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Micro-Local Approach to the Hadamard Condition in Quantum Field Theory on Curved Space-Time

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To my parents

Abstract: For the two-point distribution of a quasi-free Klein-Gordon neutral scalar quantum field on an arbitrary four dimensional globally hyperbolic curved space-time we prove the equivalence of (1) the global Hadamard condition, (2) the property that the Feynman propagator is a distinguished parametrix in the sense of Duistermaat and Hörmander, and (3) a new property referred to as the wave front set spectral condition (WFSSC), because it is reminiscent of the spectral condition in axiomatic quantum field theory on Minkowski space. Results in micro-local analysis such as the propagation of singularities theorem and the uniqueness up to C^∞ of distinguished parametrices are employed in the proof. We include a review of Kay and Wald's rigorous definition of the global Hadamard condition and the theory of distinguished parametrices, specializing to the case of the Klein-Gordon operator on a globally hyperbolic space-time. As an alternative to a recent computation of the wave front set of a globally Hadamard two-point distribution on a globally hyperbolic curved space-time, given elsewhere by Köhler (to correct an incomplete computation in [32]), we present a version of this computation that does not use a deformation argument such as that used in Fulling, Narcowich and Wald and is independent of the Cauchy evolution argument of Fulling, Sweeny and Wald (both of which are relied upon in Köhler's proof). This leads to a simple micro-local proof of the preservation of Hadamard form under Cauchy evolution (first shown by Fulling, Sweeny and Wald) relying only on the propagation of singularities theorem. In another paper [33], the equivalence theorem is used to prove a conjecture by Kay that a locally Hadamard quasi-free Klein-Gordon state on any globally hyperbolic curved space-time must be globally Hadamard.

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1. Introduction

The Hadamard condition has for some time been viewed as a necessary physical condition on quasi-free or more general states of the Klein-Gordon field on a globally hyperbolic curved space-time [5, 35, 11, 12, 20, 14, 23]. We study the Hadamard condition from the micro-local viewpoint [18] by relating the global Hadamard condition, rigorously defined in [23], to the theory of distinguished parametrices [7, 17] and to a condition on the wave front set of the two-point distribution.

Specifically, in Sect. 5 we calculate the wave front set of a two-point distribution satisfying the global Hadamard condition in neighborhoods of the form $U_x \times U_x$, where U_x is a convex normal neighborhood of x, and x ranges in a causal normal neighborhood of a Cauchy surface, and utilize the propagation of singularities theorem [7] to obtain a global wave front set satisfying a certain condition, called the *wave front set spectral condition (WFSSC)*. This condition is similar to the spectral condition of axiomatic quantum field theory [19, 34] because (in addition to specifying the location of the singularities of the two-point distribution) it requires that for each cotangent vector (k_1, k_2) in the set of directions of non-rapid decrease at (x_1, x_2), the first component must lie in the dual of the closed forward light cone and the second component must be minus the first (after parallel transport from x_1 to x_2). The wave front set of the Feynman propagator of a theory satisfying the WFSSC is then found by a symmetry argument to be that of the Feynman distinguished parametrix constructed by Duistermaat and Hörmander [7]. By the uniqueness theorem for distinguished parametrices [7], these two distributions are the same up to a smooth function. Finally, we show that any Feynman distinguished parametrix corresponds to a globally Hadamard two-point distribution. This follows from the existence of globally Hadamard parametrices. These equivalences are summarized in Theorem 5.1.

Besides clarifying the mathematical theory underlying the Hadamard condition, this equivalence theorem is useful in proving a conjecture by Kay [20, 21, 22, 14] that locally Hadamard quasi-free Klein-Gordon states must be globally Hadamard [32, 33]. In Sect. 6 we suggest some heuristic reasons for believing that the WFSSC is a natural analog of the spectral condition for linear quantum field models on curved space-times and discuss Köhler's modified WFSSC [24, 25] which is expected to hold for more general (nonlinear) models.

We note that [32] (and a previous draft of this paper) contains an error in the computation of the wave front set of a globally Hadamard two-point distribution, which was pointed out by Köhler [24, 25] and corrected by him using a deformation argument analogous to that developed by Fulling, Narcowich and Wald [11]. (The error rendered the proof valid only for the case of Minkowski space.) Here we provide an alternative computation which bypasses an argument like that of [11] and does not rely on the "Cauchy evolution argument" of [12] (on which Köhler's computation and the results of [11] depend). After the equivalence has been proven, the preservation of the Hadamard form under Cauchy evolution, originally shown by Fulling, Sweeny and Wald [12], follows easily from an application of the propagation of singularities theorem to the WFSSC.

Sections 2,3,4 contain preliminary material on the distributional approach to QFT on CST, the Hadamard condition, and distinguished parametrices respectively.

2. Distributional Approach to Quantized Fields on Curved Space-Time

A pair (M, g) is a *(curved) space-time* (CST) if M is a smooth n-dimensional pseudo-Riemannian manifold ($n \geq 2$) equipped with a smooth metric tensor field g of signature $(+-\cdots-)$. The metric g determines the notions of time-like, null, and space-like vectors $v \in T_x(M)$ at a point $x \in M$ by the conditions $g_x(v, v) > 0$, $g_x(v, v) = 0$, and $g_x(v, v) < 0$ respectively, where g_x is the value of the metric tensor field at x. Time-like, null, or space-like curves on (M, g) are smooth curves on M whose tangent vectors at every point on the curve are time-like, null, or space-like respectively. A *geodesic* is a (parametrized) curve whose tangent vector is parallel transported along itself. Points $x_1, x_2 \in M$ are *causally related* if x_1 and x_2 can be connected by a time-like or null curve in M. They are *space-like separated* if they are not causally related. They are *null related* if they may be connected by a null geodesic. The *closed light cone* V_x at x consists of all nonzero time-like and null vectors in $T_x(M)$. Clearly V_x decomposes into two components at each x. A *time orientable* CST is one in which a continuous global designation of "future" component of the closed light cone can be made. In this case the future/past (also called forward/backward) closed light cone at x is denoted by $V_x^{\pm}$. A CST (M, g) with a hypersurface S such that every inextendible causal curve in M intersects S precisely once is labelled *globally hyperbolic*. Every globally hyperbolic CST is necessarily time orientable. Some of these definitions are as in Hawking and Ellis [15] and Chapter 8 of Wald [36]. Also, a covector $k \in T_x^*(M)$ is called dual to $v \in T_x(M)$ if $k = g_x(\cdot, v)$.

For the test function space on a space-time (M, g), we use in this paper the space of smooth complex-valued functions of compact support $C_0^\infty(M)$. The dual space of $C_0^\infty(M)$ with respect to the metric volume form on (M, g) is the space of *distributions* on M and is denoted $\mathscr{D}'(M)$. See Sect. 6.3 of [18] for definitions and further discussion of distributions on a manifold.

Let $\mathscr{D}_m(M)$ denote $\bigotimes^m C_0^\infty(M)$ for $m \geq 1$ and define $\mathscr{D}_0(M) = \mathbb{C}$. For a collection of functions $\{f_m\}_{m\geq 0}$, where $f_m \in \mathscr{D}_m(M)$ and only a finite number of the f_m do not vanish, define $f = \bigoplus_{m=0}^\infty f_m$. With involution defined as $f^* = \bigoplus_{m=0}^\infty f_m^*$, where $f_m^*(x_1, \ldots, x_m) = \overline{f_m(x_m, \ldots, x_1)}$, and the product of f and $g = \bigoplus_{m=0}^\infty g_m$ defined as $f \times g = \bigoplus_{m=0}^\infty (f \times g)_m$, where $(f \times g)_m(x_1, \ldots, x_m) = \sum_{i=0}^m f_i(x_1, \ldots, x_i) g_{m-i}(x_{i+1}, \ldots, x_m)$, the set of all such f becomes an involutive algebra $\mathscr{B}(M)$, called the *Borchers algebra on* M. See [2, 8].

Let $\mathscr{D}_m'(M)$ denote the space $\bigotimes^m [\mathscr{D}'(M)]$, the dual of $\mathscr{D}_m(M)$. The direct sum topology is given to $\mathscr{B}(M) = \bigoplus_{m=0}^\infty \mathscr{D}_m(M)$. If μ is in $\mathscr{B}'(M)$, the dual of $\mathscr{B}(M)$ with respect to this topology, then for each $m \geq 0$ the *m-point distributions (or functions)* are $\mu_m = \mu|_{\mathscr{D}_m(M)} \in \mathscr{D}_m'(M)$. If $\omega \in \mathscr{B}'(M)$ satisfies $\omega_0 = 1$ and the positivity condition $\omega(f^* \times f) \geq 0$ then ω is a *state*. Suppose in addition that ω satisfies the local commutativity condition

$$\omega(\cdots \otimes f \otimes g \otimes \cdots) = \omega(\cdots \otimes g \otimes f \otimes \cdots) \tag{1}$$

for supp f and supp g space-like separated. (This is a statement of the independence of measurements (commensurability) of observables at space-like separation, a typical quantum mechanical restriction.) Then one may think of the m-point distributions $\omega_m(x_1, \ldots, x_m)$ (in generalized function notation) as representing the expectation values of the product of m field operators $\Phi_\omega(x_1), \ldots, \Phi_\omega(x_m)$ with respect to some vector Ω_ω in a Hilbert space $\mathscr{H}_\omega$, an interpretation made available by an analog of the Wightman reconstruction theorem [2, 34], which is here given the generic label of

"GNS construction" [3]. We call a triple (M, g, ω) whose ω satisfies these properties a *quantum field model on the CST* (M, g). (Note that further conditions will be needed for physical quantum field models.)

A state ω is *quasi-free* if the m-point distributions satisfy $\omega_{2m+1} = 0$ for $m \geq 0$ and

$$\omega_{2m}(f^1 \otimes \cdots \otimes f^{2m}) = \sum_{\pi \in \Pi_m} \omega_2(f^{\pi_1} \otimes f^{\pi_2}) \cdots \omega_2(f^{\pi_{2m-1}} \otimes f^{\pi_{2m}}) \qquad \text{(QF)}$$

for $m \geq 1$, where Π_m is the set of permutations $\pi\colon \{1, \ldots, 2m\} \to \{1, \ldots, 2m\}$ such that $\pi_1 < \pi_3 < \cdots < \pi_{2m-1}$ and $\pi_1 < \pi_2,\ \pi_3 < \pi_4, \ldots, \pi_{2m-1} < \pi_{2m}$. The main focus of research in quantum field theory on CST has been on states constructed from a linear wave equation via canonical quantization on CST [1]. These states turn out to satisfy (QF).

The fact that a quasi-free state ω is determined entirely by its two-point distribution leads one to direct particular attention to ω_2. Two general properties of ω_2, as implied by those for a (not necessarily quasi-free) state ω of a quantum field model on (M, g), are as follows:

Positive Type: For any $f \in C_0^\infty(M)$,

$$\omega_2(\bar{f} \otimes f) \geq 0\,. \qquad \text{(PT)}$$

This follows from the generic positivity condition on ω which in turn corresponds to the positive definiteness of the inner product on the Hilbert space $\mathscr{H}_\omega$ obtained by GNS construction from ω.

Let the *symmetric (anti-symmetric) part* of a two-point distribution u be defined by $u_\pm(f \otimes g) = \frac{1}{2}\left(u(f \otimes g) \pm u(g \otimes f)\right)$. Equation (1) implies the following necessary condition on ω_2:

Local Commutativity: For any $f, g \in C_0^\infty(M)$ such that supp f and supp g are space-like separated,

$$(\omega_2)_-(f \otimes g) = 0\,. \qquad \text{(LC)}$$

The properties (PT) and (LC) make sense for any space-time (M, g), even possibly one that is not time orientable, and are two of the basic properties for ω_2 that are necessary for the state ω to yield a physically meaningful field Φ_ω by the GNS construction. We suggest in Sect. 11 of [33] that on a time orientable CST a certain "wave front set spectral condition" is a third such condition. (It is of interest to determine if there are perhaps any more such physically necessary conditions, such as the existence of the scaling limit of the state [8] and Lorentz invariance of this scaling limit. See Chapter 4 of [32] for a discussion of "axiomatics" on a CST, and in particular, ideas for a proof of a spin-statistics theorem for theories satisfying the axioms given above. Note that the WFSSCs for m-point distributions ($m \geq 3$) that are proposed in [32] fail to hold even for quasi-free states. See Köhler [25] who has suggested an improved version of these conditions.)

A *Klein-Gordon quantum field model on* (M, g) is a quantum field model (M, g, ω) such that, in addition to (PT) and (LC), ω satisfies:

Klein-Gordon: For any $f, g \in C_0^\infty(M)$,

$$\omega_2\left((\Box + m^2)f \otimes g\right) = \omega_2\left(f \otimes (\Box + m^2)g\right) = 0\,. \qquad \text{(KG)}$$

Here, $\square = g^{\mu\nu}\nabla_\mu\nabla_\nu$, where ∇_μ is the covariant derivative on the pseudo-Riemannian manifold (M, g). The term m^2 may be replaced by a more general potential $V(x)$ and a first derivative term $-ib^\mu(x)\nabla_\mu$ may be added.

In order to have a well-posed Cauchy problem for the Klein-Gordon equation, we assume in this paper (as is usually done) that the CST for a Klein-Gordon quantum field model is globally hyperbolic. For states satisfying (KG) on a globally hyperbolic CST we also assume in this paper the property (QF) for ω as well as the following property:

Commutator: For any $f, g \in C_0^\infty(M)$,

$$(\omega_2)_-(f \otimes g) = \frac{\mathrm{i}}{2}\Delta(f \otimes g)\ , \tag{Com}$$

where $\Delta = \Delta_A - \Delta_R$ and Δ_A and Δ_R are the advanced and retarded fundamental solutions of the inhomogeneous Klein-Gordon equation. These distributions are uniquely determined by their support properties [27, 28, 29]. Condition (Com) is a direct consequence of canonically quantizing a scalar field satisfying the Klein-Gordon equation. Clearly it implies (LC).

For our purposes the *Feynman propagator* ω_F of a state ω is defined to be $\omega_F = \mathrm{i}\omega_2 + \Delta_A$. When ω_2 satisfies (QF), (PT), (KG) and (Com) the distribution $\omega_F(x_1, x_2)$ is interpreted as the time-ordered expectation value (with respect to some global time coordinate function) of the product of fields $\Phi_\omega(x_1)\Phi_\omega(x_2)$.

3. Review of the Global Hadamard Condition

We review the rigorous statement of the global Hadamard condition given by Kay and Wald [23], including the proofs of some minor lemmas for completeness. Suppose (M, g) is a globally hyperbolic curved space-time of dimension $n = 4$ with a preferred time orientation and let T be a global time coordinate function on M which is increasing toward the future. If S is a subset of M, one defines the *causal future $J^+(S)$ (causal past $J^-(S)$) to be the set of all points x of M such that there is a* future-directed (past-directed) causal curve from S to x.

Let $\mathscr{X} \subset M \times M$ be the set of causally related points (x_1, x_2) such that $J^+(x_1) \cap J^-(x_2)$ and $J^-(x_1) \cap J^+(x_2)$ (one of which may be empty) are within *convex normal neighborhoods*, where such a neighborhood is an open set $\mathscr{U}$ such that for any two points x_1 and x_2 in $\mathscr{U}$, there exists a unique geodesic *contained in* $\mathscr{U}$ which connects x_1 and x_2. The *(signed) square of the geodesic distance* from x_1 to x_2 in a convex normal neighborhood $\mathscr{U}$ is defined as

$$\sigma(x_1, x_2) = \pm\left(\int_a^b \left|g_{\mu\nu}(x(\tau))\frac{dx^\mu(\tau)}{d\tau}\frac{dx^\nu(\tau)}{d\tau}\right|^{\frac{1}{2}} d\tau\right)^2 , \tag{2}$$

where $x(\cdot)$ is a parametrization of the unique geodesic in $\mathscr{U}$ from x_1 to x_2 (i.e., $x(a) = x_1$ and $x(b) = x_2$) and the plus or minus sign is chosen according to whether $x(\cdot)$ is space-like or time-like respectively. For example, on Minkowski space $(\mathbb{R}^n, \eta)$, we have $\sigma(x_1, x_2) = -(x_1 - x_2)^2 = -(x_1^\mu - x_2^\mu)(x_{1\mu} - x_{2\mu})$.

Lemma 3.1. *There is an (open) neighborhood $\mathscr{O}$ of $\mathscr{X}$ on which σ is well-defined and smooth. Furthermore this neighborhood may be taken to be a union of sets of the form $U \times U$, where U is a convex normal neighborhood.*

Proof. Take $\mathscr{O} = \cup_{(x_1,x_2)\in\mathscr{V}} U_{(x_1,x_2)} \times U_{(x_1,x_2)}$, where for each point (x_1, x_2) in $\mathscr{V}$ the set $U_{(x_1,x_2)}$ is a convex normal neighborhood containing $J^-(x_1) \cap J^+(x_2)$ or $J^+(x_1) \cap J^-(x_2)$ (whichever is nonempty) and thus containing x_1 and x_2. ∎

Fix an integer $p \geq 1$ and a real number $\epsilon > 0$ and define for $(x_1, x_2) \in \mathscr{O}$, the complex-valued function

$$G_\epsilon^{T,p}(x_1,x_2) \quad := \quad \frac{1}{(2\pi)^2}\left(\frac{\Delta^{\frac{1}{2}}(x_1,x_2)}{\sigma_\epsilon(x_1,x_2)} + v^{(p)}(x_1,x_2)\ln[\sigma_\epsilon(x_1,x_2)]\right), \qquad (3)$$

where we define $\sigma_\epsilon(x_1,x_2) := \sigma(x_1,x_2) + 2i\epsilon[T(x_1) - T(x_2)] + \epsilon^2$, $v^{(p)}(x_1,x_2) := \sum_{m=0}^{p} v_m(x_1,x_2)\sigma^m(x_1,x_2)$, and $\Delta^{\frac{1}{2}}, v_m$ are smooth functions uniquely determined by certain recursion relations (called the *Hadamard recursion relations* [13, 5]). The function Δ is called the Van Vleck-Morette determinant and does not vanish where σ does. The branch cut for the logarithm in Eq. (3) is chosen to be on the negative real axis.

A set $\mathscr{N}$ is said to be a *causal normal neighborhood* of a Cauchy hypersurface $\mathscr{C}$ of a globally hyperbolic space-time (M, g) if $\mathscr{C}$ is a Cauchy hypersurface for $\mathscr{N}$ (considered as a space-time in its own right) and if for any points $x_1, x_2 \in \mathscr{N}$, such that $x_1 \in J^+(x_2)$, one can find a convex normal neighborhood containing $J^-(x_1) \cap J^+(x_2)$.

Lemma 3.2 (Lemma 2.2 of [23]). *Let $\mathscr{C}$ be a (space-like) Cauchy hypersurface of a globally hyperbolic space-time (M, g). Then $\mathscr{C}$ has an open causal normal neighborhood.* ∎

Let $\mathscr{W}$ be the set of pairs of points (x_1, x_2) which are causally related (hence $\mathscr{W} \supset \mathscr{V}$) and let $\mathscr{O}$ be an open neighborhood of $\mathscr{V}$ on which σ is well-defined and smooth (by Lemma 3.1).

Lemma 3.3. *In $\mathscr{N} \times \mathscr{N}$ there is an open neighborhood $\mathscr{O}'$ of $\mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$ such that the closure of $\mathscr{O}'$ in $\mathscr{N} \times \mathscr{N}$ is contained in $\mathscr{O} \cap (\mathscr{N} \times \mathscr{N})$.*

Proof. We first prove that $\mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$ is a closed subset in $\mathscr{N} \times \mathscr{N}$ with respect to the relative topology of $\mathscr{N} \times \mathscr{N}$. Suppose $\{(x^i, y^i)\}$ is a sequence converging in $M \times M$ to $(x, y) \in \mathscr{N} \times \mathscr{N}$ and $(x^i, y^i) \in \mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$ for all i. Since $(x_1, x_2) \in \mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$ implies that x_1 and x_2 are causally related and, by definition of $\mathscr{N}$, that $J^+(x_1) \cap J^-(x_2)$ and $J^-(x_1) \cap J^+(x_2)$ are in convex normal neighborhoods in M, we have $\mathscr{W} \cap (\mathscr{N} \times \mathscr{N}) \subset \mathscr{O}$, which means that σ is smooth on $\mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$. Hence $\sigma(x^i, y^i) \leq 0$ for all i implies $\sigma(x, y) \leq 0$, i.e., x and y are causally related. Hence $\mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$ is closed relative to $\mathscr{N} \times \mathscr{N}$. Since $\mathscr{O} \cap (\mathscr{N} \times \mathscr{N})$ is open relative to $\mathscr{N} \times \mathscr{N}$ and contains $\mathscr{W} \cap (\mathscr{N} \times \mathscr{N})$, there is a set $\mathscr{O}' \subset \mathscr{N} \times \mathscr{N}$ open relative to $\mathscr{N} \times \mathscr{N}$ such that

$$\mathscr{W} \cap (\mathscr{N} \times \mathscr{N}) \subset \mathscr{O}' \subset \overline{\mathscr{O}'} \subset \mathscr{O} \cap (\mathscr{N} \times \mathscr{N}),$$

where the closure is taken relative to $\mathscr{N} \times \mathscr{N}$. ∎

Now let $\chi(x_1, x_2) \in C^\infty(\mathscr{N} \times \mathscr{N})$ be chosen so that $\chi(x_1, x_2) = 0$ whenever $(x_1, x_2) \notin \mathscr{O}$ and $\chi(x_1, x_2) = 1$ whenever $(x_1, x_2) \in \overline{\mathscr{O}'}$.

Definition 3.4 (Globally Hadamard, cf. [23]). *Let ω_2 be a two-point distribution in $\mathscr{D}_2'(M)$ on a four dimensional globally hyperbolic space-time (M, g) and let T be a* *choice of global time coordinate function on M that is increasing toward the future. Let $\mathscr{C}$, $\mathscr{N}$, and χ be chosen as above. Then ω_2 is said to be* **globally Hadamard** *on $\mathscr{N} \times \mathscr{N}$ if for each integer p there exists a function $H^p \in C^p(\mathscr{N} \times \mathscr{N})$ such that for all $f_1, f_2 \in C_0^\infty(\mathscr{N})$,*

$$\omega_2(f_1 \otimes f_2) = \lim_{\epsilon \to 0^+} \int_{\mathscr{N} \times \mathscr{N}} \Lambda_\epsilon^{T,p}(x_1, x_2) f_1(x_1) f_2(x_2) d\mu_g(x_1) d\mu_g(x_2) \, , \qquad \text{(GH)}$$

where $d\mu_g(x) = \sqrt{|\det g_{\mu\nu}(x)|}\, d^4x$ on coordinate patches and

$$\Lambda_\epsilon^{T,p}(x_1, x_2) = \chi(x_1, x_2) G_\epsilon^{T,p}(x_1, x_2) + H^p(x_1, x_2) \, .$$

This means that for each choice of T and p we have $\omega_2 = \Lambda^{T,p}$ on $\mathscr{N} \times \mathscr{N}$, where $\Lambda^{T,p} := \lim_{\epsilon \to 0^+} \Lambda_\epsilon^{T,p}$ is a well-defined two-point distribution. The function χ has been chosen so that σ is smooth on supp χ. Hence $\chi(x_1, x_2) G_\epsilon^{T,p}(x_1, x_2)$ is a smooth function on $M \times M$. Since $H^p(x_1, x_2)$ is in $C^p(\mathscr{N} \times \mathscr{N})$, and p can be made as large as desired, this term effectively acts as a C^∞ contribution to ω_2. Hence the set of singular points of $\Lambda^{T,p}$ and ω_2 in $\mathscr{O}'$ is determined by those of $\Gamma^{T,p} := \lim_{\epsilon \to 0^+} \Gamma_\epsilon^{T,p}$, where $\Gamma_\epsilon^{T,p} := \chi G_\epsilon^{T,p}$. Furthermore, outside of $\mathscr{O}'$ in $\mathscr{N} \times \mathscr{N}$, the two-point distribution ω_2 is smooth. We then see that the global Hadamard condition requires that $\omega_2(x_1, x_2)$ have singularities only at points (x_1, x_2) in $\mathscr{N} \times \mathscr{N}$ such that x_1 and x_2 are related by a null geodesic totally contained within $\mathscr{N}$.

Note that in [23], (PT), (KG), (Com) are implicitly assumed in their statement of the global Hadamard condition, and that (QF) is *not* assumed (whereas in Definition 3.4 none of these four properties is assumed). In Sect. 6 we shall see that (PT) is a *consequence* (mod C^∞) of (GH), and in fact that this result has been in the literature since 1972 (see [7]).

The definition of globally Hadamard is consistent (mod C^∞) with (KG) since each Λ^p satisfies (KG), by the choice of $\Delta^{\frac{1}{2}}$ and the coefficients v_m. Consistency of the global Hadamard condition with (Com) follows from the rigorous Hadamard expansion of the advanced and retarded fundamental solutions of the inhomogeneous Klein-Gordon equation on an arbitrary globally hyperbolic CST in, e.g., Chapter 4 of Friedlander [9]. Precisely the same partial sums as in [9] are obtained by taking the imaginary (anti-symmetric) part of the Γ^p in the global Hadamard condition on $\mathscr{N} \times \mathscr{N}$.

If a two-point distribution ω_2 satisfying the global Hadamard condition on $\mathscr{N} \times \mathscr{N}$ is also required to satisfy the Klein-Gordon equation (KG) globally (as is required in [23]), then the singularity structure of ω_2 in any other neighborhood (in $M \times M$) of the form $U \times U$, where U is a convex normal neighborhood, is also of the Hadamard form, as has been shown by Fulling, Sweeny and Wald [12]. This is called "preservation of Hadamard form under Cauchy evolution." Furthermore if one chooses a different global time coordinate function T', Cauchy hypersurface $\mathscr{C}'$, causal normal neighborhood $\mathscr{N}'$, and cutoff function χ' in Definition 3.4, then the global singularity structure specified by Definition 3.4 is the same as for the first set of choices, as has been shown in [23].

4. Distinguished Parametrices

The definitions adopted for the distribution spaces $\mathscr{D}'(M), \mathscr{E}'(M)$ on a manifold M, and for pseudo-differential operators, symbols and principal symbols on M

may be found in [16, 18, 17, 32]. On a curved space-time (M, g) of dimension n, the Klein-Gordon operator $\Box + m^2$ is a pseudo-differential operator, with principal symbol $g^{\mu\nu}(x)k_\mu k_\nu$. More generally, the principal symbol of the differential operator $\sum_{|\alpha|\leq q} a_\alpha(x)(-i\partial)^\alpha$ with respect to local coordinates $(x^0, \ldots, x^{n-1})$ is $\sum_{|\alpha|=q} a_\alpha(x)k^\alpha$, where α is a multi-index.

If $u \in \mathscr{D}'(\mathbb{R}^p)$ then if $\phi \in C_0^\infty(\mathbb{R}^p)$, the distribution ϕu is in $\mathscr{E}'(\mathbb{R}^p)$. A covector $k \in \mathbb{R}^p \backslash \{0\}$ is a *direction of rapid decrease* of the Fourier transform $\widehat{\phi u}$ iff there exists a conic neighborhood $\mathscr{C}_k$ of k such that for any integer N there exists a constant C_N such that

$$|\widehat{\phi u}(\xi)| \leq C_N(1 + |\xi|)^{-N}, \ \forall \xi \in \mathscr{C}_k \,.$$

Here, $|k|$ is the Euclidean norm of k, namely,

$$|k| = \left(\sum_{i=1}^{p}(k_i)^2\right)^{\frac{1}{2}} \,.$$

Note that the set of directions of rapid decrease is open in $\mathbb{R}^p \backslash \{0\}$. The set of directions of *non-rapid decrease* $\Sigma(\phi u)$ is the complement in $\mathbb{R}^p \backslash \{0\}$ of this set and is closed in $\mathbb{R}^p \backslash \{0\}$. Now let $\Sigma_x(u)$ be the intersection of the sets $\Sigma(\phi u)$ for all $\phi \in C_0^\infty(\mathbb{R}^p)$ such that $\phi(x) \neq 0$.

Definition 4.1 (Definition 8.1.2 of [18]). *If* $u \in \mathscr{D}'(M)$ *the* **wave front set** $\mathrm{WF}(u)$ *is the union of the points* (x, k) *such that* $k \in \Sigma_x(u)$, *i.e.,*

$$\mathrm{WF}(u) = \{(x, k) \in T^*(M)\backslash \mathbf{0}\colon\ k \in \Sigma_x(u)\} \,.$$

The projection of $\mathrm{WF}(u)$ on the first variable is equal to the *singular support* of u, called sing supp u, which is the complement of the largest open set on which u is smooth. Furthermore, if $v \in \mathscr{E}'(\mathbb{R}^p)$ then the projection of $\mathrm{WF}(v)$ on the second variable is $\Sigma(v)$. Definition 4.1 extends to distributions on manifolds ($u \in \mathscr{D}'(M)$), where $\mathrm{WF}(u)$ is an invariantly defined closed conic subset of $T^*(M)\backslash \mathbf{0}$, the cotangent bundle minus the zero section [17].

Roughly speaking, if (x, k) is a point in the wave front set of u, then x specifies the location of a singularity of u and k a direction of non-rapid decrease of $\hat{u}$ (where we multiply by $\phi \in C_0^\infty$ if necessary so that $u \in \mathscr{E}'$) that contributes to this singularity. Alternatively this k may be considered a "direction of propagation" of the singularity at x. (The meaning of this statement is made precise in the propagation of singularities theorem, mentioned later.) Generally speaking, the wave front set is a valuable tool because it distinguishes between singularities propagating in different directions from the same point, a considerable improvement over the singular set, which does not.

The wave front set and similar structures find wide application in partial differential equation theory. See the notes at the end of Chapter VIII of [18] for an historical development of the concept of the wave front set. Study of the wave front sets of the m-point distributions in quantum field theory on curved space-time (and other micro-local aspects of this branch of physics) has apparently received attention only in [30] (which uses pseudo-differential operator techniques) and [6] (which uses the theory of distinguished parametrices) since the work of Duistermaat and Hörmander [7].

A pseudo-differential operator Q on a manifold M is said to be *properly supported* if for each compact set $K \subset M$, there exists a compact set $K' \subset M$ such that supp $u \subset K$ implies supp $Qu \subset K'$ and $v = 0$ on K' implies $Qv = 0$ on K. (This is Definition 18.1.21 of [17].) Any differential operator, such as $\Box + m^2$, is properly supported since one can choose $K' = K$. If Q is properly supported and E is a continuous mapping $C_0^\infty(M) \to C^\infty(M)$ then EQ and QE are well-defined operators on $C_0^\infty(M)$. If in addition (i) $QE = I$ (mod C^∞), (ii) $EQ = I$ (mod C^∞), or (iii) $QE = EQ = I$ (mod C^∞), then we call E a (i) *right*, (ii) *left*, or (iii) *two-sided parametrix* of Q. In case (iii) one usually deletes "two-sided."

On a space-time (M, g) the Schwartz nuclear theorem implies that a parametrix E corresponds to a distribution $\tilde{E} \in \mathscr{D}_2'(M)$ such that the distribution density $\tilde{E}_1$ (see e.g., Chapter 6 of [18]) associated with $\tilde{E}$ satisfies

$$\tilde{E}_1(f \otimes h) = \int f(Eh) d\mu_g \ ,$$

for $f, h \in C_0^\infty(M)$. Henceforth we denote the parametrix E, the corresponding distribution $\tilde{E}$, and the associated distribution density $\tilde{E}_1$ by the same symbol E.

We now review pp. 217–218 of [7], preliminary material for the existence and uniqueness theorem for distinguished parametrices. We work out the details for the special case $Q = \Box + m^2$ on a globally hyperbolic space-time (M, g). Since only the principal symbol of $\Box + m^2$ plays a rôle in what follows, one may replace m^2 by any other lower derivative terms. (This would change, e.g., the distinguished parametrices of $\Box + m^2$, but not their wave front sets.)

For Q a properly supported pseudo-differential operator with principal symbol q, the *bicharacteristic strips of* Q are the curves on the submanifold of $T^*(M)\backslash\mathbf{0}$ defined by $q = 0$ which are generated by the Hamiltonian flow, where the Hamiltonian is taken to be q. (This definition is consistent because Hamiltonian flow lines remain within the submanifold defined by $q = 0$.) The *bicharacteristic curves* of Q are the projections of these strips onto M itself.

On a curved space-time (M, g) a *null geodesic strip* is a curve in $T^*(M)$ of the form $\{(\gamma(\lambda), k(\lambda))\colon \lambda \in \mathbb{R}\}$, where $\gamma(\cdot)$ is a null geodesic (with affine parameter λ) and $k(\lambda)$ is the dual of the tangent vector to γ at λ. We denote it by (γ, k).

Proposition 4.2. *On a curved space-time (M, g), the bicharacteristic strips of $\Box + m^2$ are the null geodesic strips in $T^*(M)$ and its bicharacteristic curves are the null geodesics on M.*

The proof is elementary and may be found, for example, in [9] and [32] (where the computation of bicharacteristic strips is evident in the proof). ■

A properly supported Q is *of real principal type in* M if its principal part q is real and homogeneous of some order m and no complete bicharacteristic strip of Q stays over a compact set in M.

Proposition 4.3. *For (M, g) a globally hyperbolic space-time, $\Box + m^2$ is of real principal type on M.*

Proof. Since the principal symbol $g^{\mu\nu}(x)k_\mu k_\nu$ is manifestly real and homogeneous of degree 2, it remains to show that no complete null geodesic remains inside a compact set in M. Lemma 8.3.8 of [36], which states that the globally hyperbolic space-time (M, g) is strongly causal, and Lemma 8.2.1 of [36] together imply that if a complete null geodesic γ is confined to a compact set $K \subset M$, then γ must have its past and future endpoints in K. But since the domain of a complete null geodesic is $(-\infty, \infty)$, we have $\dot{\gamma}(\tau) \to 0$ as $\tau \to \pm\infty$. This implies $\dot{\gamma}(\tau) = 0$ for all $\tau \in \mathbb{R}$ (since a geodesic parallel transports its tangent vector), so that $\gamma(\tau) = x_0$, a constant, contrary to assumption. ■

For Q a properly supported pseudo-differential operator of real principal type in a manifold M, we say that M is *pseudo-convex* with respect to Q if for every compact set $K \subset M$, there is another compact set $K' \subset M$ such that K' contains any interval on a bicharacteristic curve with respect to Q having both endpoints in K.

Proposition 4.4. *For (M, g) a globally hyperbolic space-time (of any dimension), M is pseudo-convex with respect to $\square + m^2$.*

Proof. The Corollary to Proposition 6.6.1 of Hawking and Ellis [15] states that if (M, g) is globally hyperbolic and K_1 and K_2 are compact, then $J^+(K_1) \cap J^-(K_2)$ is compact. If K is compact, then by this Corollary, $K' = J^+(K) \cap J^-(K)$ is compact, and if γ is a null geodesic with endpoints in K, then clearly $\gamma \subset K'$. See also Proposition 4.2 of [6]. ■

For Q a pseudo-differential operator with principal symbol q, define N to be the set

$$N = \{(x, k) \in T^*(M)\backslash\mathbf{0}\colon\ q(x, k) = 0\} \tag{4}$$

and for $x \in M$ let

$$N_x = \{k \in T^*_x(M)\backslash\{0\}\colon\ q(x, k) = 0\}\ . \tag{5}$$

For a properly supported pseudo-differential operator Q of real principal type, with respect to which M is pseudo-convex, the *bicharacteristic relation* C for Q is the set

$$C = \{((x_1, k_1), (x_2, k_2)) \in N \times N\colon (x_1, k_1) \approx (x_2, k_2)\}\ , \tag{6}$$

where $(x_1, k_1) \approx (x_2, k_2)$ means that (x_1, k_1) and (x_2, k_2) are on the same bicharacteristic strip of Q. (As noted in [7], p. 217, canonical transformations on q leave the bicharacteristic relation of Q fixed, and if a is everywhere nonzero, aq defines the same bicharacteristic relation.)

For the operator $\square + m^2$, we have $N = \{(x, k) \in T^*(M)\backslash\mathbf{0}\colon g^{\mu\nu}(x)k_\mu k_\nu = 0\}$ and the bicharacteristic relation is

$$C = \{((x_1, k_1), (x_2, k_2)) \in N \times N\colon (x_1, k_1) \sim (x_2, k_2)\}\ ,$$

where by $(x_1, k_1) \sim (x_2, k_2)$ we mean that (x_1, k_1) and (x_2, k_2) are on the same null geodesic strip (γ, k) in $T^*(M)$. Since they are tangent vectors to the geodesic γ, k_1^μ and k_2^μ are parallel transports of each other along γ.

Let Δ_N be the diagonal of $N \times N$:

$$\Delta_N = \{((x_1, k_1), (x_2, k_2)) \in N \times N\colon x_1 = x_2, k_1 = k_2\}\ . \tag{7}$$

Then $C\backslash\Delta_N$ decomposes into the open sets

$$C^\pm = \{((x_1, k_1), (x_2, k_2)) \in N \times N\colon (x_1, k_1) \underset{\prec}{\succ} (x_2, k_2)\}\ , \tag{8}$$

where $(x_1, k_1) \underset{\prec}{\succ} (x_2, k_2)$ means $(x_1, k_1) \approx (x_2, k_2)$ and (x_1, k_1) comes after/before (x_2, k_2) with respect to the time parameter of the bicharacteristic curve.

Specializing to the case $Q = \square + m^2$ on a globally hyperbolic space-time (M, g), if $k \in T^*_x(M)$ we introduce the notation $k_i \underset{\triangleleft}{\triangleright} 0$, meaning $k_i \in (V_x^\pm)^d$, the dual of the future/past closed light cone at x. Then we have that

$$C^+ = \{((x_1,k_1),(x_2,k_2)) \in C\colon\ x_1 \in J^+(x_2) \text{ if } k_1 \rhd 0 \text{ or } x_1 \in J^-(x_2) \text{ if } k_1 \lhd 0\},$$

$$C^- = \{((x_1,k_1),(x_2,k_2)) \in C\colon x_1 \in J^+(x_2) \text{ if } k_1 \lhd 0 \text{ or } x_1 \in J^-(x_2) \text{ if } k_1 \rhd 0\}\ .$$

An *orientation of* C is a splitting (C^1, C^2) of $C\backslash\Delta_N = C^1 \cup C^2$ into two disjoint subsets C^1 and C^2 which are open in $C\backslash\Delta_N$ and are inverse relations in the sense that $((x_1,k_1),(x_2,k_2)) \in C^1$ if and only if $((x_2,k_2),(x_1,k_1)) \in C^2$. Because C^1, C^2 are inverse relations, neither set can be empty (or $C\backslash\Delta_N$). Note that C^j is both open and closed (it is the complement of an open set in $C\backslash\Delta_N$). Hence C^1 (and C^2) must be a union of connected components of $C\backslash\Delta_N$.

Next we show explicitly how each orientation is associated to a union of connected components of N. We include these details to facilitate further uses of distinguished parametrices, i.e., for higher order operators in QFT on CST. Furthermore, the constructions will later be used to explain why the primed wave front set of a distinguished parametrix (i.e., a parametrix uniquely determined up to C^∞ by its wave front set) must be the union of an orientation set C^1 or C^2 and the diagonal set $\Delta^* = \{((x_1,k_1),(x_1,k_1))\colon (x_1,k_1) \in T^*(M)\backslash\mathbf{0}\}$.

As in [7] (p. 218), define $B(x,k)$ to be the complete bicharacteristic strip of Q through (x,k) and let $C^\pm(x,k) = C^\pm \cap (B(x,k) \times B(x,k))$. If (C^1, C^2) is an orientation of C, then for each $j = 1,2$, and for each (x,k), we have

$$C^+(x,k) \subset C^j \text{ or } C^+(x,k) \cap C^j = \emptyset\ , \tag{9}$$

since C^j is a union of connected components of $C\backslash\Delta_N$ and $C^+(x,k)$ is a connected set.

Define for $j = 1,2$ the set $N^j = \{(x,k) \in N\colon C^+(x,k) \subset C^j\}$. For $(x,k) \in N$, the set $C^+(x,k)$ must be in one of the sets C^1, C^2 since $C^1 \cup C^2 = C\backslash\Delta_N$. Hence we must have $N^1 \cup N^2 = N$. Furthermore, N^1 and N^2 are disjoint, by Eq. (9), and are open sets in N. Hence the N^j are unions of connected components of N.

We can reconstitute C^1 and C^2 by

$$C^1 = \Big(\bigcup_{(x,k)\in N^1} C^+(x,k)\Big) \cup \Big(\bigcup_{(x,k)\in N^2} C^-(x,k)\Big)\ , \tag{10}$$

$$C^2 = \Big(\bigcup_{(x,k)\in N^2} C^+(x,k)\Big) \cup \Big(\bigcup_{(x,k)\in N^1} C^-(x,k)\Big)\ . \tag{11}$$

Indeed, if $C^+(x,k) \subset C^1$ then $C^-(x,k) \subset C^2$ since C^1, C^2 are inverse relations. If $(x,k) \in N^1$ then $C^+(x,k) \subset C^1$ and if $(x',k') \in N^2$ then $C^-(x',k') \subset C^1$. Hence

$$C^1 \supset \Big(\bigcup_{(x,k)\in N^1} C^+(x,k)\Big) \cup \Big(\bigcup_{(x,k)\in N^2} C^-(x,k)\Big)\ ,$$

$$C^2 \supset \Big(\bigcup_{(x,k)\in N^2} C^+(x,k)\Big) \cup \Big(\bigcup_{(x,k)\in N^1} C^-(x,k)\Big)\ .$$

Finally, $C^1 \cup C^2 = C^+ \cup C^- = C\backslash\Delta_N$ implies that equality holds in the above two expressions. Hence orientations of C are classified by the power set of the components of N. For a general Q satisfying the hypotheses of Theorem 4.5, if N has k components, then there are 2^k orientations of C.

Denote the set of all components of N by $\tilde{N}$, and let ν denote a collection of components of N, i.e., $\nu \subset \tilde{N}$. Let N_ν^+, N_ν^- be the unions of all the sets in ν, $\tilde{N}\backslash\nu$

respectively. Let (C_ν^+, C_ν^-) be the orientation of C corresponding to N_ν^+, N_ν^-. Note that $(C_\nu^-, C_\nu^+) = (C_{\tilde{N}\setminus\nu}^+, C_{\tilde{N}\setminus\nu}^-)$.

In the case of $Q = \Box + m^2$, the set $N = \{(x,k) \in T^*(M)\backslash\mathbf{0}: g^{\mu\nu}(x)k_\mu k_\nu = 0\}$ has two connected components in $n \geq 3$ dimensions (four for $n = 2$), namely

$$N_+ = \{(x,k) \in N: k \rhd 0\} ,$$

$$N_- = \{(x,k) \in N: k \lhd 0\} .$$

Hence there are $2^2 = 4$ orientations in $n \geq 3$ dimensions (and $4^2 = 16$ for two dimensions). The choices for $\nu \subset \tilde{N}$ are $\{N_+, N_-\}, \{N_+\}, \{N_-\}, \emptyset$, with corresponding N_ν^+ equal to $N, N_+, N_-, \emptyset$. Letting these be N_1, N_2, N_3, N_4 respectively, we obtain orientations (C_i^1, C_i^2), $i = 1, \ldots, 4$, where

$$C_i^1 = (\bigcup_{N_i} C^+(x,k)) \cup (\bigcup_{N\setminus N_i} C^-(x,k))$$

and similarly for C_i^2. Hence

$$C_1^1 = \bigcup_N C^+(x,k) = C_4^2 ,$$

$$C_2^1 = \bigcup_{N_+} C^+(x,k) \cup \bigcup_{N_-} C^-(x,k) = C_3^2 ,$$

$$C_3^1 = \bigcup_{N_-} C^+(x,k) \cup \bigcup_{N_+} C^-(x,k) = C_2^2 ,$$

$$C_4^1 = \bigcup_N C^-(x,k) = C_1^2 .$$

The different possible orientations of C are thus (C_1^1, C_4^1), (C_2^1, C_3^1), (C_3^1, C_2^1), (C_4^1, C_1^1).

The sets $C_1^1, C_2^1, C_3^1, C_4^1$ are shown in Fig. 1 for $n = 3$. Note that in these diagrams x_2 is fixed at the vertices of the cones and only the directions of the vectors k_1 are shown. Those of k_2 are left undisplayed for simplicity.

If $E \in \mathscr{D}_2'(M)$, then let the *primed wave front set* of E be

$$\begin{aligned}\mathrm{WF}'(E) &= \{((x_1,k_1),(x_2,k_2)) \in T^*(M \times M)\backslash\mathbf{0}: \\ &\qquad ((x_1,k_1),(x_2,-k_2)) \in \mathrm{WF}(E)\} .\end{aligned}$$

We restate the existence and uniqueness theorem for distinguished parametrices [7]:

Theorem 4.5 (Theorem 6.5.3 of [7]). *Let Q be of real principal type in M and assume that M is pseudo-convex with respect to Q. For every orientation $C\backslash\Delta_N = C_\nu^+ \cup C_\nu^-$ one can find parametrices E_ν^+ and E_ν^- of Q with*

$$\mathrm{WF}'(E_\nu^+) = \Delta^* \cup C_\nu^+, \quad \mathrm{WF}'(E_\nu^-) = \Delta^* \cup C_\nu^- ,$$

where Δ^* is the diagonal in $T^*(M)\backslash\mathbf{0} \times T^*(M)\backslash\mathbf{0}$. Any right or left parametrix E with $\mathrm{WF}'(E)$ contained in $\Delta^* \cup C_\nu^+$ resp. $\Delta^* \cup C_\nu^-$ must be equal to E_ν^+ resp. E_ν^- modulo C^∞. ■

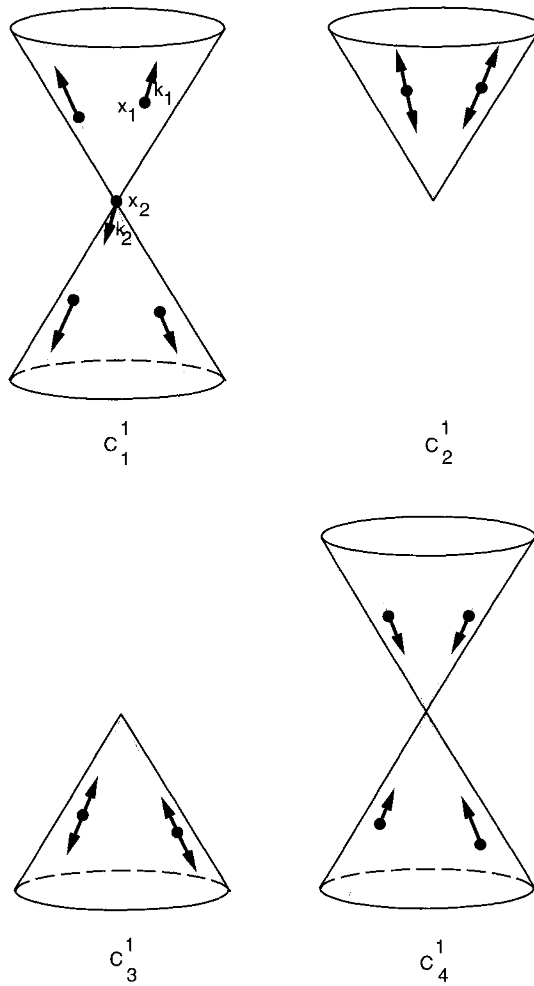

Fig. 1. Sets $C_1^1, C_2^1, C_3^1, C_4^1$ making up orientations of C for $n = 3$. In these diagrams x_2 is fixed at the vertices of the cones and only the directions of the vectors k_1 are shown, those of k_2 being left undisplayed for simplicity (except for the labelled points in C_1^1 where k_2 is shown).

In the case $Q = P = \Box + m^2$ we identify the parametrices corresponding to $C_1^1, C_2^1, C_3^1, C_4^1$ as follows. By virtue of the fact that the wave front sets C_2^1/C_3^1 have support only for x_1 in the future/past of x_2, we deduce that $E_2 = E_{N_+}^+$ and $E_3 = E_{N_-}^+$ must be (up to C^∞) the retarded and advanced fundamental solutions Δ_R, Δ_A to the inhomogeneous Klein-Gordon equation, i.e., $E_2 = \Delta_R$, $E_3 = \Delta_A$. For example, $\Delta_A(x_1, f) = \int \Delta_A(x_1, x_2) f(x_2) dx_2$ is the solution of $(\Box + m^2)u = f$ ($f \in C_0^\infty$) with support to the past of supp f, hence only points (x_1, x_2) for which $x_1 \in J^-(x_2)$ are in supp Δ_A.

In Sect. 6.6 of [7] the parametrices E_1 and E_4 are *labelled* the Feynman and anti-Feynman propagators E_F and $E_{\bar{F}}$ respectively. In this paper we call these the Feynman and anti-Feynman distinguished *parametrices* respectively, because we must regard E_F as logically distinct from the distribution ω_F, which in Sect. 2 is denoted the Feynman propagator *associated to a state* ω. In the next section E_F and ω_F are shown to be in fact identical mod C^∞ precisely when ω_2 is globally Hadamard and satisfies (KG), (Com) up to C^∞.

Note that the wave front set of E_F gives precise meaning to the statement often found in the physics literature that "the Feynman propagator propagates positive frequencies to the future and negative frequencies to the past." According to Theorem 2.5.14 of [16], if $u \in \mathscr{E}'(M)$ then $\mathrm{WF}(E_F u) = \mathrm{WF}'(E_F) \circ \mathrm{WF}(u)$, where the $\circ$ operator maps sets in $T^*(M)\backslash\mathbf{0}$ to sets in $T^*(M)\backslash\mathbf{0}$, i.e., if $(y,l) \in \mathrm{WF}(u)$ then $\mathrm{WF}(E_F u)$ contains any points (x,k) such that $((x,k),(y,l)) \in \mathrm{WF}'(E_F)$. Hence if $\mathrm{WF}(u)$ contains any points of the form (y,l), where l is null and $l \rhd 0$ resp. $l \lhd 0$ then $\mathrm{WF}(E_F u)$ will contain the null geodesic strip to the future resp. past of (y,l). Otherwise, $\mathrm{WF}(E_F u)$ contains only $\mathrm{WF}(u)$ (this comes from the Δ^* part in $\mathrm{WF}'(E_F)$), i.e., singularities with non-null covectors are not propagated anywhere. Furthermore, because of Theorem 4.5, one can say that the Feynman parametrix is (mod C^∞) the *unique* parametrix of $\Box + m^2$ that propagates positive frequencies to the future and negative frequencies to the past *as seen in the wave front set.* (Note that this interpretation requires only global hyperbolicity, not asymptotic flatness.)

The parametrices E_ν^+, E_ν^- are called *distinguished* because no other parametrix E of Q is uniquely determined up to C^∞ by its wave front set $\mathrm{WF}(E)$. See Proposition 6.6.8 of [7].

The following *propagation of singularities theorem* (PST) is also of use here (see Sect. 6.1 of [7], p. 196).

Theorem 4.6 (Theorem 6.1.1 of [7]). *Assume that* $Q \in L^m(M)$ *is properly supported and has a real principal part* q *which is homogeneous of degree* m. *If* $u \in \mathscr{D}'(M)$ *and* $Qu = f$ *it follows that* $\mathrm{WF}(u)\backslash\mathrm{WF}(f)$ *is contained in* $q^{-1}(0)$ *and is invariant under the Hamiltonian vector field* H_q. ∎

For the definition of the symbol class $L^m(M) = L^m_{1,0}(M)$ (also called $P^m(M)$), see Chapter 2 of [16].

For the case that $f \in C^\infty$, and with the choices $Q = (\Box + m^2) \otimes \mathbf{1}, \mathbf{1} \otimes (\Box + m^2)$, applied to a two-point distribution $\mu_2(x_1,x_2)$ on a globally hyperbolic CST, the PST implies that $\mathrm{WF}(\mu_2)$ must be a union of sets of the form $B(x_1,k_1) \times B(x_2,k_2)$, where $(x_1,k_1),(x_2,k_2) \in N$.

At this point, we provide an explanation for why the wave front set of a distinguished parametrix must be one of the sets of an orientation $C_\nu^\pm$ union Δ^*. In the proof of Lemma 6.5.4 of [7], which is needed to prove the existence part of Theorem 4.5, the identity operator I is broken up into $\sum T_i$, where each T_i is a pseudo-differential operator whose kernel has support in a conic region V_i, and $\{V_i\}$ is a locally finite covering of $T^*(M)\backslash\mathbf{0}$. Intermediate parametrices $F_i^\pm$ are constructed such that $PF_i^\pm = T_i + R_i^\pm$, where $\mathrm{WF}'(F_i^\pm) \subset \Delta^* \cup C_\nu^\pm$ and $R_i^\pm$ is a certain Fourier integral operator whose primed wave front set is contained in $C_\nu^\pm$. (Under the hypotheses of Theorem 4.5, the sum of the $R_i^\pm$ may be expressed as $PG^\pm$ mod C^∞, where $\mathrm{WF}'(G^\pm) \subset C_\nu^\pm$, which finishes the construction of the distinguished parametrices.) In the case that $\mathrm{WF}(T_i)$ is in a sufficiently small conic neighborhood of (x_0,k_0) such that $p(x_0,k_0) = 0$, it is clear from the construction of $F_i^\pm$ that the part of C_ν^+ in which $\mathrm{WF}'(F_i^+)$ is contained is a conic neighborhood in C^+ of $C^+(x_0,k_0)$ if $(x_0,k_0) \in N_\nu^+$, or a conic neighborhood in C^- of $C^-(x_0,k_0)$ if $(x_0,k_0) \in N_\nu^-$. Moreover, each $(x,k) \in N$ will give rise to a contribution of either $C^+(x,k)$ or $C^-(x,k)$

(not both) in the wave front set of the sum $\sum F_i^+ - G^+$ (the constructed distinguished parametrix E_ν^+). Note that if *both* $C^+(x,k)$ and $C^-(x,k)$ are included in the wave front set of E_ν^+ then the uniqueness argument would fail; see, e.g., Proposition 6.5.11 of [7]. Hence E_ν^+ must have wave front set

$$\mathrm{WF}'(E_\nu^+) = \bigcup_{N^1} C^+(x,k) \cup \bigcup_{N^2} C^-(x,k) \cup \Delta^* ,$$

where N^1 and N^2 are complements of each other in N. However, since $\mathrm{WF}'(E_\nu^+)$ is a closed subset of $T^*(M \times M)\backslash\mathbf{0}$, N^1, N^2 must be closed subsets of N, i.e., they give rise to an orientation by Eqs. (10) and (11).

5. Equivalence Theorem

Following is the main theorem of this paper, referred to here as the "equivalence theorem." We specialize to the case $n = 4$. Note that "ω_2 satisfies (KG) mod C^∞" means "$(\Box + m^2)\omega_2 = h_1$ and $\omega_2(\Box + m^2) = h_2$ for some smooth h_1, h_2."

Theorem 5.1. *Let (M, g) be a four dimensional globally hyperbolic space-time, let $P = \Box + m^2$, and suppose ω_2 is an element of $\mathscr{D}_2'(M)$. Choose a Cauchy hypersurface $\mathscr{C}$, a causal normal neighborhood $\mathscr{N}$ of $\mathscr{C}$ and time function T. Then the following three conditions are equivalent:*

1. *ω_2 is globally Hadamard on $\mathscr{N} \times \mathscr{N}$, and satisfies (KG) and (Com) mod C^∞.*
2. *The Feynman propagator ω_F of ω is the distinguished parametrix E_F of P modulo C^∞.*
3. *ω_2 satisfies (KG) and (Com) mod C^∞, and*

$$\begin{aligned} \mathrm{WF}(\omega_2) \;=\; & \{((x_1,k_1),(x_2,k_2)) \in T^*(M)\backslash\mathbf{0} \times T^*(M)\backslash\mathbf{0}: \\ & (x_1,k_1) \sim (x_2,-k_2), k_1 \rhd 0\} \,. \end{aligned}$$

Please refer to the Note Added in Proof, in which we show (KG) can be dropped from Condition 3. The consistency of Condition 1 with (KG) and (Com) has been shown earlier. Note that Condition (PT) is not mentioned in Theorem 5.1. A result of Duistermaat and Hörmander [7] will be used later to show that (PT) is a consequence (mod C^∞) of any of the above three (equivalent) conditions.

(i) 1 $\Longrightarrow$ 3. In [32] and an earlier version of this paper a proof of this implication was given, but it was valid only for the flat case ($\sigma(x_1,x_2) = -(x_1-x_2)^2$). Köhler [24, 25] has completed this proof for the general case using a deformation argument analogous to that of Fulling, Narcowich and Wald [11]. Whereas Köhler's argument depends on the results of Fulling, Sweeny and Wald [12] (namely that Cauchy evolution preserves the Hadamard expression), here we present a direct computation of the wave front set of ω_2 in the region $\mathscr{N} \times \mathscr{N}$, which does not rely on the Cauchy evolution argument of [12], nor does it use a deformation argument of [11].

Let $\mathbb{M}$ denote four dimensional Minkowski space $\mathbb{R}^4$ with the usual metric $\eta_{\mu\nu}$. The first step in our computation is to compute the wave front set of the following distributions in $\mathscr{D}'(\mathbb{M})$:

$$u_1(y) := \lim_{\epsilon \to 0^+} \left(-y_\epsilon^2\right)^{-1} ,$$

$$u_2(y) := \lim_{\epsilon \to 0^+} \ln\left(-y_\epsilon^2\right) ,$$

where $y_\epsilon^\mu = (y^0 - \mathrm{i}\epsilon, y^1, y^2, y^3)$. The wave front sets of the distributions

$$v_1(x_1, x_2) := \lim_{\epsilon \to 0^+} \sigma_\epsilon^{-1}(x_1, x_2)$$

$$v_2(x_1, x_2) := \lim_{\epsilon \to 0^+} \ln(\sigma_\epsilon(x_1, x_2))$$

(where $\sigma_\epsilon(x_1, x_2) = \sigma(x_1, x_2) + 2\mathrm{i}\epsilon(T(x_1) - T(x_2)) + \epsilon^2$) on a convex normal neighborhood of a general space-time M will then be deduced through a judicious choice of coordinates on the *product manifold* $M \times M$.

Define the distribution $u_1^m(y)$ on $\mathbb{M}$ by setting the Fourier transform to be

$$\widehat{u_1^m}(k) = \frac{1}{2\pi}\theta(k_0)\delta(k^2 - m^2) , \tag{12}$$

which is in $\mathscr{S}'(\mathbb{M})$. By inserting a "convergence factor" $\exp(-\epsilon k_0)$ and taking the limit $\epsilon \to 0^+$, one can show that u_1^m is given by

$$u_1^m(y) = \lim_{\epsilon \to 0^+}\left[\frac{1}{-y_\epsilon^2} + f(m)\ln(-y_\epsilon^2)\right] + \cdots , \tag{13}$$

where the omitted terms are C^∞ and vanish when $m = 0$ and $f(0) = 0, f(m) \neq 0$ for $m > 0$. As in the definition of $G_\epsilon^{T,p}$ in Eq. (3), the branch cut is along the negative real axis in the logarithm. $\omega_2(x_1, x_2) = \frac{1}{(2\pi)^2} u_1^m(x_1 - x_2)$ is the two-point distribution of the free field of mass m on Minkowski space.

It is clear from Eq. (13) that sing supp $u_1^m = \{y: y^2 = 0\}$. Furthermore, from Eq. (12) we have $(\Box + m^2)u_1^m = 0$.

By the propagation of singularities theorem for the operator $\Box + m^2$ applied to u_1^m, if $(x, k) \in \mathrm{WF}(u_1^m)$ then so is (x', k'), where $(x', k') \sim (x, k)$ and $k^2 = (k')^2 = 0$. On Minkowski space $\mathbb{M}$ we have $k' = k$.

Observation 1. If $(x, k) \in \mathrm{WF}(u_1^m)$, so that $x^2 = 0$, and if $x \neq 0$, then k is parallel to x, since otherwise by the PST we may generate singularities off the light cone $x^2 = 0$.

Lemma 8.1.7 of [18] states,

Lemma 5.2. *If* $v \in \mathscr{S}'(\mathbb{R}^p)$ *then* $\mathrm{WF}(v) \subset \mathbb{R}^p \times F$, *where* F *is the limit cone of* supp $\hat{v}$ *at* ∞, *by which we mean the set of all limits of sequences* $t_j x_j$, *where* $x_j \in$ supp $\hat{v}$ *and* $t_j > 0$ *and* $\lim_{j\to\infty} t_j = 0$. ■

Using this we arrive at

Observation 2. We have $\mathrm{WF}(u_1^m) \subset \mathbb{M} \times F$, where the limit cone F of supp $\widehat{u_1^m}$ is precisely

$$F = \{k \in \mathbb{M}\backslash\{0\}: \ k_0 \geq 0, \ k^2 = 0\} .$$

If we let

$$A = \{(x, k) \in T^*(\mathbb{M})\backslash\mathbf{0}: \ k \parallel x \neq 0, \ k_0 \geq 0, \ k^2 = 0\} , \tag{14}$$

$$B = \{(0, k) \in T^*(\mathbb{M})\backslash\mathbf{0}: \ k_0 \geq 0, \ k^2 = 0\} , \tag{15}$$

then Observations 1 and 2 imply that

$$\mathrm{WF}(u_1^m) \subset A \cup B = \{(x,k) \in T^*(\mathbb{M})\backslash\mathbf{0}\colon\ \exists s \in \mathbb{R},\ x = sk,\ k_0 \geq 0,\ k^2 = 0\}\ . \quad (16)$$

Now if $x^2 = 0$ and $x \neq 0$, there must be a nonzero covector $k \in \mathbb{M}$ such that $(x,k) \in \mathrm{WF}(u_1^m)$ since $u_1^m(x)$ must have a singularity at such an x. Hence $\mathrm{WF}(u_1^m) \supset A$. Furthermore, the points $(0,k)$ with $k^2 = 0$ and $k_0 \geq 0$ are also in $\mathrm{WF}(u_1^m)$ because we may pick a point $(x,k) \in A$ and by the propagation of singularities theorem propagate (x,k) to $(0,k)$ to produce a point in B. Hence we conclude that equality holds in Ineq. (16), i.e.,

$$\mathrm{WF}(u_1^m) = A \cup B\ .$$

This determines the wave front set for $u_1 = u_1^0$, for $u_1^m(y) - u_1^0(y) = \lim_{\epsilon\to 0^+} f(m) \ln(-y_\epsilon^2) + C^\infty$, with $m \neq 0$, and hence for $u_2(y)$.

Following is the computation of the wave front set of a two-point distribution $\omega_2(x_1,x_2)$ satisfying Condition 1 for the case of a general four dimensional globally hyperbolic space-time (M,g). Choose a Cauchy hypersurface $\mathscr{C} \subset \mathscr{M}$, a causal normal neighborhood $\mathscr{N}$, and a convex normal neighborhood U in $\mathscr{N}$. Consider the mapping $\varphi\colon M \times M \longrightarrow M \times \mathbb{M}$ defined as follows. For each pair $(x_1,x_2) \in U \times U$, let $\varphi(x_1,x_2) = (x, y(x_1,x_2))$, where $x = x_2$ and $y^\mu(x_1,x_2), \mu = 0,\ldots,3$ are the coordinates of the point x_1 with respect to the *Riemann normal coordinate system* at x_2. (See e.g., Fulling [10].) Hence φ is a diffeomorphism and $\sigma(x_1,x_2) = -y^2(x_1,x_2) = -\eta_{\mu\nu}y^\mu(x_1,x_2)y^\nu(x_1,x_2)$. The arguments of [23] which show that the definition of Hadamard is independent of the choice of T can be modified to show that $T(x_1) - T(x_2)$ may be replaced by $y^0(x_1,x_2)$ (both of which are positive when $x_1 \in J^+(x_2)$) in the definition of σ_ϵ without changing the global Hadamard definition, so that under the mapping φ^{-1} the distributions $v_1(x_1,x_2), v_2(x_1,x_2)$ become $\tilde{u}_1(x,y), \tilde{u}_2(x,y)$, which are the elements of $\mathscr{D}'(M\times\mathbb{M})$ defined by $\tilde{u}_1 = 1 \otimes u_1, \tilde{u}_2 = 1 \otimes u_2$.

Now clearly one has for $i = 1,2$,

$$\begin{aligned}\mathrm{WF}(\tilde{u}_i) &= \{((x,0),(y,k)) \in T^*(M \times \mathbb{M})\backslash\mathbf{0}\colon (y,k) \in \mathrm{WF}(u_i)\} \\ &= \{((x,0),(y,k)) \in T^*(M \times \mathbb{M})\backslash\mathbf{0}\colon \\ &\qquad \exists s \in \mathbb{R}, y^\mu = sk^\mu, k^2 = 0, k_0 \geq 0\}\ .\end{aligned}$$

Hence it remains to apply the following theorem, from which we deduce how to compute the wave front set of the pullback of a distribution:

Theorem 5.3 (Theorem 2.5.11′ of [16]). *Let X and Y be manifolds and $\varphi\colon Y \to X$ be a C^∞ map, and let*

$$N_\varphi = \{(\varphi(y),\xi) \in T^*(X)\colon d\varphi^t(y)\xi = 0\}$$

be the set of normals of the map. If $u \in \mathscr{D}'(X)$ and $\mathrm{WF}(u) \cap N_\varphi = \emptyset$ we can define the pullback $\varphi^* u$ in one and only one way so that it is equal to the composition $u \circ \varphi$ when u is a continuous function and is sequentially continuous from $\mathscr{D}'_\Gamma(X)$ to $\mathscr{D}'(Y)$ for any closed cone $\Gamma \subset T^*(X)\backslash\mathbf{0}$ with $\Gamma \cap N_\varphi = \emptyset$. Moreover,

$$\mathrm{WF}(\varphi^* u) \subset \varphi^*\mathrm{WF}(u) = \{(y, d\varphi^t(y)\xi)\colon\ (\varphi(y),\xi) \in \mathrm{WF}(u)\}\ .$$

Refer to [16] for the definition of the pseudo-topologies given to the sets of distributions $\mathscr{D}'_\Gamma(X) = \{u \in \mathscr{D}'(X)\colon \mathrm{WF}(u) \subset \Gamma\}$. Transposition is denoted by ^{t}. When φ is a diffeomorphism, N_φ is contained in the zero section $\mathbf{0}$ and $N_\varphi \cap \mathrm{WF}(u)$ is empty. Since φ^{-1} is also a diffeomorphism, we have

$$\mathrm{WF}(\varphi^* u) = \varphi^* \mathrm{WF}(u) .$$

For our choice of φ, replacing y by (x_1, x_2) and ξ by $[0,k]^t$, and changing to space-time tensor notation, $d\varphi^t(y)\xi$ becomes $d\varphi^t(x_1,x_2)[0,k]^t$, which is

$$\begin{bmatrix} 0 & \left(\frac{\partial y}{\partial x_1}\right)^t \\ 1 & \left(\frac{\partial y}{\partial x_2}\right)^t \end{bmatrix} \begin{bmatrix} 0 \\ k \end{bmatrix} = \begin{bmatrix} y^\mu_{,\alpha_1} k_\mu \\ y^\mu_{,\alpha_2} k_\mu \end{bmatrix} . \tag{17}$$

Here the subscript $1,2$ on the index α indicates that the derivative (indicated by a comma) is with respect to the coordinates x_1, x_2 respectively. Now the wave front sets of $\tilde{u}_i, i = 1,2$ contain points $((x,y),(0,k)), k \neq 0$ such that $y_\mu = sk_\mu$ for some $s \in \mathbb{R}$. We deal with the three cases $s > 0, s < 0, s = 0$ separately. If $s > 0$, then the right hand side of Eq. (17) for $\mathrm{WF}(\varphi^* \tilde{u}_i), i = 1,2$ is

$$\begin{bmatrix} -\frac{1}{2s}\sigma_{,\alpha_1} \\ -\frac{1}{2s}\sigma_{,\alpha_2} \end{bmatrix} .$$

Now recall (see e.g., Fulling [10]) that the vectors $\sigma^{\alpha_i} := \sigma^{,\alpha_i} = g^{\alpha_i\beta_i}\nabla_{\beta_i}\sigma$ for $i = 1,2$ are the tangent vectors to the geodesic from x_1 to x_2 (within the convex normal neighborhood) at x_1, x_2 pointing toward the other point along the geodesic, with magnitude equal to twice the length of the geodesic. (Our definition of σ is equal to the more common definition of σ times -2.) The first vector σ^{α_1} is minus the parallel transport of the second σ^{α_2} along the geodesic from x_2 to x_1. Since $k_0 > 0$, k^μ is a forward pointing null vector, which means that $x_1 \succ x_2$, i.e., x_1 and x_2 are connected by a null geodesic γ and x_1 is advanced in time with respect to x_2. Hence $k_1 = -\frac{1}{2s}\sigma^{\alpha_1}$ is the forward pointing tangent vector to γ at x_1, and $k_2 = -\frac{1}{2s}\sigma^{\alpha_2}$ is minus the parallel transport of k_1 along γ from x_1 to x_2.

For the case $s < 0$, we have $x_1 \prec x_2$ and one finds that k_1 defined above is forward pointing and that k_2 defined above is minus the parallel transport of k_1 along γ from x_1 to x_2. For the case $s = 0$, the points x_1, x_2 coincide, $k_1 = -k_2$, $k_1^2 = 0$, and $k_1 \rhd 0$ as follows from continuity from the other two cases. Hence $\mathrm{WF}(v_i), i = 1,2$ consists of all points $((x_1,k_1),(x_2,k_2))$ in $T^*(U \times U)$ such that $(x_1,k_1) \sim (x_2,-k_2)$ and for which $k_1 \rhd 0$.

Now define the distribution $\Gamma^{T,p}(x_1,x_2)$ on the set $\mathscr{O}$ defined in Lemma 3.1 to be $\lim_{\epsilon\to 0^+} \chi(x_1,x_2) G^{T,p}_\epsilon(x_1,x_2)$, where $G^{T,p}$ is defined in Eq. (3). Clearly we have on $\mathscr{O}$

$$\begin{aligned} \Gamma^{T,p}(x_1,x_2) &= \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^2}\chi(x_1,x_2)\Big\{ \frac{\Delta^{\frac{1}{2}}(x_1,x_2)}{\sigma_\epsilon(x_1,x_2)} \\ &\quad + v^{(p)}(x_1,x_2)\ln\Big(\sigma_\epsilon(x_1,x_2)\Big)\Big\} \\ &= \frac{1}{(2\pi)^2}\chi(x_1,x_2)\Big(\Delta^{\frac{1}{2}}(x_1,x_2)v_1(x_1,x_2) \\ &\quad + v^{(p)}(x_1,x_2)v_2(x_1,x_2)\Big) , \end{aligned}$$

where $\sigma_\epsilon(x_1,x_2) = \sigma(x_1,x_2) + 2i\epsilon y^0(x_1,x_2) + \epsilon^2$.

To simplify the notation in the following, we drop the T in $\Lambda^{T,p}$ and $\Gamma^{T,p}$. Note that we may choose the causal normal neighborhood $\mathcal{N}$ to be close enough to $\mathscr{C}$ and the set $\mathscr{O}$ to be close enough to $\mathcal{N} \times \mathcal{N}$ so that $\Delta^{\frac{1}{2}}(x_1,x_2) \neq 0$ for $(x_1,x_2) \in \mathscr{O}$. In the following we shall also use the fact that for any $y \in M$, and any $\phi \in C^\infty$ such that $\phi(y) \neq 0$, and any $u \in \mathscr{D}'(M)$, we have $\Sigma_y(\phi u) = \Sigma_y(u)$.

Now since $\mathrm{WF}(v_i), i = 1,2$ is determined on any set of the form $U \times U$, where U is a convex normal neighborhood, and since $\mathscr{O}$ is constructed as a union of such sets by Lemma 3.1, $\mathrm{WF}(v_i), i = 1,2$ is thus determined on all of $\mathscr{O}$ to be

$$\{((x_1,k_1),(x_2,k_2)) \in T^*(M \times M)\backslash\mathbf{0}\colon\ (x_1,k_1) \sim (x_2,-k_2), k_1 \rhd 0\}\ .$$

Hence by the above facts and the fact that $\Gamma^p = 0$ outside $\mathscr{O}$, we have that

$$\begin{aligned}\mathrm{WF}(\Gamma^p)\Big|_{\mathcal{N}\times\mathcal{N}} &= \{((x_1,k_1),(x_2,k_2)) \in T^*(M \times M)\backslash\mathbf{0}\colon \\ &\qquad (x_1,k_1) \sim (x_2,-k_2),\ k_1 \rhd 0\}\ .\end{aligned}$$

For any pair $(x_1,x_2) \in \mathcal{N} \times \mathcal{N}$, choose a function ϕ such that $\phi(x_1,x_2) \neq 0$ and with compact support in $U_1 \times U_2$, where U_i are small coordinate neighborhoods of $x_i,\ i = 1,2$. Hence we may compute the Fourier transform of ϕH^p with respect to the coordinates on $U_1 \times U_2$ to be

$$\left|(\phi H^p)^\frown(k_1,k_2)\right| \le C_p(1 + |k|)^{-p}$$

for some constant C_p, and for any $k = (k_1,k_2)$. Since $\Lambda^p = \Gamma^p + H^p$ for any p, we deduce that the wave front set over $\mathcal{N}\times\mathcal{N}$ of a two-point distribution ω_2 satisfying Condition 1 is

$$\begin{aligned}\mathrm{WF}(\omega_2) &= \{((x_1,k_1),(x_2,k_2)) \in T^*(M \times M)\backslash\mathbf{0}\colon \\ &\qquad (x_1,k_1) \sim (x_2,-k_2),\ k_1 \rhd 0\}\ .\end{aligned}$$

By the PST and the absence of singularities of $\omega_2(x_1,x_2)$ at points x_1,x_2 which are space-like separated in $\mathcal{N}$, we conclude that the above equation is true on $M \times M$. Hence $\mathrm{WF}(\omega_2)$ is as given in Condition 3.

(ii) 3 $\Longrightarrow$ 2. We wish to show that if Condition 3 holds, then $\omega_F = E_F \bmod C^\infty$, where $\omega_F = i\omega_2 + \Delta_A$ is the Feynman propagator of ω and E_F is the Feynman distinguished parametrix.

First, it follows easily from (Com) that $\omega_F = i(\omega_2)_+ + \frac{1}{2}(\Delta_A + \Delta_R)$, and since $\Delta_A(x_1,x_2) = \Delta_R(x_2,x_1)$, the symmetry of ω_F is manifest.

When restricted to points $((x_1,k_1),(x_2,k_2)) \in T^*(M \times M)\backslash\mathbf{0}$ such that $x_1 \notin J^-(x_2)$, the distribution $\Delta_A(x_1,x_2)$ vanishes, and hence $\mathrm{WF}(\omega_F) = \mathrm{WF}(\omega_2)$ for $x_1 \notin J^-(x_2)$. It is easily verified that the wave front set of a symmetric two-point distribution is a symmetric set. Hence

$$\begin{aligned}&\mathrm{WF}'(\omega_F)|_{x_1\neq x_2} \\ &= \{((x_1,k_1),(x_2,k_2)) \in T^*(M)\backslash\mathbf{0} \times T^*(M)\backslash\mathbf{0}\colon (x_1,k_1) \sim (x_2,k_2), \\ &\qquad k_1 \rhd 0 \text{ if } x_1 \succ x_2 \text{ and } k_1 \lhd 0 \text{ if } x_1 \prec x_2\}.\end{aligned}$$

This set is just C_1^1, shown in Fig. 1.

The last step is to show that $\mathrm{WF}'(\omega_F)|_{x_1=x_2} = \Delta^*$, where

$$\Delta^* = \{((x,k),(x,k)) : (x,k) \in T^*(M)\backslash\mathbf{0}\} .$$

Remark that $P\omega_F = \omega_F P = I$ up to C^∞, where $P = \Box + m^2$, since this is true for Δ_A and ω_2 is (mod C^∞) a bisolution of P. Now by the pseudo-local property of pseudo-differential operators,

$$\mathrm{WF}'(\omega_F) \supset \mathrm{WF}'(P\omega_F) = \mathrm{WF}'(I) = \Delta^* . \tag{18}$$

However, $\mathrm{WF}'(\Delta_A) = \Delta^* \cup C_3^1$. (See Fig. 1 for the definition of C_3^1.) Note that $C_3^1|_{x_1=x_2} \subset \Delta^*$ and that $\mathrm{WF}'(\omega_2)|_{x_1=x_2} \subset \Delta^*$. Therefore, $\mathrm{WF}'(\omega_F)|_{x_1=x_2} \subset \mathrm{WF}'(\omega_2)|_{x_1=x_2} \cup \mathrm{WF}'(\Delta_A)|_{x_1=x_2} \subset \Delta^*$. Thus we have established that

$$\begin{aligned} &\mathrm{WF}'(\omega_F) \\ &= \Delta^* \cup \{((x_1,k_1),(x_2,k_2)) \in T^*(M)\backslash\mathbf{0} \times T^*(M)\backslash\mathbf{0} : (x_1,k_1) \sim (x_2,k_2), \\ &\quad k_1 \rhd 0 \text{ if } x_1 \succ x_2 \text{ and } k_1 \lhd 0 \text{ if } x_1 \prec x_2\}. \end{aligned}$$

Finally, since ω_F is a parametrix of P, the uniqueness (mod C^∞) of distinguished parametrices (Theorem 4.5) implies $\omega_F = E_F$ mod C^∞. This proves (ii).

(iii) 2 $\Longrightarrow$ 1. First, note that Condition 2 implies $\omega_2 = -\mathrm{i}(\omega_F - \Delta_A) = -\mathrm{i}(E_F - \Delta_A)$ mod C^∞ satisfies (KG) mod C^∞, since E_F and Δ_A are parametrices of P. Next,

$$\begin{aligned} (\omega_2)_- &= -\mathrm{i}((\omega_F)_- - (\Delta_A)_-) \\ &= \frac{\mathrm{i}}{2}(\Delta_A - \Delta_R) = \frac{\mathrm{i}}{2}\Delta \quad (\mathrm{mod}\ C^\infty) . \end{aligned}$$

Therefore (Com) is satisfied mod C^∞.

Finally, we need to show that if $\omega_F = E_F$ mod C^∞ then C^p functions H^p exist such that $\omega_2 = \Lambda^p$ on $\mathcal{N} \times \mathcal{N}$ for all p, where $\Lambda^p = \Gamma^p + H^p$ (see discussion following Definition 3.4). This follows easily from the existence of a globally Hadamard *parametrix* $\lambda_2(x_1,x_2)$ on $\mathcal{N} \times \mathcal{N}$ since then we have $\lambda_F = E_F$ mod C^∞ and thus $\omega_2 = \lambda_2$ mod C^∞. See, e.g., [12] for the construction of such a parametrix, or Chapter 4 of Friedlander [9] for this construction for the advanced and retarded fundamental solutions, which is readily extendible to the globally Hadamard case. (Note that to construct this parametrix one does not need to use a Cauchy evolution argument, nor does one need to show the existence of a globally Hadamard two-point distribution satisfying (PT), (Com), and (KG) exactly, as is done in [11].) This completes the proof of Theorem 5.1. ∎

Now since the proof of Theorem 5.1 has not relied upon the "preservation of Hadamard form under Cauchy evolution" result of Fulling, Sweeny and Wald [12], we have an alternative *micro-local* proof of their results as follows: If (Com) and (KG) hold mod C^∞ (globally), then the Hadamard condition on $\mathcal{N} \times \mathcal{N}$ is equivalent to the WFSSC on $\mathcal{N} \times \mathcal{N}$. If $\mathcal{N}'$ is another causal normal neighborhood on M, then all points $((y_1,l_1),(y_2,l_2))$ in $\mathcal{N}' \times \mathcal{N}'$ of the form $(y_1,l_1) \sim (y_2,-l_2)$ with $l_1 \rhd 0$ are in the wave front set of ω_2 since they are easily seen to come from $\mathrm{WF}(\omega_2)$ on $\mathcal{N} \times \mathcal{N}$ by the PST. It is also clear that there are no other points in $\mathrm{WF}(\omega_2)$ on $\mathcal{N}' \times \mathcal{N}'$ since these would propagate back to pairs $((x_1,k_1),(x_2,k_2))$ not allowed by the WFSSC on $\mathcal{N} \times \mathcal{N}$. Hence the WFSSC holds in $\mathcal{N}' \times \mathcal{N}'$ which, along with (Com), (KG) mod C^∞, implies (GH) on this set. Hence the global Hadamard condition "propagates" throughout the space-time.

6. Discussion

In anticipation of quantum field models satisfying a more general linear wave equation and having a different form for the commutator, we isolate the condition on the wave front set from Condition 3 of Theorem 5.1, calling it the *wave front set spectral condition* (WFSSC):

Definition 6.1. *The two-point distribution* ω_2 *is said to satisfy the* **wave front set spectral condition** *(WFSSC) if*

$$\begin{aligned} \mathrm{WF}'(\omega_2) &= \{((x_1,k_1),(x_2,k_2)) \in T^*(M)\backslash\mathbf{0} \times T^*(M)\backslash\mathbf{0}: \\ &\qquad (x_1,k_1) \sim (x_2,k_2), k_1 \rhd 0\}\,. \end{aligned}$$

As stated in the Introduction, the WFSSC is analogous to the ordinary spectral condition for the two-point distribution in axiomatic quantum field theory. We may see this as follows:

First, on Minkowski space $\mathbb{M} = (\mathbb{R}^4, \eta)$, the spectral condition in axiomatic QFT requires that $\omega_2 \in \mathscr{S}'(\mathbb{M}^2)$ and that

$$\mathrm{supp}\,\widehat{\omega_2} \subset \left\{(k_1,k_2) \in \mathbb{M}\backslash\{0\} \times \mathbb{M}\backslash\{0\}: k_1 \in V^+,\ k_1 + k_2 = 0\right\} \cup \{0\}\,,$$

where $V^+ = \{k \in \mathbb{M}\colon\ \eta^{\mu\nu}k_\mu k_\nu \geq 0,\ k_0 \geq 0\}$ is the closed forward light cone. By Lemma 5.2 this implies

$$\pi_2\mathrm{WF}(\omega_2) \subset \left\{(k_1,k_2) \in \mathbb{M}\backslash\{0\} \times \mathbb{M}\backslash\{0\}:\ k_1 \in V^+,\ k_1 + k_2 = 0\right\}.$$

Hence for each point $(x_1,x_2) \in \mathbb{M}^2$,

$$\Sigma_{(x_1,x_2)}(\omega_2) \subset \left\{(k_1,k_2) \in \mathbb{M}\backslash\{0\} \times \mathbb{M}\backslash\{0\}:\ k_1 \in V^+,\ k_1 + k_2 = 0\right\}.$$

Second, on an arbitrary globally hyperbolic space-time (M, g), the WFSSC states that for null-related x_1 and x_2,

$$\begin{aligned} \Sigma_{(x_1,x_2)}(\omega_2) \quad \subset \quad & \Big\{(k_1,k_2) \in T^*_{x_1}(M)\backslash\{0\} \times T^*_{x_2}(M)\backslash\{0\}: \\ & \quad k_1^2 = 0,\ k_1 \rhd 0,\ k_2 = -T^{x_1}_{x_2}k_1\Big\}\,, \end{aligned}$$

where the operator $T^{x_1}_{x_2}$ parallel transports vectors along the null geodesic from x_1 to x_2, and for other points (x_1,x_2),

$$\Sigma_{(x_1,x_2)}(\omega_2) = \emptyset.$$

The resemblance of the two conditions is manifest, justifying the terminology "wave front set *spectral* condition."

Recently Köhler has proposed a modified WFSSC (called MWFSSC in this paper) which allows for nontrivial examples that do not satisfy WFSSC at conjugate points (i.e., points x_1, x_2 which can be connected by more than one null geodesic). See [24, 25, 33] for more discussion. Note that the WFSSC given here is entirely adequate for linear models.

We remark that the WFSSC (or MWFSSC) contains qualitatively different kinds of information than the spectral condition. The WFSSC specifies the location of the singularities of ω_2 and indicates the directions of non-rapid decrease at these points (but does not restrict the support of the Fourier transform of ω_2), whereas the spectral condition only places a restriction on the support of the Fourier transform without explicitly specifying the location of the singularities. Now from axiomatic QFT on $\mathbb{M}$ it is known that in general, $\omega_2(x_1, x_2)$ is smooth for space-like separated points x_1, x_2, if ω_2 satisfies the spectral condition and Lorentz invariance. Hence the WFSSC may be viewed as a combination of these two conditions *modulo* C^∞ on curved space-time.

For m-point distributions ($m \geq 3$), a wave front set condition has been proposed by Köhler [25, 4] (see also [32] which contains a first attempt at such a condition, but was shown not to be satisfied in the quasi-free case for the Einstein cylinder by Köhler [26]), and it is of interest to investigate the consequences of the wave front set property and other properties as is done in axiomatic quantum field theory [34, 19].

Various authors have viewed the Hadamard condition as a necessary physical condition on quasi-free Klein-Gordon states in a globally hyperbolic curved space-time [5, 35, 11, 12, 14, 23], and in particular as a remnant of the spectral condition via the equivalence principle (see, e.g., [31]). Theorem 5.1 provides a stronger connection between the Hadamard condition and the spectral condition, namely through the WFSSC. This connection could perhaps have been anticipated by the following heuristic argument: If $\omega_2 \in \mathscr{S}'(\mathbb{M}^2)$ and (supp $\widehat{\omega_2}$) consists of points (k_1, k_2) such that k_1 is in the closed forward light cone V^+ and $k_2 = -k_1$, then multiplication by a smooth cutoff function $\phi \in C_0^\infty(\mathbb{M}^2)$ will result in a violation of the spectral condition: e.g., $\pi_1(\text{supp } \widehat{\phi\omega_2}) \not\subset V^+$. However, the directions (k_1, k_2) of non-rapid decrease of $\widehat{\phi\omega_2}$ are still such that $k_1 \in V^+$ and $k_2 = -k_1$. When considering distributions on curved space-times, it is natural to use a partition of unity to split up ω_2 into $\phi\omega_2 \in \mathscr{E}'(M \times M)$, where ϕ is localized near a point (x_1, x_2), and to map $\phi\omega_2$ to $\mathscr{E}'(\mathbb{R}^4 \times \mathbb{R}^4)$ using a coordinate chart. It is sensible to then make some sort of restriction on the directions (k_1, k_2) of non-rapid decrease of $\widehat{\phi\omega_2}$ so that k_1 is in the forward light cone, and k_2 is in the backward light cone. Since the metric on $\mathbb{R}^4$ is no longer flat, and k_1, k_2 are considered to be covectors localized near x_1, x_2 resp., there may not be a simple relation between k_1 and k_2 (such as $k_2 = -k_1$ on flat space). However, parallel transporting k_2 to x_1 and requiring $k_1 = -Tk_2$ appears to be a natural thing to do in the curved case. In the limit as the support of ϕ goes to (x_1, x_2) this condition becomes an exact condition on the wave front set of ω_2, and it only remains to decide, e.g., along which curves parallel transport should be taken. In any case, such an argument suggests that using wave front sets may be an appropriate way of generalizing the restrictions suggested by the spectral condition on flat space to a curved space-time.

Next, we quote a result by Duistermaat and Hörmander [7] demonstrating that the global Hadamard condition for Klein-Gordon two-point distributions is sufficient to guarantee positivity (PT) mod C^∞.

If $\tilde{n} \in \tilde{N}$ is a component of N, defined in Sect. 5, then one defines the two-point distribution $S_{\tilde{n}}$ to be the difference $E^+_{\tilde{n}} - E^+_{\emptyset}$ of the distinguished parametrices corresponding to $\tilde{n}$ and $\emptyset$ respectively of a properly supported pseudo-differential operator Q, with respect to which M is pseudo-convex. As shown in Sect. 6.6 of [7], if ν is any subset of $\tilde{N}$, then

$$E^+_\nu = E^+_\emptyset + \sum_{\tilde{n} \in \nu} S_{\tilde{n}}. \tag{19}$$

We refer to [7] for more properties of $S_{\tilde{n}}$. Of interest to us here is the following slightly modified version of the main result from Sect. 6.6 of [7].

The operator Q is called *Hermitian* if $(Qu, v)_M = (u, Qv)_M$ for all $u, v \in C_0^\infty(M)$, and $(u, v)_M = \int u(x)v(x)d\mu_g(x)$.

Theorem 6.2 (Theorem 6.6.2 of [7]). *Let Q be Hermitian and of real principal type in M, and assume that M is pseudo-convex with respect to Q. Then one can choose $S_{\tilde{n}}$ anti-Hermitian so that for $u \in C_0^\infty(M)$,*

$$(\mathrm{i}^{-1} S_{\tilde{n}} u, u)_M \geq 0. \blacksquare$$

Refer to [7] for the proof. This theorem implies that if $\nu_1 \supset \nu_2$ then

$$-\mathrm{i}(E^+_{\nu_1} - E^+_{\nu_2}) = -\mathrm{i} \sum_{\tilde{n} \in \nu_1 \setminus \nu_2} S_{\tilde{n}}$$

is of positive type up to C^∞.

When we consider the case of $Q = \Box + m^2$ on a globally hyperbolic space-time (M, g), and choose the distinguished parametrices E_F and Δ_A, whose subsets ν are $N_+ \cup N_-$ and N_- respectively (see Sect. 4 for the definition of these sets), we see that $S_{N_+} = E_F - \Delta_A$. Hence the above theorem informs us that $-\mathrm{i}(E_F - \Delta_A)$ is of positive type up to C^∞ (here we recall the correspondence between continuous linear mappings of $C_0^\infty(M)$ to $C^\infty(M)$ and elements of $\mathscr{D}_2'(M)$). Therefore, we have the following result.

Theorem 6.3. *If ω_2 is a two-point distribution satisfying (KG) and (Com) and the global Hadamard condition on a globally hyperbolic space-time (M, g) then there is a function $f \in C^\infty(M \times M)$ such that $\omega_2 + f$ satisfies (PT).* $\blacksquare$

Hence whereas positivity (mod C^∞) was not needed to define the global Hadamard condition, it is not only consistent with the global Hadamard condition but is also a consequence of it.

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Note Added in Proof: One can drop the condition (KG) from Condition 3 of Theorem 5.1; it is implied by the other properties of Condition 3. To see this, let $A_0 = (\square + m^2) \otimes \mathbf{1}$, $A_2 = \mathbf{1} \otimes (\square + m^2)$, and note that $A_1 \varDelta = A_2 \varDelta = 0$. Since $(\omega_2)_+$ is symmetric, we have $(A_1(\omega_2)_+)(x_1, x_2) = (A_2(\omega_2)_+)(x_2, x_1)$ and hence $\mathrm{WF}(A_1(\omega_2)_+) = \mathrm{WF}(A_2(\omega_2)_+)^t$, where ^{t} interchanges (x_1, k_1) and (x_2, k_2) in the wave front set. Also, A_1 and A_2 are pseudo-differential, hence $\mathrm{WF}(A_1(\omega_2)_+) = \mathrm{WF}(A_1 \omega_2) \subset \mathrm{WF}(\omega_2)$ and $\mathrm{WF}(A_1(\omega_2)_+)^t = \mathrm{WF}(A_2(\omega_2)_+) \subset \mathrm{WF}(\omega_2)$, and since only $k_1 \rhd 0$, $k_2 \lhd 0$ appear in $\mathrm{WF}(\omega_2)$, we see that $\mathrm{WF}(A_1(\omega_2)_+)$ must be empty. Similarly for $\mathrm{WF}(A_2(\omega_2)_+)$. Thus ω_2 satisfies (KG) modulo C^∞.

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