilde{\mathcal{J}}_r^* \tilde{\mathcal{J}}_r C_r u_\emptyset, u_\emptyset\rangle \geq 0.\end{aligned}$$

This proves the theorem. □

Before proceeding, we now discuss generalized inverses for P_I when P_I is not invertible, rather merely Fredholm. Note that since $\mathcal{C}^\infty(X)$ is dense in $\mathcal{Y}_I = H^{s_I - m+1}$, the closed subspace of finite codimension $\mathrm{Ran}_I\, P$ has a complementary subspace $\mathcal{Z}_I \subset \mathcal{C}^\infty(X)$ in $\mathcal{Y}_I$: indeed, the orthocomplement of $\mathrm{Ran}_I\, P$ in the Hilbert space $\mathcal{Y}_I$ is finite dimensional, and approximating an orthonormal basis for it by elements of $\mathcal{C}^\infty(X)$ gives the desired complementary space. We now can decompose an arbitrary $f \in \mathcal{Y}_I$ as $f = f_1 + f_2$, $f_1 \in \mathrm{Ran}_I\, P$, $f_2 \in \mathcal{Z}_I$ and then, letting $\mathcal{W}_I$ be a complementary subspace of $\mathcal{X}_I$ to $\mathrm{Ker}_I P$, $f_1 = Pu$ for a unique $u \in \mathcal{W}_I$; we let $P_I^{-1} f = u$, so P_I^{-1} is a *generalized inverse* for P. Note that as $\mathcal{Z}_I \subset \mathcal{C}^\infty(X)$, $\mathrm{WF}^\sigma(f_1) = \mathrm{WF}^\sigma(f)$ for all σ. The propagation of singularities, for $f \in H^\sigma$, $\sigma > -(m-1)/2$, $Pu = f_1$, $u \in \mathcal{X}_I$ shows that $\mathrm{WF}^{\sigma+m-1}(u) \subset \cup_{j\in I}\Lambda_{j,-} \cup \cup_{j\in I^c}\Lambda_{j,+}$. This suffices for all the arguments below.

An immediate corollary of Theorem 1 is the Duistermaat-Hörmander theorem:

Corollary 4. *(cf. Duistermaat and Hörmander* [6, Theorem 6.6.2]*) Suppose that P is as in Theorem 1 (in particular, $P_\emptyset$, P_{J_k} are invertible). For all I, there exists an operator $\tilde{S}_I$ such that $P_I^{-1} - P_\emptyset^{-1}$ differs from $\tilde{S}_I$ by an operator that is smoothing away from $\Lambda_\pm$ in the sense that $\phi \in \mathcal{C}^{-\infty}(X)$, $\mathrm{WF}^\sigma(\phi) \cap (\Lambda_+ \cup \Lambda_-) = \emptyset$, $\sigma > -(m-1)/2$, implies $\mathrm{WF}((P_I^{-1} - P_\emptyset^{-1} - \tilde{S}_I)\phi) \subset \Lambda_+ \cup \Lambda_-$, and such that $\tilde{S}_I$ is skew-adjoint and $\imath\tilde{S}_I$ is positive.*

Here, if P_I is not invertible (i.e. is only Fredholm), the statement holds if in addition $\phi \in \mathrm{Ran}\, P_I$ in the sense of Remark 3, and more generally for all ϕ as above if P_I^{-1} is a generalized inverse of P_I defined on $\mathcal{Y}_I$ using a complement $\mathcal{Z}_I$ to $\mathrm{Ran}\, P_I$ which is a subspace of $\mathcal{C}^\infty$, as defined above.

Thus, here smoothing is understood e.g. as a statement that for $\phi \in H^\sigma(X)$, where $\sigma > -(m-1)/2$, the operator in question maps to $\mathcal{C}^\infty(X)$, microlocally away from $\Lambda_\pm$. In fact, as all the operators in question can naturally be applied to distributions with wave front set away from $\Lambda_\pm$ (by suitable choice of the order function s), which is the context of the Duistermaat-Hörmander result, and smoothing holds in this extended context as well, as stated in the corollary.

Remark 5. In the case of $P_\emptyset$ and P_{J_k}, in Remark 3 we showed that if $\mathrm{Ker}_\emptyset P, \mathrm{Ker}_{J_k} P \subset \mathcal{C}^\infty(X)$, then we have canonical generalized inverses $P_\emptyset^{-1}$, $P_{J_k}^{-1}$ which satisfy the properties (3)-(4). Thus, relaxing the invertibility hypothesis for $P_\emptyset$, P_{J_k}, but under this additional assumption on the kernels of these operators, conclusion of this Corollary still holds.

Proof. In the following discussion we assume that P_I is invertible. In fact, all the arguments go through for a generalized inverse as in the statement of the theorem, but it is more convenient to not have to write out repeatedly decompositions with respect to which the generalized inverse is taken.

We use a microlocal partition of unity $\sum_{j=0}^k B_j$, $B_j = B_j^*$, with B_0 having wave front set in the elliptic set, B_j, $j \geq 1$ having wave front set disjoint from the components Σ_l, $l \neq j$, of the characteristic set. Let

$$T_j = B_j(P_{J_k}^{-1} - P_\emptyset^{-1})B_j.$$

Then for any I,

$$\tilde{S}_I = \sum_{j \in I} T_j$$

has the required properties, with skew-adjointness of $\tilde{S}_I$ and positivity of $\imath\tilde{S}_I$ following from the main theorem above.

To see the parametrix property, note that for $j \neq 0$, $B_j = \mathrm{Id}$ microlocally near Σ_j, while $B_l = 0$ microlocally near Σ_j for $l \neq j$. Thus, for $\phi \in H^\sigma(X)$, where $\sigma > -(m-1)/2$,

$$P(P_\emptyset^{-1} + \tilde{S}_I)\phi = \phi + \sum_{j \in I}[P, B_j](P_{J_k}^{-1} - P_\emptyset^{-1})B_j\phi,$$

with the wave front set of the commutator, and thus of all but the first term, being in the elliptic set. But $P(P_{J_k}^{-1} - P_\emptyset^{-1})B_j\phi = 0$, so microlocal elliptic regularity shows that $[P, B_j](P_{J_k}^{-1} - P_\emptyset^{-1})B_j\phi \in \mathcal{C}^\infty(X)$.

Notice that microlocal elliptic regularity also shows that all parametrices are microlocally the same in the elliptic set: if $Pu - Pv \in \mathcal{C}^\infty(X)$, then $u - v$ has wave front set disjoint from the elliptic set of P. So in order to analyze our parametrix, it suffices to consider the characteristic set.

Microlocally near Σ_j, $P_\emptyset^{-1}f$, resp. $P_{J_k}^{-1}f$, $f \in H^\sigma(X)$, solve $Pu - f \in \mathcal{C}^\infty(X)$, with $\mathrm{WF}^{\sigma+m-1}(u) \subset \Lambda_{+,j}$, resp. $\mathrm{WF}^{\sigma+m-1}(u) \subset \Lambda_{-,j}$. Further $P_I^{-1}f$ has the same property as one of these, depending on whether $j \notin I$ or $j \in I$. In particular, for $j \notin I$, $u = P_I^{-1}\phi - P_\emptyset^{-1}\phi$ solves $Pu = 0$, with $\mathrm{WF}^{\sigma+m-1}(u) \cap \Sigma_j \subset \Lambda_{+,j}$, which implies by propagation of singularities (including the version at the radial points in $\Lambda_{-,j}$, where u is a priori in a better space than the threshold Sobolev regularity) that in fact $\mathrm{WF}(u) \cap \Sigma_j \subset \Lambda_{+,j}$. Since microlocally near Σ_j, $(P_\emptyset^{-1} + \tilde{S}_I)\phi$ is the same as $P_\emptyset^{-1}\phi$ if $j \notin I$, we deduce that $P_I^{-1} - (P_\emptyset^{-1} + \tilde{S}_I)$ is smoothing near such j, in the sense that in this neighborhood of Σ_j, $\mathrm{WF}(P_I^{-1}\phi - (P_\emptyset^{-1} + \tilde{S}_I)\phi)$ is contained in $\Lambda_{+,j}$, so we only need to consider $j \in I$.

Since $B_j\phi$ and ϕ are the same microlocally near Σ_j, by the propagation of singularities, again using the a priori better than threshold Sobolev regularity at $\Lambda_{+,j}$, $u = P_{J_k}^{-1}(\phi - B_j\phi)$ has $\mathrm{WF}(u) \cap \Sigma_j \subset \Lambda_{-,j}$, and similarly for $P_\emptyset^{-1}(\phi - B_j\phi)$ (for $\Lambda_{+,j}$). In view of B_j being microlocally the identity near Σ_j, and trivial near Σ_k, $k \neq j$, we deduce that the intersection of the wave front set of $P_\emptyset^{-1}\phi - B_jP_\emptyset^{-1}B_j\phi$ with Σ_j is in $\Lambda_{+,j}$. Similar arguments give that for $j \in I$ the intersection of the wave front set of $P_I^{-1}\phi - B_jP_{J_k}^{-1}B_j\phi$ with Σ_j is in $\Lambda_{-,j}$. The conclusion is that, microlocally near Σ_j, $j \in I$, the wave front set of $(P_\emptyset^{-1} + \tilde{S}_I)\phi - P_I^{-1}\phi$ is in $\Lambda_{+,j} \cup \Lambda_{-,j}$. This proves that $P_I^{-1} - P_\emptyset^{-1}$ differs from $\tilde{S}_I$ by an operator that is smoothing away from $\Lambda_\pm$, completing the proof of the corollary. $\square$

Notice that while it is a distinguished parametrix in the Duistermaat-Hörmander sense, $P_\emptyset^{-1}+\tilde{S}_I$ is in principle not necessarily one of our distinguished inverses, P_I^{-1}. Indeed, while P_I^{-1} maps $\phi\in\mathcal{C}^\infty(X)$ to have wave front set disjoint from $\Lambda_{j,+}$ for $j\in I$, on the other hand, for $j\in I$ the difference of $P_\emptyset^{-1}\phi$ and $B_jP_\emptyset^{-1}B_j\phi$ at $\Lambda_{j,+}$ is not necessarily smooth, though it does have wave front set (locally) contained in $\Lambda_{j,+}$ (i.e. the difference is smoothing away from $\Lambda_{j,+}$ within Σ_j). If B_j can be arranged to commute with P, however, this statement can be improved.

2. Positivity in Melrose's b-pseudodifferential algebra

There are natural extensions to b- and scattering settings of Melrose (see [23] for a general treatment of the b-setting, [22] for the scattering setting), such as the wave equation and the Klein-Gordon equation on asymptotically Minkowski spaces, in the sense of 'Lorentzian scattering metrics' of Baskin, Vasy and Wunsch, see [1] and [19, Section 5]. This in particular includes the physically relevant example of Minkowski space (and perturbations of an appropriate type) that motivated this part of the Duistermaat-Hörmander work. Since no new analytic work is necessary in these new settings (i.e. one essentially verbatim repeats the proof of Theorem 1 and Corollary 4, changing various bundles, etc.), we only briefly recall the setups and state the corresponding theorems, explaining any (minor) new features.

Before proceeding, we recall that Melrose's b-analysis is induced by the analysis of totally characteristic, or b-, differential operators, i.e. ones generated (over $\mathcal{C}^\infty(M)$, as finite sums of products) by vector fields $V\in\mathcal{V}_{\mathrm{b}}(M)$ tangent to the boundary of a manifold with boundary M. Locally near some point in $X=\partial M$, with the boundary defined by a function x (so it vanishes non-degenerately and exactly at ∂M), and with y_j, $j=1,\dots,n-1$, local coordinates on X, extended to M, these vector fields are linear combinations of the vector fields $x\partial_x$ and ∂_{y_j} with smooth coefficients, i.e. are of the form $a_0(x\partial_x)+\sum a_j\partial_{y_j}$. Correspondingly, they are exactly the set of all smooth sections of a vector bundle, ${}^{\mathrm{b}}TM$. Thus, the dual bundle ${}^{\mathrm{b}}T^*M$ has smooth sections locally of the form $b_0\,\frac{dx}{x}+\sum b_j\,dy_j$, with b_j smooth. Then (classical) b-pseudodifferential operators $P\in\Psi_{\mathrm{b}}^m(M)$ have principal symbols p which are homogeneous degree m functions on ${}^{\mathrm{b}}T^*M\setminus o$.

Thus, in the b-setting, where this setup was described by Gell-Redman, Haber and Vasy [8], we require for the strengthened Fredholm framework that $P\in\Psi_{\mathrm{b}}^m(M)$ is formally self-adjoint, and the bicharacteristic dynamics in ${}^{\mathrm{b}}S^*M$ is as before, i.e. with sources and sinks at $L=L_+\cup L_-\subset{}^{\mathrm{b}}S^*M=({}^{\mathrm{b}}T^*M\setminus o)/\mathbb{R}^+$ (with $L_+=\Lambda_+/\mathbb{R}^+$ in the previous notation, where Λ was conic). Examples include a modified conjugate of the Minkowski wave operator, and more generally non-trapping Lorentzian scattering metrics, namely if x is a boundary defining function, then the relevant operator is $P=x^{-(n-2)/2-2}\Box_g x^{(n-2)/2}$ (symmetric with respect to the b-density $x^n\,|dg|$); see [19]. The characteristic set Σ satisfies $\Sigma\subset{}^{\mathrm{b}}S^*M$, and is a union of connected components Σ_j, $j=1,\dots,k$, just as in the boundaryless setting. Again, choosing a subset I of J_k, we require the order s to be increasing along the H_p-flow on Σ_j, $j\in I$, decreasing otherwise, so in Σ_j, $j\in I$ estimates are propagated backwards, for $j\in I^c$ forwards. The additional ingredient is to have a weight $\ell\in\mathbb{R}$; we then work with the variable order b-Sobolev spaces $H_{\mathrm{b}}^{s,\ell}$. The actual numerology of the function spaces arises from the sources and sinks, namely with x being a boundary defining function as before and ρ_∞ being a defining function of fiber infinity in $\overline{{}^{\mathrm{b}}T^*M}$ (so e.g. can be taken as a homogenous degree -1

function on ${}^{\mathrm{b}}T^*M$ away from the zero section), both $H_p x$ and $H_p\rho_\infty$ play a role. A general numerology is discussed in [19, Proposition 2.1] for saddle points, with an analogous numerology also available for other sources/sinks but is discussed only for $P = x^{-(n-2)/2-2}\Box_g x^{(n-2)/2}$ in [19, Section 5]. Thus, here for simplicity, we only consider the numerology of $P = x^{-(n-2)/2-2}\Box_g x^{(n-2)/2}$, though we remark that *for ultrahyperbolic equations corresponding to quadratic forms on $\mathbb{R}^n$ the numerology is identical.* The requirement at L then for obtaining the estimates needed to establish Fredholm properties is $s+\ell > (m-1)/2$ (with $m=2$ for the wave operator) at the components $L_{\pm,j}$ from which one wants to propagate estimates, and $s+\ell < (m-1)/2$ to which one wants to propagate estimates. This (plus the required monotonicity of s along bicharacteristics) is still not sufficient, it only gives estimates of the form

$$\|u\|_{H_{\mathrm{b}}^{s,\ell}} \leq C(\|Pu\|_{H_{\mathrm{b}}^{s-m+1,\ell}} + \|u\|_{H_{\mathrm{b}}^{\tilde{s},\ell}}),$$

with $\tilde{s} < s$; here the problem is that the inclusion $H_{\mathrm{b}}^{s,\ell} \to H_{\mathrm{b}}^{\tilde{s},\ell}$ is *not* compact, because there is no gain in the decay order, ℓ. Thus, one needs an additional condition involving the Mellin transformed normal operator, $\hat{P}(.)$.

One arrives at the normal operator by 'freezing coefficients' at $X = \partial M$, namely by using a collar neighborhood $X \times [0,\epsilon)_x$ of X, including it in $X \times [0,\infty)$, obtaining an operator by evaluating the coefficients of P at $x = 0$ (which can be done in a natural sense) and then regarding the resulting $N(P)$ as a dilation invariant operator on $X \times \mathbb{R}^+$, with dilations acting in the second factor. The Mellin transform then is simply the Mellin transform in the $\mathbb{R}^+$-factor. Thus, the Mellin transformed normal operator is a family of operators, $\mathbb{C} \ni \sigma \mapsto \hat{P}(\sigma)$, on $X = \partial M$. In fact, this is an analytic Fredholm family by the boundaryless analysis explained above (with the dynamical assumptions on P implying those for $\hat{P}(\sigma)$), which in addition has the property that for any $C > 0$ it is invertible in $|\operatorname{Im}\sigma| < C$ for $|\sigma|$ large (with 'large' depending on C), due to the high energy, or semiclassical version, of these Fredholm estimates. The poles of the inverse are called resonances and form a discrete set of $\mathbb{C}$, with only finitely many in any strip $|\operatorname{Im}\sigma| < C$. If ℓ is chosen so that there are no resonances with $\operatorname{Im}\sigma = -\ell$, and if the requirement on s is strengthened to $s+\ell-1 > (m-1)/2$ at the components from which we propagate estimates then $P : \mathcal{X} \to \mathcal{Y}$ is Fredholm, where

$$\mathcal{X} = \{u \in H_{\mathrm{b}}^{s,\ell} :\ Pu \in H_{\mathrm{b}}^{s-m+1,\ell}\},\ \mathcal{Y} = H_{\mathrm{b}}^{s-m+1,\ell}.$$

(Here the stronger requirement $s+\ell-1 > (m-1)/2$ enters when combining the normal operator estimates with the symbolic estimates, see [19, Proposition 2.3 and Section 5] and [8, Theorem 3.3].) Again, for given ℓ, if P is actually invertible, P^{-1} only depends on the choice of I (modulo the natural identification), so we write P_I^{-1}; if we allow ℓ to vary it is still independent of ℓ as long as we do not cross any resonances, i.e. if ℓ and ℓ' are such that there are no resonances σ with $-\operatorname{Im}\sigma \in [\ell,\ell']$ (if $\ell < \ell'$). Then the arguments given above, with regularization $\mathcal{J}_r$ needed only in the differentiability (not decay) sense, so $\mathcal{J}_r \in \Psi_{\mathrm{b}}^{-N}(M)$ for $r > 0$, uniformly bounded in $\Psi_{\mathrm{b}}^0(M)$, converging to Id in $\Psi_{\mathrm{b}}^\epsilon(M)$ for any $\epsilon > 0$ apply if we take the decay order to be $\ell = 0$, i.e. work with spaces $H_{\mathrm{b}}^{s,0}$, the point being that $[P,\mathcal{J}_r] \to 0$ in $\Psi_{\mathrm{b}}^{m-1+\epsilon}$ then (there is no extra decay at X), so we need to make sure that u_I lie in a weighted space with weight 0 to get the required boundedness and convergence properties. In summary, this show immediately the following theorem and corollary, with the analogue of Remark 3 also valid:

Theorem 6. *Suppose $P = P^* \in \Psi_{\mathrm{b}}^m(M)$ is as above, and suppose that no resonances lie on the real line,* $\operatorname{Im}\sigma = 0$. *If $P_{J_k}^{-1}$, $P_\emptyset^{-1}$ exist (rather than P being merely Fredholm between the appropriate spaces) then the operator $\imath(P_{J_k}^{-1} - P_\emptyset^{-1})$ is positive, i.e. it is symmetric and for all $\phi \in \dot{\mathcal{C}}^\infty(M)$,*

$$\langle \imath(P_{J_k}^{-1} - P_\emptyset^{-1})\phi, \phi\rangle \geq 0.$$

Corollary 7. *(cf. Duistermaat and Hörmander* [6, Theorem 6.6.2]*) Suppose that P is as in Theorem 6 (in particular, $P_\emptyset$, P_{J_k} are invertible). For all I, there exists an operator $\tilde{S}_I$ such that $P_I^{-1} - P_\emptyset^{-1}$ differs from $\tilde{S}_I$ by an operator that is smoothing away from $L_\pm$ in the sense that* $\mathrm{WF}_{\mathrm{b}}^{\sigma,0}(\phi) \cap (L_+ \cup L_-) = \emptyset$, *$\sigma > 1 - \frac{m-1}{2}$, implies that* $\mathrm{WF}_{\mathrm{b}}^{\infty,0}((P_I^{-1} - P_\emptyset^{-1} - \tilde{S}_I)\phi) \subset L_+ \cup L_-$, *and such that $\tilde{S}_I$ is skew-adjoint and $\imath\tilde{S}_I$ is positive.*

If P_I is not invertible, P_I^{-1} is understood as a generalized inverse, using a $\dot{\mathcal{C}}^\infty(M)$-complement to $\operatorname{Ran}_I P$, *similarly to the discussion preceding Corollary 4.*

3. Positivity in Melrose's scattering pseudodifferential algebra

The scattering setting, $P \in \Psi_{\mathrm{sc}}^m(M)$ (one can also have a weight l; this is irrelevant here), is analogous to the b-setting, except that all the principal symbols are functions (there is no normal operator family), but they are objects on two intersecting boundary hypersurfaces of the cotangent bundles: fiber infinity ${}^{\mathrm{sc}}S^*M$, and base infinity $\overline{{}^{\mathrm{sc}}T^*}_{\partial M}M$, and (full) ellipticity is the invertibility of both of these. (Note that these two parts of the principal symbol agree at the corner ${}^{\mathrm{sc}}S^*_{\partial M}M = \partial\overline{{}^{\mathrm{sc}}T^*}_{\partial M}M$ of $\overline{{}^{\mathrm{sc}}T^*}M$.) While here we used the invariant formulation, an example to which it can *always* be locally reduced is the radial compactification $M = \overline{\mathbb{R}^n}$ of $\mathbb{R}^n$; in that case ${}^{\mathrm{sc}}T^*M = \overline{\mathbb{R}^n} \times \mathbb{R}^n$ with basis of sections of ${}^{\mathrm{sc}}T^*M$ given by the lifts of the standard coordinate differentials dz_j, $j = 1, \ldots, n$, and $\overline{{}^{\mathrm{sc}}T^*}M = \overline{\mathbb{R}^n} \times \overline{\mathbb{R}^n}$. This is the setting which Melrose introduced for studying the scattering theory of asymptotically Euclidean spaces [22]; these are compactified Riemannian manifolds M (so one has a Riemannian metric on M°) which are asymptotically the large ends of cones. For Melrose's problem, the operator $P = \Delta - \lambda$ is elliptic at fiber infinity, ${}^{\mathrm{sc}}S^*M$; note that λ is *not* lower order than Δ in the sense of the relevant principal symbol, namely at base infinity.

For such scattering problems the previous discussion can be repeated almost verbatim. Here one works with variable order scattering Sobolev spaces $H_{\mathrm{sc}}^{s,\ell}(M)$, with ℓ being necessarily variable now due to the ellipticity at ${}^{\mathrm{sc}}S^*M$, see [32]. Again, the relevant dynamical assumption is source/sink bundles $L_\pm$, where now since we have ellipticity at ${}^{\mathrm{sc}}S^*M$, we have $L_\pm \subset \overline{{}^{\mathrm{sc}}T^*}_{\partial M}M$, where now the requirement is $\ell > -1/2$ at the components from which we want to propagate estimates, and $\ell < -1/2$ at the components towards which we want to propagate estimates. (For a general operator of order l, the threshold would be $(l-1)/2$, i.e. l simply plays the analogue of the differential order m discussed in the compact setting X.) Actually as above, one can weaken the assumptions on the dynamics significantly, so one does not even need a source/sink manifold: one needs a source/sink region, with suitable behavior in the normal variables. (So for instance, the more typical lower dimensional sources/sinks/saddles of [15] are fine as well for this analysis; one regards the whole region on the 'outgoing' side a sink, on the 'incoming' side a source, regardless of the detailed dynamical behavior.) One then has that $P : \mathcal{X} \to \mathcal{Y}$ is Fredholm, where

$$\mathcal{X} = \{u \in H_{\mathrm{sc}}^{s,\ell} :\ Pu \in H_{\mathrm{sc}}^{s-m,\ell-1}\},\ \mathcal{Y} = H_{\mathrm{sc}}^{s-m,\ell-1}.$$

Now our 'smoothing' $\mathcal{J}_r$ is actually just decay gaining, i.e. spatial regularization, corresponding to ℓ; this does not affect the proof of the analogue of the main theorem. We thus have, with the above notation, with the analogue of Remark 3 also holding:

Theorem 8. *Suppose $P = P^* \in \Psi_{\mathrm{sc}}^m(M)$ is as above, in particular elliptic at ${}^{\mathrm{sc}}S^*M$. If $P_{J_k}^{-1}$, $P_\emptyset^{-1}$ exist (rather than P being merely Fredholm between the appropriate spaces) then the operator $\imath(P_{J_k}^{-1} - P_\emptyset^{-1})$ is positive, i.e. it is symmetric and for all $\phi \in \dot{\mathcal{C}}^\infty(M)$,*

$$\langle \imath(P_{J_k}^{-1} - P_\emptyset^{-1})\phi, \phi\rangle \geq 0.$$

Corollary 9. *(cf. Duistermaat and Hörmander* [6, Theorem 6.6.2]*) Suppose that P is as in Theorem 8 (in particular, $P_\emptyset$, P_{J_k} are invertible). For all I, there exists an operator $\tilde{S}_I$ such that $P_I^{-1} - P_\emptyset^{-1}$ differs from $\tilde{S}_I$ by an operator that is smoothing away from $L_\pm$ in the sense that $\mathrm{WF}_{\mathrm{sc}}^{s-m,\mu}(\phi) \cap (L_+ \cup L_-) = \emptyset$, $\mu > 1/2$, implies $\mathrm{WF}_{\mathrm{sc}}((P_I^{-1} - P_\emptyset^{-1} - \tilde{S}_I)\phi) \subset L_+ \cup L_-$, and such that $\tilde{S}_I$ is skew-adjoint and $\imath\tilde{S}_I$ is positive.*

If P_I is not invertible, P_I^{-1} is understood as a generalized inverse, using a $\dot{\mathcal{C}}^\infty(M)$-complement to $\mathrm{Ran}_I P$*, similarly to the discussion preceding Corollary 4.*

Notice that in this setting in fact P is actually self-adjoint on $L^2_{\mathrm{sc}}(M) = H_{\mathrm{sc}}^{0,0}(M)$ as an unbounded operator, which in turn follows from the invertibility of

$$P \pm \imath : H_{\mathrm{sc}}^{s,\ell} \to H_{\mathrm{sc}}^{s-m,\ell}$$

for any s, ℓ; note that $P \pm \imath$ is fully elliptic so invertibility as a map between any such pair of Sobolev spaces is equivalent to invertibility between any other pair. In the case of $P = \Delta_g + V - \lambda$, g as scattering metric, $V \in x\mathcal{C}^\infty(M)$ real, this problem was studied by Melrose [22], but of course there is extensive literature in Euclidean scattering theory from much earlier. Then for $\lambda > 0$ the limits

$$(P \pm \imath 0)^{-1} = \lim_{\epsilon \to 0} (P \pm \imath\epsilon)^{-1}$$

exist in appropriate function spaces (this is the limiting absorption principle), and

$$\imath(P_{J_k}^{-1} - P_\emptyset^{-1}) = \imath((P + \imath 0)^{-1} - (P - \imath 0)^{-1})$$

is, up to a positive factor, the density of the spectral measure by Stone's theorem. A direct scattering theory formula for it, implying its positivity, was given in [16, Lemma 5.2] using the Poisson operators; this formula in turn arose from 'boundary pairings'. This explains in detail the earlier statement that our result is a generalization of the positivity of the spectral measure in a natural sense.

This also gives rise to another interesting example, namely an asymptotically Euclidean space whose boundary has two connected components, e.g. two copies of $\mathbb{R}^n$ glued in a compact region. Then the previous theory applies in particular, with the Feynman and anti-Feynman propagators giving the limiting absorption principle resolvents. However, one can also work with different function spaces, propagating estimates forward in one component of the boundary (and hence the characteristic set), and backward in the other, relative to the Hamilton flow. The resulting problem is Fredholm, though the invertibility properties are unclear. This problem is an analogue of the retarded and advanced propagators (and thus the Cauchy problem) for the wave equation.

We now discuss the comments in the final paragraph of Remark 3 in more detail. For operators of the kind $P = \Delta_g + V - \lambda$, g as scattering metric, $V \in x\mathcal{C}^\infty(M)$ real, using the boundary pairing formula Melrose showed in [22] that the nullspaces of $P_\emptyset$ and P_{J_k} are necessarily in $\dot{\mathcal{C}}^\infty(M)$; he then used Hörmander's unique continuation theorem to show that in fact these nullspaces are trivial. There is a more robust proof of these results by a different commutator approach which, as far as the author knows, goes back to Isozaki's work in N-body scattering [21, Lemma 4.5]. In a geometric N-body setting this proof was adapted by Vasy in [27, Proposition 17.8]; it in particular applies to operators like $P = \Delta_g + V - \lambda$. The argument relies on a family of commutants given by functions which are *not* (uniformly) bounded in the relevant space of (scattering) pseudodifferential operators, but for which the commutators themselves *are* bounded, and have a sign modulo lower order terms. In the general setting of pseudodifferential operators, an analogous argument works provided one uses the functional calculus for an elliptic operator (the weight in the commutant). One has to be rather careful here because the commutant family is not bounded: this is the reason that the argument only implies that elements of the nullspace are in $\dot{\mathcal{C}}^\infty(M)$, not that those with $Pu \in \dot{\mathcal{C}}^\infty(M)$ are such; for pairings involving the commutant and Pu must vanish identically. This point will be addressed in a future paper in full detail. Notice that this result *only* applies to $P_\emptyset$ and P_{J_k} as illustrated by the two Euclidean end problem in a particularly simple setting: the line $\mathbb{R}_z$ with $V = 0$, $\lambda = 1$. Then the complex exponentials $e^{\pm \imath z \cdot \zeta}$ are incoming at one end, outgoing at the other, thus are in the nullspace of P_I, resp. P_{I^c}, for I corresponding to the appropriate non-Feynman choice.

The simplest non-elliptic (in the usual sense) interesting example in the scattering setting is the Klein-Gordon equation on asymptotically Minkowski like spaces (in the same sense as above, in the b-case, i.e. Lorentzian scattering spaces of [1]). Here one works with variable order scattering Sobolev spaces $H^{s,\ell}_{\mathrm{sc}}(M)$, see [32]. Let ρ_∞ be a defining function for fiber infinity, ${}^{\mathrm{sc}}S^*M$, and $\rho_{\partial M}$ a defining function for base infinity $\overline{{}^{\mathrm{sc}}T^*}_{\partial M}M$. Again, the relevant dynamical assumption is source/sink bundles $L_\pm$, where now for simplicity we assume that $L_\pm \subset \overline{{}^{\mathrm{sc}}T^*}_{\partial M}M$ transversal to the boundary of the fiber compactification and now $\beta_0 = \mp \rho_\infty^{m-1} \rho_{\partial M}^{-1} H_p \rho_{\partial M}$ is positive at $L_\pm$ while $\rho_\infty^{m-2} H_p \rho_\infty$ vanishes there. In this case, as shown in [32, Proposition 0.11] (where the roles of ρ_∞ and $\rho_{\partial M}$ are reversed), the requirement for propagation estimates at the sources/sinks is $\ell > -1/2$ at the components from which we want to propagate estimates, and $\ell < -1/2$ at the components towards which we want to propagate estimates. Actually as above, one can weaken the assumptions on the dynamics significantly, so one does not even need a source/sink manifold: one needs a source/sink region, with suitable behavior in the normal variables. (So for instance, the more typical lower dimensional sources/sinks/saddles of [15] are fine as well for this analysis; one regards the whole region on the 'outgoing' side a sink, on the 'incoming' side a source, regardless of the detailed dynamical behavior.) With ℓ chosen monotone along the H_p-flow, satisfying these inequalities, and with the dynamics being non-trapping in the same sense as before, one then has that $P : \mathcal{X} \to \mathcal{Y}$ is Fredholm, where

$$\mathcal{X} = \{u \in H_{\mathrm{sc}}^{s,\ell} :\ Pu \in H_{\mathrm{sc}}^{s-m+1,\ell-1}\},\ \mathcal{Y} = H_{\mathrm{sc}}^{s-m+1,\ell-1}.$$

Since there are no restrictions on s, we may simply take it high enough so that there are no issues with pairings, etc., as far as s is concerned, and so we do not need to regularize in s. Thus, with the above notation and with the same proof, with $\mathcal{J}_r$ regularizing only in decay:

Theorem 10. *Suppose $P = P^* \in \Psi_{\mathrm{sc}}^m(M)$ is as above. If $P_{J_k}^{-1}$, $P_\emptyset^{-1}$ exist (rather than P being merely Fredholm between the appropriate spaces) then the operator $\imath(P_{J_k}^{-1} - P_\emptyset^{-1})$ is positive, i.e. it is symmetric and for all $\phi \in \dot{\mathcal{C}}^\infty(M)$,*

$$\langle \imath(P_{J_k}^{-1} - P_\emptyset^{-1})\phi, \phi\rangle \geq 0.$$

Corollary 11. *(cf. Duistermaat and Hörmander* [6, Theorem 6.6.2]*) Suppose that P is as in Theorem 10 (in particular, $P_\emptyset$, P_{J_k} are invertible). For all I, there exists an operator $\tilde{S}_I$ such that $P_I^{-1} - P_\emptyset^{-1}$ differs from $\tilde{S}_I$ by an operator that is smoothing away from $L_\pm$ in the sense that $\mathrm{WF}_{\mathrm{sc}}^{s-m+1,\mu}(\phi) \cap (L_+ \cup L_-) = \emptyset$, $\mu > 1/2$, implies $\mathrm{WF}_{\mathrm{sc}}((P_I^{-1} - P_\emptyset^{-1} - \tilde{S}_I)\phi) \subset L_+ \cup L_-$, and such that $\tilde{S}_I$ is skew-adjoint and $\imath\tilde{S}_I$ is positive.*

If P_I is not invertible, P_I^{-1} is understood as a generalized inverse, using a $\dot{\mathcal{C}}^\infty(M)$-complement to $\mathrm{Ran}_I\, P$, similarly to the discussion preceding Corollary 4.

4. Asymptotically de Sitter problems

We end this paper by discussing a new direction. An interesting class of Lorentzian spaces whose behavior is more complicated is asymptotically de Sitter spaces. As shown in [31], [30] and [33], the Klein-Gordon operator $\Box_{X_0} - (n-1)^2/4 - \sigma^2$ on these spaces X_0 can be analyzed by 'capping them off' with asymptotically hyperbolic spaces $X_\pm$ to obtain a compact manifold without boundary X. (In general, for topological reasons, one needs two copies of the asymptotically de Sitter spaces, see [33, Section 3].) Then on X one has exactly the setup analyzed at the beginning of this paper. In particular, with the characteristic set having two components (if only a single connected asymptotically de Sitter space was used) one has forward and backward propagators, which propagate estimates in the opposite direction relative to the Hamilton flow in the two components, as well as Feynman and anti-Feynman propagators which propagate either forward everywhere along the Hamilton flow or backward everywhere. In the aforementioned papers the connection between the forward and backward propagators on X and the resolvents of the Laplacian on $X_\pm$ as well as the forward and backward propagators on X_0 is explained; see in particular [33, Section 4]. For instance, if $F = \{j\}$, where Σ_j is the component of Σ on which the de Sitter time function is decreasing along the bicharacteristics, then P_F^{-1} gives rise to the forward propagator

$$(\Box_{X_0} - (n-1)^2/4 - \sigma^2)^{-1}_{\mathrm{future}} = x_{X_0}^{-\imath\sigma+(n-1)/2} P_F^{-1} x_{X_0}^{\imath\sigma-(n-1)/2-2},$$

where x_{X_0} is a boundary defining function of X_0 (which is thus time-like near ∂X_0). In particular, these global propagators on X can be used to analyze the local objects on X_0 and $X_\pm$; this is essentially a consequence of the evolution equation nature of the wave equation in the de Sitter region. Thus, for instance, it does not matter how one caps off X_0 above, the forward propagator on X, in the appropriate sense (conjugation and multiplication) restricts to the forward propagator on X_0 — an object independent of the choice of the caps $X_\pm$!

A natural question is then whether this method allows one to define a canonical Feynman propagator on X_0. Certainly one choice arises by taking $P_\emptyset^{-1}$ on X, and letting

$$(\Box_{X_0} - (n-1)^2/4 - \sigma^2)^{-1}_{\text{Feynman}} = x_{X_0}^{-\imath\sigma+(n-1)/2} P_\emptyset^{-1} x_{X_0}^{\imath\sigma-(n-1)/2-2}.$$

One expects that this operator does depend on the choice of the caps $X_\pm$, and thus it is important to understand this dependence. In particular, one would ideally like to replace these conditions depending on the caps by boundary conditions at ∂X_0. Recall that in [31] one defines $\mu = -x_{X_0}^2$, so from the perspective of the extended problem, on X, $\mu > 0$ in $X_+ \cup X_-$, $\mu < 0$ in X_0, and μ vanishes simply at ∂X_0 with respect to the smooth structure of X. Now, $P_\emptyset^{-1}$ is characterized by $P_\emptyset^{-1}\psi$, $\psi \in \mathcal{C}^\infty(X)$, having only the $(\mu + \imath 0)^{\imath\sigma}$-type conormal behavior at $\mu = 0$ (i.e. potential wave front set in the corresponding half of the conormal bundle of $\partial X_0 = \{\mu = 0\}$), not the $(\mu - \imath 0)^{\imath\sigma}$ behavior (i.e. no wave front set in the corresponding half of the conormal bundle of $\partial X_0 = \{\mu = 0\}$), namely having the form

$$(\mu + \imath 0)^{\imath\sigma} b_+ + b_-,$$

with $b_\pm$ smooth, since $(\mu + \imath 0)^{\imath\sigma}$ has wave front set in the sink, where the dual variable ξ of μ is positive. Restricting to X_0 near the joint boundary Y_+ with X_+, this has the form

$$x_0^{2\imath\sigma} a_{X_0,+}^+ + a_{X_0,+}^-,$$

with $a_{X_0,+}^\pm$ smooth (and even), while restricting to X_+ near Y_+ we get the form

$$x_+^{2\imath\sigma} a_{X_+}^+ + a_{X_+}^-,$$

where, with tilde denoting restriction to Y_+,

$$\tilde a_{X_0,+}^- = \tilde b_- = \tilde a_{X_+}^-,\ \tilde a_{X_0,+}^+ = e^{-\pi\sigma}\tilde b_+ = e^{-\pi\sigma}\tilde a_{X_+}^+.$$

Thus, if ϕ is supported in X_0, $x_{X_0}^{-\imath\sigma+(n-1)/2} P_\emptyset^{-1} x_{X_0}^{\imath\sigma-(n-1)/2-2}\phi$ is a generalized eigenfunction of $\Delta_{X_+} - (n-1)^2/4 - \sigma^2$ with asymptotic behavior

$$x_+^{\imath\sigma+(n-1)/2} a_{X_+}^+ + x_+^{-\imath\sigma+(n-1)/2} a_{X_+}^-,$$

with the result that

$$\tilde a_{X_+}^- = \mathcal{S}_{X_+}(\sigma)\tilde a_{X_+}^+,$$

where $\mathcal{S}_{X_+}(\sigma)$ is the scattering matrix of the asymptotically hyperbolic problem. In terms of X_0 we thus have

$$\tilde a_{X_0,+}^- = e^{\pi\sigma}\mathcal{S}_{X_+}(\sigma)\tilde a_{X_0,+}^+.$$

Since a similar statement also holds at Y_-, this Feynman propagator corresponds to the non-local boundary conditions

$$a_{X_0,\pm}^-|_{Y_\pm} = e^{\pi\sigma}\mathcal{S}_{X_\pm}(\sigma) a_{X_0,\pm}^+|_{Y_\pm},$$

where all $\pm$ signs are consistent on this line. The anti-Feynman propagator on X produces $(\mu - \imath 0)^{\imath\sigma}$ type conormal distributions, with the result that

$$a_{X_0,\pm}^-|_{Y_\pm} = e^{-\pi\sigma}\mathcal{S}_{X_\pm}(\sigma) a_{X_0,\pm}^+|_{Y_\pm},$$

then. It would then be an interesting question to study these boundary conditions directly, as well as more general boundary conditions where the scattering matrices are replaced by more general pseudodifferential operators on $Y_\pm$ of order $-2\imath\sigma$, perhaps even simply $\Delta_{Y_\pm}^{-\imath\sigma}$, which would give a canonical propagator even in this case. Of course, if one wants to use a pseudodifferential operator that *is* actually the scattering matrix for a suitable asymptotically hyperbolic space, one is set!

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