

Adiabatic Vacuum States on General Spacetime Manifolds: Definition, Construction, and Physical Properties

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Abstract

Adiabatic vacuum states are a well-known class of physical states for linear quantum fields on Robertson-Walker spacetimes. We extend the definition of adiabatic vacua to general spacetime manifolds by using the notion of the Sobolev wavefront set. This definition is also applicable to interacting field theories. Hadamard states form a special subclass of the adiabatic vacua. We analyze physical properties of adiabatic vacuum representations of the Klein-Gordon field on globally hyperbolic spacetime manifolds (factoriality, quasiequivalence, local definiteness, Haag duality) and construct them explicitly, if the manifold has a compact Cauchy surface.

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Contents

1	Introduction	2
2	The Klein-Gordon field in globally hyperbolic spacetimes	3
3	Definition of adiabatic states	9
4	The algebraic structure of adiabatic vacuum representations	12
4.1	Primarity and local quasiequivalence of adiabatic and Hadamard states . . .	12
4.2	Local definiteness and Haag duality	28
5	Construction of adiabatic vacuum states	33
5.1	Criteria for initial data of adiabatic vacuum states	34
5.2	Construction on a compact Cauchy surface	41
6	Adiabatic vacua on Robertson-Walker spaces	45
7	Physical interpretation	52
A	Sobolev spaces	56
B	Microlocal analysis with finite Sobolev regularity	58

1 Introduction

It has always been one of the main problems of quantum field theory on curved spacetimes to single out a class of physical states among the huge set of positive linear functionals on the algebra of observables. One prominent choice for linear field theories is the class of Hadamard states. It has been much investigated in the past, but only recently gained a deeper understanding due to the work of Radzikowski [41]. He showed that the Hadamard states are characterized by the wavefront set of their two-point functions (see Definition 3.1). This characterization immediately allows for a generalization to interacting fields [8] and puts all the techniques of microlocal analysis at our disposal [27, 28, 29]. They have made possible the construction of the free field theory [31] and the perturbation theory [7] on general spacetime manifolds.

On the other hand, there is another well-known class of states for linear field theories on Robertson-Walker spaces, the so-called adiabatic vacuum states. They were introduced by Parker [38] to describe the particle creation by the expansion of cosmological spacetime models. Much work has also been devoted to the investigation of the physical (for a review see [18]) and mathematical [35] properties of these states, but it has never been known how to extend their definition to field theories on general spacetime manifolds. Hollands [24] recently defined these states for Dirac fields on Robertson-Walker spaces and observed that

they are in general not of the Hadamard form (correcting an erroneous claim in [31]). It has been the aim of the present work to find a microlocal definition of adiabatic vacuum states which makes sense on arbitrary spacetime manifolds and can be extended to interacting fields, in close analogy to the Hadamard states. It turned out that the notion of the Sobolev (or H^s -) wavefront set is the appropriate mathematical tool for this purpose. In Appendix B we review this notion and the calculus related to it. After an introduction to the structure of the algebra of observables of the Klein-Gordon quantum field on a globally hyperbolic spacetime manifold (\mathcal{M}, g) in Section 2 we present our definition of adiabatic states of order N (Definition 3.2) in Section 3. It contains the Hadamard states as a special case: they are adiabatic states “of infinite order”. To decide which order of adiabatic vacuum is physically admissible we investigate the algebraic structure of the corresponding GNS-representations. Haag, Narnhofer & Stein [23] suggested as a criterion for physical representations that they should locally generate von Neumann factors that have all the same set of normal states (in other words, the representations are locally primary and quasiequivalent). We show in Section 4.1 (Theorem 4.5 and Theorem 4.7) that this is generally the case if $N > 5/2$. For the case of pure states on a spacetime with compact Cauchy surface, which often occurs in applications, we improve the admissible order to $N > 3/2$. In addition, in Section 4.2 we show that adiabatic vacua of order $N > 5/2$ satisfy the properties of local definiteness (Corollary 4.13) and those of order $N > 3/2$ Haag duality (Theorem 4.15). These results extend corresponding statements for adiabatic vacuum states on Robertson-Walker spacetimes due to Lüders & Roberts [35], and for Hadamard states due to Verch [49]; for their discussion in the framework of algebraic quantum field theory we refer to [21]. In Section 5 we explicitly construct pure adiabatic vacuum states on an arbitrary spacetime manifold with compact Cauchy surface (Theorem 5.10). In Section 6 we show that our adiabatic states are indeed a generalization of the well-known adiabatic vacua on Robertson-Walker spaces: Theorem 6.3 states that the adiabatic vacua of order n (according to the definition of [35]) on a Robertson-Walker spacetime with compact spatial section are adiabatic vacua of order $2n$ in the sense of our microlocal Definition 3.2. We conclude in Section 7 by summarizing the physical interpretation of our mathematical analysis and calculating the response of an Unruh detector to an adiabatic vacuum state. It allows in principle to physically distinguish adiabatic states of different orders. Appendix A provides a survey of the Sobolev spaces which are used in this paper.

2 The Klein-Gordon field in globally hyperbolic spacetimes

We assume that spacetime is modeled by a 4-dimensional paracompact \mathcal{C}^∞ -manifold \mathcal{M} without boundary endowed with a Lorentzian metric g of signature $(+ - - -)$ such that (\mathcal{M}, g) is globally hyperbolic. This means that there is a 3-dimensional smooth spacelike hypersurface Σ (without boundary) which is intersected by each inextendible causal (null or

timelike) curve in \mathcal{M} exactly once. As a consequence \mathcal{M} is time-orientable, and we fix one orientation once and for all defining “future” and “past”. Σ is also assumed to be orientable. Our units are chosen such that $\hbar = c = G = 1$.

In this work, we are concerned with the quantum theory of the linear Klein-Gordon field in globally hyperbolic spacetimes. We first present the properties of the classical scalar field in order to introduce the phase space that underlies the quantization procedure. Then we construct the Weyl algebra and define the set of quasifree states on it. The material in this section is based on the papers [36, 13, 32]. Here, all function spaces are considered to be spaces of *real*-valued functions.

Let us start with the Klein-Gordon equation

$$\begin{aligned} (\square_g + m^2)\Phi &= (g^{\mu\nu}\nabla_\mu\nabla_\nu + m^2)\Phi \\ &= \frac{1}{\sqrt{\mathfrak{g}}}\partial_\mu(g^{\mu\nu}\sqrt{\mathfrak{g}}\partial_\nu\Phi) + m^2\Phi = 0 \end{aligned} \tag{1}$$

for a scalar field $\Phi : \mathcal{M} \rightarrow \mathbb{R}$ on a globally hyperbolic spacetime (\mathcal{M}, g) where $g^{\mu\nu}$ is the inverse matrix of $g = (g_{\mu\nu})$, $\mathfrak{g} := |\det(g_{\mu\nu})|$, ∇_μ the Levi-Civita connection associated to g and $m > 0$ the mass of the field. Since (1) is a hyperbolic differential equation, the Cauchy problem on a globally hyperbolic space is well-posed. As a consequence (see e.g. [13]), there are two unique continuous linear operators

$$E^{R,A} : \mathcal{D}(\mathcal{M}) \rightarrow \mathcal{C}^\infty(\mathcal{M})$$

with the properties

$$\begin{aligned} (\square_g + m^2)E^{R,A}f &= E^{R,A}(\square_g + m^2)f = f \\ \text{supp}(E^A f) &\subset J^-(\text{supp } f) \\ \text{supp}(E^R f) &\subset J^+(\text{supp } f) \end{aligned}$$

for $f \in \mathcal{D}(\mathcal{M})$ where $J^{\pm}(S)$ denotes the causal future/past of a set $S \subset \mathcal{M}$, i.e. the set of all points $x \in \mathcal{M}$ that can be reached by future/past-directed causal (i.e. null or timelike) curves emanating from S . They are called the advanced (E^A) and retarded (E^R) fundamental solutions of the Klein-Gordon equation (1). $E := E^R - E^A$ is called the fundamental solution or classical propagator of (1). It has the properties

$$\begin{aligned} (\square_g + m^2)Ef &= E(\square_g + m^2)f = 0 \\ \text{supp}(Ef) &\subset J^+(\text{supp } f) \cup J^-(\text{supp } f) \end{aligned} \tag{2}$$

for $f \in \mathcal{D}(\mathcal{M})$. E^R, E^A and E can be continuously extended to the adjoint operators

$$E^{R'}, E^{A'}, E' : \mathcal{E}'(\mathcal{M}) \rightarrow \mathcal{D}'(\mathcal{M})$$

by $E^{R'} = E^A$, $E^{A'} = E^R$, $E' = -E$.

Let Σ be a given Cauchy surface of \mathcal{M} with future-directed unit normal field n^α . Then we

denote by

$$\begin{aligned}
\rho_0 : \mathcal{C}^\infty(\mathcal{M}) &\rightarrow \mathcal{C}^\infty(\Sigma) \\
u &\mapsto u|_\Sigma \\
\rho_1 : \mathcal{C}^\infty(\mathcal{M}) &\rightarrow \mathcal{C}^\infty(\Sigma) \\
u &\mapsto \partial_n u|_\Sigma := (n^\alpha \nabla_\alpha u)|_\Sigma
\end{aligned} \tag{3}$$

the usual restriction operators, while $\rho'_0, \rho'_1 : \mathcal{E}'(\Sigma) \rightarrow \mathcal{E}'(\mathcal{M})$ denote their adjoints. Dimock [13] proves the following existence and uniqueness result for the Cauchy problem:

Proposition 2.1 (a) $E\rho'_0, E\rho'_1$ restrict to continuous operators from $\mathcal{D}(\Sigma) (\subset \mathcal{E}'(\Sigma))$ to $\mathcal{E}(\mathcal{M}) (\subset \mathcal{D}'(\mathcal{M}))$, and the unique solution of the Cauchy problem (1) with initial data $u_0, u_1 \in \mathcal{D}(\Sigma)$ is given by

$$u = E\rho'_0 u_1 - E\rho'_1 u_0. \tag{4}$$

(b) Furthermore, (4) also holds in the sense of distributions, i.e. given $u_0, u_1 \in \mathcal{D}'(\Sigma)$, there exists a unique distribution $u \in \mathcal{D}'(\mathcal{M})$ which is a (weak) solution of (1) and has initial data $u_0 = \rho_0 u, u_1 = \rho_1 u$ (the restrictions in the sense of Proposition B.7). It is given by

$$u(f) = -u_1(\rho_0 E f) + u_0(\rho_1 E f)$$

for $f \in \mathcal{D}(\mathcal{M})$.

(c) If u is a smooth solution of (1) with $\text{supp } u_{0,1}$ contained in a bounded subset $\mathcal{O} \subset \Sigma$ then, for any open neighborhood \mathcal{U} of \mathcal{O} in \mathcal{M} , there exists an $f \in \mathcal{D}(\mathcal{U})$ with $u = E f$.

Inserting $u = E f$ into both sides of Eq. (4) we get the identity

$$E = E\rho'_0 \rho_1 E - E\rho'_1 \rho_0 E \tag{5}$$

on $\mathcal{D}(\mathcal{M})$. Proposition 2.1 allows us to describe the phase space of the classical field theory and the local observable algebras of the quantum field theory in two different (but equivalent) ways. One uses test functions in $\mathcal{D}(\mathcal{M})$, the other the Cauchy data with compact support on Σ . The relation between them is then established with the help of the fundamental solution E and Proposition 2.1:

Let $(\tilde{\Gamma}, \tilde{\sigma})$ be the real linear symplectic space defined by $\tilde{\Gamma} := \mathcal{D}(\mathcal{M})/\ker E$, $\tilde{\sigma}([f_1], [f_2]) := \langle f_1, E f_2 \rangle$. $\tilde{\sigma}$ is independent of the choice of representatives $f_1, f_2 \in \mathcal{D}(\mathcal{M})$ and defines a non-degenerate symplectic bilinear form on $\tilde{\Gamma}$. For any open $\mathcal{U} \subset \mathcal{M}$ there is a local symplectic subspace $(\tilde{\Gamma}(\mathcal{U}), \tilde{\sigma})$ of $(\tilde{\Gamma}, \tilde{\sigma})$ defined by $\tilde{\Gamma}(\mathcal{U}) := \mathcal{D}(\mathcal{U})/\ker E$. To a symplectic space $(\tilde{\Gamma}, \tilde{\sigma})$ there is associated (uniquely up to $*$ -isomorphism) a Weyl algebra $\mathcal{A}[\tilde{\Gamma}, \tilde{\sigma}]$, which is a simple abstract C^* -algebra generated by the elements $W([f])$, $[f] \in \tilde{\Gamma}$, that satisfy

$$\begin{aligned}
W([f])^* &= W([f])^{-1} = W([-f]) \quad (\text{unitarity}) \\
W([f_1])W([f_2]) &= e^{-\frac{i}{2}\tilde{\sigma}([f_1], [f_2])} W([f_1 + f_2]) \quad (\text{Weyl relations})
\end{aligned} \tag{6}$$

for all $[f], [f_1], [f_2] \in \tilde{\Gamma}$ (see e.g. [3]). The Weyl elements satisfy the “field equation” $W([\square_g + m^2]f) = W(0) = \mathbf{1}$. (In a regular representation we can think of the elements $W([f])$ as the unitary operators $e^{i\hat{\Phi}([f])}$ where $\hat{\Phi}([f])$ is the usual field operator smeared with test functions $f \in \mathcal{D}(\mathcal{M})$ and satisfying the field equation $(\square_g + m^2)\hat{\Phi}([f]) = \hat{\Phi}([\square_g + m^2]f) = 0$. (6) then corresponds to the canonical commutation relations.) A local subalgebra $\mathcal{A}(\mathcal{U})$ (\mathcal{U} an open bounded subset of \mathcal{M}) is then given by $\mathcal{A}[\tilde{\Gamma}(\mathcal{U}), \tilde{\sigma}]$. It is the C^* -algebra generated by the elements $W([f])$ with $\text{supp } f \subset \mathcal{U}$ and contains the quantum observables measurable in the spacetime region \mathcal{U} . Then $\mathcal{A}[\tilde{\Gamma}, \tilde{\sigma}] = C^*(\bigcup_{\mathcal{U}} \mathcal{A}(\mathcal{U}))$.

Dimock [13] has shown that $\mathcal{U} \mapsto \mathcal{A}(\mathcal{U})$ is a net of local observable algebras in the sense of Haag and Kastler [22], i.e. it satisfies

- (i) $\mathcal{U}_1 \subset \mathcal{U}_2 \Rightarrow \mathcal{A}(\mathcal{U}_1) \subset \mathcal{A}(\mathcal{U}_2)$ (isotony).
- (ii) \mathcal{U}_1 spacelike separated from $\mathcal{U}_2 \Rightarrow [\mathcal{A}(\mathcal{U}_1), \mathcal{A}(\mathcal{U}_2)] = \{0\}$ (locality).
- (iii) There is a faithful irreducible representation of \mathcal{A} (primitivity).
- (iv) $\mathcal{U}_1 \subset D(\mathcal{U}_2) \Rightarrow \mathcal{A}(\mathcal{U}_1) \subset \mathcal{A}(\mathcal{U}_2)$.
- (v) For any isometry $\kappa : (\mathcal{M}, g) \rightarrow (\mathcal{M}, g)$ there is an isomorphism $\alpha_\kappa : \mathcal{A} \rightarrow \mathcal{A}$ such that $\alpha_\kappa[\mathcal{A}(\mathcal{U})] = \mathcal{A}(\kappa(\mathcal{U}))$ and $\alpha_{\kappa_1} \circ \alpha_{\kappa_2} = \alpha_{\kappa_1 \circ \kappa_2}$ (covariance).

In (iv), $D(\mathcal{U})$ denotes the domain of dependence of $\mathcal{U} \subset \mathcal{M}$, i.e. the set of all points $x \in \mathcal{M}$ such that every inextendible causal curve through x passes through \mathcal{U} .

Since we are dealing with a linear field equation we can equivalently use the time zero algebras for the description of the quantum field theory. To this end we pick a Cauchy surface Σ with volume element $d^3\sigma := \sqrt{\mathfrak{h}} d^3x$, where $\mathfrak{h} := \det(h_{ij})$ and h_{ij} is the Riemannian metric induced on Σ by g , and define a classical phase space (Γ, σ) of the Klein-Gordon field by the space $\Gamma := \mathcal{D}(\Sigma) \oplus \mathcal{D}(\Sigma)$ of real-valued initial data with compact support and the real symplectic bilinear form

$$\begin{aligned} \sigma : \Gamma \times \Gamma &\rightarrow \mathbb{R} \\ (F_1, F_2) &\mapsto - \int_{\Sigma} [q_1 p_2 - q_2 p_1] d^3\sigma, \end{aligned} \quad (7)$$

$F_i := (q_i, p_i) \in \Gamma, i = 1, 2$. In this case, the local subspaces $\Gamma(\mathcal{O}) := \mathcal{D}(\mathcal{O}) \oplus \mathcal{D}(\mathcal{O})$ are associated to bounded open subsets $\mathcal{O} \subset \Sigma$. The next proposition establishes the equivalence between the two formulations of the phase space:

Proposition 2.2 *The spaces $(\Gamma(\mathcal{O}), \sigma)$ and $(\tilde{\Gamma}(D(\mathcal{O})), \tilde{\sigma})$ are symplectically isomorphic. The isomorphism is given by*

$$\begin{aligned} \rho_{\Sigma} : \tilde{\Gamma}(D(\mathcal{O})) &\rightarrow \Gamma(\mathcal{O}) \\ [f] &\mapsto (\rho_0 E f, \rho_1 E f). \end{aligned}$$

The proof of the proposition is a simple application of Proposition 2.1 and Eq. (5). It shows in particular that the symplectic form σ , Eq. (7), is independent of the choice of Cauchy surface Σ .

Now, to (Γ, σ) we can associate the Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ with its local subalgebras $\mathcal{A}(\mathcal{O}) := \mathcal{A}[\Gamma(\mathcal{O}), \sigma]$. By uniqueness, $\mathcal{A}(\mathcal{O})$ is isomorphic (as a C^* -algebra) to $\mathcal{A}(D(\mathcal{O}))$ which should justify our misuse of the same letter \mathcal{A} . The $*$ -isomorphism is explicitly given by

$$\alpha : \mathcal{A}(D(\mathcal{O})) \rightarrow \mathcal{A}(\mathcal{O}), \quad \alpha W([f]) := W(\rho_\Sigma([f])).$$

In the rest of the paper we will only have to deal with the net $\mathcal{O} \mapsto \mathcal{A}(\mathcal{O})$ of local time zero algebras, since they naturally occur when one discusses properties of a linear quantum field theory. Nevertheless, by the above isomorphism, one can translate all properties of this net easily into statements about the net $\mathcal{U} \mapsto \mathcal{A}(\mathcal{U})$ and vice versa. Let us only mention here that locality of the time zero algebras means that $[\mathcal{A}(\mathcal{O}_1), \mathcal{A}(\mathcal{O}_2)] = \{0\}$ if $\mathcal{O}_1 \cap \mathcal{O}_2 = \emptyset$.

The states on an observable algebra \mathcal{A} are the linear functionals $\omega : \mathcal{A} \rightarrow \mathbf{C}$ satisfying $\omega(\mathbf{1}) = 1$ (normalization) and $\omega(A^*A) \geq 0 \forall A \in \mathcal{A}$ (positivity). The set of states on our Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ is by far too large to be tractable in a concrete way. Therefore, for linear systems, one usually restricts oneself to the quasifree states, all of whose truncated n -point functions vanish for $n \neq 2$:

Definition 2.3 *Let $\mu : \Gamma \times \Gamma \rightarrow \mathbb{R}$ be a real scalar product satisfying*

$$\frac{1}{4} |\sigma(F_1, F_2)|^2 \leq \mu(F_1, F_1) \mu(F_2, F_2) \quad (8)$$

for all $F_1, F_2 \in \Gamma$. Then the **quasifree state** ω_μ associated with μ is given by

$$\omega_\mu(W(F)) = e^{-\frac{1}{2}\mu(F, F)}.$$

If ω_μ is pure it is called a **Fock state**.

The connection between this algebraic notion of a quasifree state and the usual notion of “vacuum state” in a Hilbert space is established by the following proposition which we cite from [32]:

Proposition 2.4 *Let ω_μ be a quasifree state on $\mathcal{A}[\Gamma, \sigma]$.*

(a) *There exists a **one-particle Hilbert space structure**, i.e. a Hilbert space \mathcal{H} and a real-linear map $k : \Gamma \rightarrow \mathcal{H}$ such that*

- (i) $k\Gamma + ik\Gamma$ is dense in \mathcal{H} ,
- (ii) $\mu(F_1, F_2) = \operatorname{Re}\langle kF_1, kF_2 \rangle_{\mathcal{H}} \forall F_1, F_2 \in \Gamma$,
- (iii) $\sigma(F_1, F_2) = 2\operatorname{Im}\langle kF_1, kF_2 \rangle_{\mathcal{H}} \forall F_1, F_2 \in \Gamma$.

The pair (k, \mathcal{H}) is uniquely determined up to unitary equivalence.

Moreover: ω_μ is pure $\Leftrightarrow k(\Gamma)$ is dense in \mathcal{H} .

(b) *The GNS-triple $(\mathcal{H}_{\omega_\mu}, \pi_{\omega_\mu}, \Omega_{\omega_\mu})$ of the state ω_μ can be represented as $(\mathcal{F}^s(\mathcal{H}), \rho_\mu, \Omega^{\mathcal{F}})$, where*

- (i) $\mathcal{F}^s(\mathcal{H})$ is the symmetric Fock space over the one-particle Hilbert space \mathcal{H} ,

(ii) $\rho_\mu[W(F)] = \exp\{-i\overline{[a^*(kF) + a(kF)]}\}$, where a^* and a are the standard creation and annihilation operators on $\mathcal{F}^s(\mathcal{H})$ satisfying

$$[a(u), a^*(v)] = \langle u, v \rangle_{\mathcal{H}} \text{ and } a(u)\Omega^{\mathcal{F}} = 0$$

for $u, v \in \mathcal{H}$. (The bar over $a^*(kF) + a(kF)$ indicates that we take the closure of this operator initially defined on the space of vectors of finite particle number.)

(iii) $\Omega^{\mathcal{F}} := \mathbf{1} \oplus \mathbf{0} \oplus \mathbf{0} \oplus \dots$ is the (cyclic) Fock vacuum.

Moreover: ω_μ is pure $\Leftrightarrow \rho_\mu$ is irreducible.

Thus, ω_μ can also be represented as $\omega_\mu(W(F)) = \exp\{-\frac{1}{2}\|kF\|_{\mathcal{H}}^2\}$ (by (a)) or $\omega_\mu(W(F)) = \langle \Omega^{\mathcal{F}}, \rho_\mu(F)\Omega^{\mathcal{F}} \rangle$ (by (b)). $\hat{\Phi}(F) := \overline{a^*(kF) + a(kF)}$ is the usual field operator on $\mathcal{F}^s(\mathcal{H})$ and we can determine the (“symplectically smeared”) two-point function as

$$\begin{aligned} \lambda(F_1, F_2) &= \langle \Omega^{\mathcal{F}}, \hat{\Phi}(F_1)\hat{\Phi}(F_2)\Omega^{\mathcal{F}} \rangle \\ &= \langle kF_1, kF_2 \rangle_{\mathcal{H}} \\ &= \mu(F_1, F_2) + \frac{i}{2}\sigma(F_1, F_2) \end{aligned} \quad (9)$$

for $F_1, F_2 \in \Gamma$, resp. the Wightman two-point function Λ as

$$\Lambda(f_1, f_2) = \lambda \left(\begin{pmatrix} \rho_0 E f_1 \\ \rho_1 E f_1 \end{pmatrix}, \begin{pmatrix} \rho_0 E f_2 \\ \rho_1 E f_2 \end{pmatrix} \right) \quad (10)$$

for $f_1, f_2 \in \mathcal{D}(\mathcal{M})$. The fact that the antisymmetric (= imaginary) part of λ is the symplectic form σ implies for Λ :

$$\begin{aligned} \text{Im } \Lambda(f_1, f_2) &= -\frac{1}{2} \int_{\Sigma} [f_1 E' \rho'_0 \rho_1 E f_2 - f_1 E' \rho'_1 \rho_0 E f_2] d^3\sigma \\ &= \frac{1}{2} \langle f_1, E f_2 \rangle \end{aligned} \quad (11)$$

by Eq. (5). All the other n -point functions can also be calculated, one finds that they vanish if n is odd and that the n -point functions for n even are sums of products of two-point functions.

Once a (quasifree) state ω on the algebra \mathcal{A} has been chosen the GNS-representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ of Proposition 2.4 allows us to represent all the algebras $\mathcal{A}(\mathcal{O})$ as concrete algebras $\pi_\omega(\mathcal{A}(\mathcal{O}))$ of bounded operators on \mathcal{H}_ω . The weak closure of $\pi_\omega(\mathcal{A}(\mathcal{O}))$ in $\mathcal{B}(\mathcal{H}_\omega)$, which, by von Neumann’s double commutant theorem, is equal to $\pi_\omega(\mathcal{A}(\mathcal{O}))''$ (the prime denoting the commutant of a subalgebra of $\mathcal{B}(\mathcal{H}_\omega)$), is denoted by $\mathcal{R}_\omega(\mathcal{O})$. It is the net of von Neumann algebras $\mathcal{O} \mapsto \mathcal{R}_\omega(\mathcal{O})$ which contains all the physical information of the theory and is therefore the main object of study in algebraic quantum field theory (see e.g. [21]). One of the most straightforward properties is the so-called additivity. It states that if an

open bounded subset $\mathcal{O} \subset \Sigma$ is the union of open subsets $\mathcal{O} = \bigcup_i \mathcal{O}_i$ then the von Neumann algebra $\mathcal{R}_\omega(\mathcal{O})$ is generated by the subalgebras $\mathcal{R}_\omega(\mathcal{O}_i)$, i.e.

$$\mathcal{R}_\omega(\mathcal{O}) = \left(\bigcup_i \mathcal{R}_\omega(\mathcal{O}_i) \right)'' . \quad (12)$$

Additivity expresses the fact that the physical information contained in $\mathcal{R}_\omega(\mathcal{O})$ is entirely encoded in the observables that are localized in arbitrarily small subsets of \mathcal{O} . The following result is well-known:

Lemma 2.5 *Let ω be a quasifree state of the Weyl algebra, \mathcal{O} an open bounded subset of Σ . Then $\mathcal{R}_\omega(\mathcal{O})$ is additive.*

Proof: Let (k, \mathcal{H}) be the one-particle Hilbert space structure of ω (Proposition 2.4). According to results of Araki [1, 34] Eq. (12) holds iff

$$\overline{k\Gamma(\mathcal{O})} = \overline{\text{span } k\Gamma(\mathcal{O}_i)} \quad (13)$$

where the closure is taken w.r.t. the norm in \mathcal{H} . With the help of a partition of unity $\{\chi_i; \text{supp } \chi_i \subset \mathcal{O}_i\}$ it is clear that any $u = k(F) \in k\Gamma(\mathcal{O})$, $F \in \Gamma(\mathcal{O})$, can be written as $u = \sum_i k(\chi_i F) \in \text{span } k\Gamma(\mathcal{O}_i)$ (note that the sum is finite since F has compact support in \mathcal{O}), and therefore $k\Gamma(\mathcal{O}) \subset \text{span } k\Gamma(\mathcal{O}_i)$. The converse inclusion is obvious, and therefore also (13) holds. \blacksquare

(More generally, additivity even holds for arbitrary states since already the Weyl algebra $\mathcal{A}(\mathcal{O})$ has an analogous property, cf. [3].) Other, more specific, properties of the net of von Neumann algebras will not hold in such general circumstances, but will depend on a judicious selection of (a class of) physically relevant states ω . For the choice of states we make in Section 3 we will investigate the properties of the local von Neumann algebras $\mathcal{R}_\omega(\mathcal{O})$ in Section 4.

3 Definition of adiabatic states

As we have seen in the last section, the algebra of observables can easily be defined on any globally hyperbolic spacetime manifold. This is essentially due to the fact that there is a well defined global causal structure on such a manifold, which allows to solve the classical Cauchy problem and formulate the canonical commutation relations, Eq.s (6) and (11). Symmetries of the spacetime do not play any role. This changes when one asks for the physical states of the theory. For quantum field theory on Minkowski space the state space is built on the vacuum state which is defined to be the Poincaré invariant state of lowest energy. A generic spacetime manifold however neither admits any symmetries nor the notion of energy, and it has always been the main problem of quantum field theory on curved spacetime to find a specification of the physical states of the theory in such a situation.

Using Hadamard's elementary solution of the wave equation DeWitt & Brehme [11] wrote down an asymptotic expansion of the singular kernel of a distribution which they called the Feynman propagator of a quantum field on a generic spacetime manifold. Since then quantum states whose two-point functions exhibit these prescribed local short-distance singularities have been called Hadamard states. Much work has been devoted to the investigation of the mathematical and physical properties of these states (for the literature see e.g. [32]), but only Kay & Wald [32] succeeded in giving a rigorous mathematical definition of them. Shortly later, in a seminal paper Radzikowski [41] found a characterization of the Hadamard states in terms of the wavefront set of their two-point functions. This result proved to be fundamental to all ensuing work on quantum field theory in gravitational background fields. Since we do not want to recall the old definition of Hadamard states (it does not play any role in this paper) we reformulate Radzikowski's main theorem as a *definition* of Hadamard states:

Definition 3.1 *A quasifree state ω_H on the Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ of the Klein-Gordon field on (\mathcal{M}, g) is called an **Hadamard state** if its two-point function is a distribution $\Lambda_H \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ that satisfies the following wavefront set condition*

$$WF'(\Lambda_H) = C^+. \quad (14)$$

Here, C^+ is the positive frequency component of the bicharacteristic relation $C = C^+ \dot{\cup} C^-$ that is associated to the principal symbol of the Klein-Gordon operator $\square_g + m^2$ (for this notion see [16]), more precisely

$$C := \{((x_1, \xi_1; x_2, \xi_2) \in T^*(\mathcal{M} \times \mathcal{M}) \setminus 0; g^{\mu\nu}(x_1)\xi_{1\mu}\xi_{1\nu} = 0, \\ g^{\mu\nu}(x_2)\xi_{2\mu}\xi_{2\nu} = 0, (x_1, \xi_1) \sim (x_2, \xi_2))\} \quad (15)$$

$$C^\pm := \{(x_1, \xi_1; x_2, \xi_2) \in C; \xi_1^0 \geq 0, \xi_2^0 \geq 0\} \quad (16)$$

where $(x_1, \xi_1) \sim (x_2, \xi_2)$ means that there is a null geodesic $\gamma : \tau \mapsto x(\tau)$ such that $x(\tau_1) = x_1, x(\tau_2) = x_2$ and $\xi_{1\nu} = \dot{x}^\mu(\tau_1)g_{\mu\nu}(x_1), \xi_{2\nu} = \dot{x}^\mu(\tau_2)g_{\mu\nu}(x_2)$, i.e. ξ_1, ξ_2 are cotangent to the null geodesic γ at x_1 resp. x_2 and parallel transports of each other along γ .

The fact that only positive frequencies occur in (14) can be viewed as a remnant of the spectrum condition in flat spacetime, therefore (14) (and its generalization to higher n -point functions in [8]) is also called microlocal spectrum condition. However, condition (14) does not fix a unique state, but a class of states that generate locally quasiequivalent GNS-representations [48].

Now to which extent is condition (14) also *necessary* to characterize locally quasiequivalent states? In [31] one of us gave a construction of Hadamard states by a microlocal separation of positive and negative frequency solutions of the Klein-Gordon equation. From these solutions we observed that a truncation of the corresponding asymptotic expansions destroys the microlocal spectrum condition (14) but preserves local quasiequivalence, at least if the Sobolev order of the perturbation is sufficiently low (for Dirac fields an analogous observation

was made by Hollands [24]). In other words, the positive frequency condition in (14) is not necessary to have local quasiequivalence, but can be perturbed by non-positive frequency or even non-local singularities of sufficiently low order. We formalize this observation by defining a new class of states with the help of the Sobolev (or H^s -) wavefront set. For a definition and explanation of this notion see Appendix B.

Definition 3.2 *A quasifree state ω_N on the Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ of the Klein-Gordon field on (\mathcal{M}, g) is called an **adiabatic state of order $N \in \mathbb{R}$** if its two-point function Λ_N is a distribution that satisfies the following H^s -wavefront set condition for all $s < N + \frac{3}{2}$*

$$WF'^s(\Lambda_N) \subset C^+. \quad (17)$$

Note, that we did not specify WF'^s for $s \geq N + \frac{3}{2}$ in the definition. Hence every adiabatic state of order N is also one of order $N' \leq N$. In particular, every Hadamard state is also an adiabatic state (of any order). Now the task is to identify those adiabatic states that are physically admissible, i.e. generate the same local quasiequivalence class as the Hadamard states. In [31, Section 3.6] an example of an adiabatic state of order -1 was given that does not satisfy this condition. In Theorem 4.7 we will prove that for $N > 5/2$ (and in the special case of pure states on a spacetime with compact Cauchy surface already for $N > 3/2$) the condition is satisfied (and the gap in between will remain unexplored in this paper). For this purpose the following simple lemma will be fundamental:

Lemma 3.3 *Let Λ_H and Λ_N be the two-point functions of an arbitrary Hadamard state and an adiabatic state of order N , respectively, of the Klein-Gordon field on (\mathcal{M}, g) . Then*

$$WF^s(\Lambda_H - \Lambda_N) = \emptyset \quad \forall s < N + \frac{3}{2}. \quad (18)$$

Proof: From Lemma 5.2 it follows that

$$WF'^s(\Lambda_H) = \begin{cases} \emptyset, & s < -\frac{1}{2} \\ C^+, & -\frac{1}{2} \leq s \end{cases}$$

and therefore

$$WF'^s(\Lambda_H - \Lambda_N) \subset WF'^s(\Lambda_H) \cup WF'^s(\Lambda_N) \subset C^+, \quad s < N + \frac{3}{2}. \quad (19)$$

On the other hand, since Λ_H and Λ_N have the same antisymmetric part $\tilde{\sigma}$, $\Lambda_H - \Lambda_N$ must be a symmetric distribution, and thus also $WF^s(\Lambda_H - \Lambda_N)$ must be a symmetric subset of $T^*(\mathcal{M} \times \mathcal{M})$, i.e. $WF'^s(\Lambda_H - \Lambda_N)$ antisymmetric. However, the only antisymmetric subset of the right hand side of (19) is the empty set and hence $WF^s(\Lambda_H - \Lambda_N) = \emptyset$ for $s < N + \frac{3}{2}$. ■

In the next section we will use this lemma to prove the result mentioned above and some other algebraic properties of the Hilbert space representations generated by our new states.

In Section 5 we will explicitly construct these states and in Section 6 we will show that the old and well-known class of adiabatic vacuum states on Robertson-Walker spacetimes satisfies our Definition 3.2 (the comparison with the order of these states led us to the normalization of s chosen in Definition 3.2). Contrary to an erroneous claim in [31], these states are in general no Hadamard states, but in fact “adiabatic states” in our sense. This justifies our naming of the new class of quantum states on curved spacetimes in Definition 3.2.

4 The algebraic structure of adiabatic vacuum representations

4.1 Primarity and local quasiequivalence of adiabatic and Hadamard states

Let $\mathcal{A} := \mathcal{A}[\Gamma, \sigma]$ be the Weyl algebra associated to our phase space (Γ, σ) introduced in Section 2 and $\mathcal{A}(\mathcal{O}) := \mathcal{A}[\Gamma(\mathcal{O}), \sigma]$ the subalgebra of observables localized in an open, relatively compact subset $\mathcal{O} \subset \Sigma$. Let ω_H denote some Hadamard state on \mathcal{A} and ω_N an adiabatic vacuum state of order N . It is the main aim of this section to show that ω_H and ω_N are locally quasiequivalent states for all sufficiently large N , i.e. the GNS-representations π_{ω_H} and π_{ω_N} are quasiequivalent when restricted to $\mathcal{A}(\mathcal{O})$, or, equivalently, there is an isomorphism τ between the von Neumann algebras $\pi_{\omega_H}(\mathcal{A}(\mathcal{O}))''$ and $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ such that $\tau \circ \pi_{\omega_H} = \pi_{\omega_N}$ on $\mathcal{A}(\mathcal{O})$ (see e.g. [6, Section 2.4]).

To prove this statement we will proceed as follows: We first notice that $\pi_{\omega_H} \upharpoonright \mathcal{A}(\mathcal{O})$ is quasiequivalent to $\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O})$ if $\pi_{\omega_H} \upharpoonright \mathcal{A}(\tilde{\mathcal{O}})$ is quasiequivalent to $\pi_{\omega_N} \upharpoonright \mathcal{A}(\tilde{\mathcal{O}})$ for some $\tilde{\mathcal{O}} \supset \mathcal{O}$. Since to any open, relatively compact set \mathcal{O} we can find an open, relatively compact set $\tilde{\mathcal{O}}$ containing \mathcal{O} and having a smooth boundary we can assume without loss of generality that \mathcal{O} has a smooth boundary. Under this assumption we first show that $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ is a factor (for $N > 3/2$, Theorem 4.5). Now we note that the GNS-representation $(\pi_{\tilde{\omega}}, \mathcal{H}_{\tilde{\omega}}, \Omega_{\tilde{\omega}})$ of the partial state $\tilde{\omega} := \omega_N \upharpoonright \mathcal{A}(\mathcal{O})$ is a subrepresentation of $(\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O}), \mathcal{H}_{\omega_N}, \Omega_{\omega_N})$. This is easy to see: $\mathcal{K} := \overline{\{\pi_{\omega_N}(A)\Omega_{\omega_N}; A \in \mathcal{A}(\mathcal{O})\}}$ is a closed subspace of \mathcal{H}_{ω_N} which is left invariant by $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))$. Since for all $A \in \mathcal{A}(\mathcal{O})$

$$(\Omega_{\tilde{\omega}}, \pi_{\tilde{\omega}}(A)\Omega_{\tilde{\omega}}) = \tilde{\omega}(A) = \omega_N(A) = (\Omega_{\omega_N}, \pi_{\omega_N}(A)\Omega_{\omega_N}),$$

the uniqueness of the GNS-representation implies that $\pi_{\tilde{\omega}}$ and $\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O})$ coincide on \mathcal{K} and $(\pi_{\tilde{\omega}}, \mathcal{H}_{\tilde{\omega}}, \Omega_{\tilde{\omega}})$ can be identified with $(\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O}), \mathcal{K}, \Omega_{\omega_N})$ (up to unitary equivalence).

We recall that a primary representation (which means that the corresponding von Neumann algebra is a factor) is quasiequivalent to all its (non-trivial) subrepresentations (see [14, Prop. 5.3.5]). Therefore, $\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O})$ is quasiequivalent to $\pi_{\tilde{\omega}} = \pi_{(\omega_N \upharpoonright \mathcal{A}(\mathcal{O}))}$, and analogously $\pi_{\omega_H} \upharpoonright \mathcal{A}(\mathcal{O})$ is quasiequivalent to $\pi_{(\omega_H \upharpoonright \mathcal{A}(\mathcal{O}))}$. To prove that $\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O})$ and $\pi_{\omega_H} \upharpoonright \mathcal{A}(\mathcal{O})$ are quasiequivalent it is therefore sufficient to prove the quasiequivalence of the GNS-representations $\pi_{(\omega_N \upharpoonright \mathcal{A}(\mathcal{O}))}$ and $\pi_{(\omega_H \upharpoonright \mathcal{A}(\mathcal{O}))}$ of the partial states. This will be done in Theorem

4.7 for $N > 5/2$.

To get started we have to prove in a first step that the real scalar products μ_N and μ_H associated to the states ω_N and ω_H , respectively, induce the same topology on $\Gamma(\mathcal{O}) = \mathcal{C}_0^\infty(\mathcal{O}) \oplus \mathcal{C}_0^\infty(\mathcal{O})$. Let us denote by $\mathcal{H}_{\mu_N}(\mathcal{O})$ and $\mathcal{H}_{\mu_H}(\mathcal{O})$ the completion of $\Gamma(\mathcal{O})$ w.r.t. μ_N and μ_H , respectively. R. Verch showed the following result [49, Prop. 3.5]:

Proposition 4.1 *For every open, relatively compact set $\mathcal{O} \subset \Sigma$ there exist positive constants C_1, C_2 such that*

$$C_1 \left(\|q\|_{H^{1/2}(\mathcal{O})}^2 + \|p\|_{H^{-1/2}(\mathcal{O})}^2 \right) \leq \mu_H \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) \leq C_2 \left(\|q\|_{H^{1/2}(\mathcal{O})}^2 + \|p\|_{H^{-1/2}(\mathcal{O})}^2 \right)$$

for all $\begin{pmatrix} q \\ p \end{pmatrix} \in \Gamma(\mathcal{O})$.

Theorem 4.2 *The topology of $\mathcal{H}_{\mu_N}(\mathcal{O})$ coincides with that of $\mathcal{H}_{\mu_H}(\mathcal{O})$ whenever Λ_N satisfies (17) for $N > 3/2$.*

Proof: If (Σ, h) is not a complete Riemannian manifold we can find a function $f \in \mathcal{C}^\infty(\Sigma)$, $f > 0$, with $f|_{\overline{\mathcal{O}}} = \text{const.}$ such that $(\Sigma, \tilde{h} := fh)$ is complete [12, Ch. XX.18, Problem 6]. Then the Laplace-Beltrami operator $\Delta_{\tilde{h}}$ associated with \tilde{h} is essentially selfadjoint on $\mathcal{C}_0^\infty(\Sigma)$ [9]. The topology on $\Gamma(\mathcal{O})$ will not be affected by switching from h to \tilde{h} . Without loss of generality we can therefore assume that Δ is selfadjoint. Lemma 3.3 shows that

$$\Lambda_H - \Lambda_N \in H_{loc}^s(\mathcal{M} \times \mathcal{M}) \quad \forall s < N + \frac{3}{2}.$$

In view of the fact that Σ is a hyperplane, Proposition B.7 implies that, for $1 < s < N + 3/2$,

$$(\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} \in H_{loc}^{s-1}(\Sigma \times \Sigma) \quad (20)$$

$$\partial_{n_1}(\Lambda_H - \Lambda_N), \partial_{n_2}(\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} \in H_{loc}^{s-2}(\Sigma \times \Sigma) \quad (21)$$

$$\partial_{n_1} \partial_{n_2}(\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} \in H_{loc}^{s-3}(\Sigma \times \Sigma). \quad (22)$$

Here, ∂_{n_1} and ∂_{n_2} denote the normal derivatives with respect to the first and second variable, respectively. We denote by λ_H and λ_N the scalar products on Γ induced via Eq. (10) by Λ_H and Λ_N , respectively. Since Λ_H and Λ_N have the same antisymmetric parts we have

$$(\mu_H - \mu_N) \left(\begin{pmatrix} q_1 \\ p_1 \end{pmatrix}, \begin{pmatrix} q_2 \\ p_2 \end{pmatrix} \right) = (\lambda_H - \lambda_N) \left(\begin{pmatrix} q_1 \\ p_1 \end{pmatrix}, \begin{pmatrix} q_2 \\ p_2 \end{pmatrix} \right) = \left\langle \begin{pmatrix} q_1 \\ p_1 \end{pmatrix}, \mathbb{M} \begin{pmatrix} q_2 \\ p_2 \end{pmatrix} \right\rangle_{L^2(\Sigma) \oplus L^2(\Sigma)} \quad (23)$$

for $\begin{pmatrix} q_1 \\ p_1 \end{pmatrix}, \begin{pmatrix} q_2 \\ p_2 \end{pmatrix} \in \Gamma$, where \mathbb{M} is the integral operator with the kernel function

$$M(x, y) = \begin{pmatrix} \partial_{n_1} \partial_{n_2}(\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} & -\partial_{n_1}(\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} \\ -\partial_{n_2}(\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} & (\Lambda_H - \Lambda_N)|_{\Sigma \times \Sigma} \end{pmatrix}. \quad (24)$$

Note that $M(x, y) = M(y, x)^*$. We next fix a neighborhood $\tilde{\mathcal{O}}$ of \mathcal{O} and a function $K = K(x, y) \in \mathcal{C}_0^\infty(\Sigma \times \Sigma)$ taking values in 2×2 real matrices such that $K(x, y) = K(y, x)^*$, $x, y \in \Sigma$, and the entries K_{ij} of K and M_{ij} of M satisfy the relations

$$\begin{aligned} \|K_{11} - M_{11}\|_{L^2(\tilde{\mathcal{O}} \times \tilde{\mathcal{O}})} &< \epsilon & \|K_{12} - M_{12}\|_{H^{1/2}(\tilde{\mathcal{O}} \times \tilde{\mathcal{O}})} &< \epsilon \\ \|K_{21} - M_{21}\|_{H^{1/2}(\tilde{\mathcal{O}} \times \tilde{\mathcal{O}})} &< \epsilon & \|K_{22} - M_{22}\|_{H^1(\tilde{\mathcal{O}} \times \tilde{\mathcal{O}})} &< \epsilon, \end{aligned} \quad (25)$$

where $\epsilon > 0$ is to be specified later on. By \mathbb{K} we denote the integral operator induced by K . We let

$$\begin{aligned} \mu'_N &:= \mu_H + \langle \cdot, (\mathbb{K} - \mathbb{M}) \cdot \rangle = \mu_N + \langle \cdot, \mathbb{K} \cdot \rangle \\ \lambda'_N &:= \mu'_N + \frac{i}{2} \sigma. \end{aligned}$$

By Λ'_N we denote the associated bilinear form on $\mathcal{C}_0^\infty(\mathcal{M}) \times \mathcal{C}_0^\infty(\mathcal{M})$

$$\Lambda'_N(f, g) := \lambda'_N \left(\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} Ef, \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} Eg \right) \quad (26)$$

(note that, in spite of our notation, Λ'_N is not the two-point function of a quasifree state in general). Recall from (3) that ρ_0, ρ_1 are the usual restriction operators. The definition of Λ'_N makes sense, since both $\rho_0 Eg$ and $\rho_1 Eg$ have compact support in Σ so that λ'_N can be applied. In view of the fact that \mathbb{K} is an integral operator with a smooth kernel, also $\lambda'_N - \lambda_N = \mu'_N - \mu_N$ is given by a smooth kernel. We claim that also $\Lambda'_N - \Lambda_N$ is smooth on $\mathcal{M} \times \mathcal{M}$: In fact,

$$(\Lambda'_N - \Lambda_N)(f, g) = \left\langle \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} Ef, \mathbb{K} \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} Eg \right\rangle$$

is given by the Schwartz kernel

$$\left(\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} E \right)^* K \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} E.$$

Since E is a Lagrangian distribution of order $\mu = -3/2$ (for more details see Section 5 below), while K is a compactly supported smooth function, the calculus of Fourier integral operators [28, Thm.s 25.2.2, 25.2.3] show that the composition is also smooth.

It follows from an argument of Verch [48, Prop. 3.8] that there are functions $\phi_j, \psi_j \in \mathcal{C}_0^\infty(\mathcal{M})$, $j = 1, 2, \dots$, such that

$$\Lambda'_N(f, g) - \Lambda_N(f, g) = \sum_{j=1}^{\infty} \sigma(f, \phi_j) \sigma(g, \psi_j)$$

for all $f, g \in \mathcal{C}_0^\infty(D(\mathcal{O}))$, satisfying moreover

$$\sum_{j=1}^{\infty} \Lambda_N(\phi_j, \phi_j)^{1/2} \Lambda_N(\psi_j, \psi_j)^{1/2} < \infty.$$

(An inspection of the proof of [48, Prop. 3.8] shows that it is sufficient for the validity of these statements that Λ_N is the two-point function of a quasifree state, Λ'_N need not be one.) It follows that

$$\begin{aligned}
|\Lambda'_N(f, f) - \Lambda_N(f, f)| &\leq \sum_j |\sigma(f, \phi_j)\sigma(f, \psi_j)| \\
&\leq \sum_j 4\Lambda_N(f, f)^{1/2}\Lambda_N(\phi_j, \phi_j)^{1/2}\Lambda_N(f, f)^{1/2}\Lambda_N(\psi_j, \psi_j)^{1/2} \\
&= 4\Lambda_N(f, f) \sum_j \Lambda_N(\phi_j, \phi_j)^{1/2}\Lambda_N(\psi_j, \psi_j)^{1/2} \\
&\leq C\Lambda_N(f, f).
\end{aligned}$$

Therefore

$$|\Lambda'_N(f, f)| \leq (1 + C)\Lambda_N(f, f).$$

Given $q, p \in \mathcal{C}_0^\infty(\mathcal{O})$, we can find $f \in \mathcal{C}_0^\infty(D(\mathcal{O}))$ such that $q = \rho_0 Ef$, $p = \rho_1 Ef$ (cf. Proposition 2.1). Hence

$$\begin{aligned}
\mu'_N \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) &= \lambda'_N \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) = \Lambda'_N(f, f) \leq (1 + C)\Lambda_N(f, f) \\
&= (1 + C)\lambda_N \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) = (1 + C)\mu_N \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right). \quad (27)
\end{aligned}$$

We next claim that for all $\begin{pmatrix} q \\ p \end{pmatrix} \in \Gamma(\mathcal{O})$

$$\left| \left\langle \begin{pmatrix} q \\ p \end{pmatrix}, \mathbb{M} \begin{pmatrix} q \\ p \end{pmatrix} \right\rangle \right| \leq C_3 \left(\|q\|_{H^{1/2}(\mathcal{O})}^2 + \|p\|_{H^{-1/2}(\mathcal{O})}^2 \right) \quad (28)$$

and

$$\left| \left\langle \begin{pmatrix} q \\ p \end{pmatrix}, (\mathbb{K} - \mathbb{M}) \begin{pmatrix} q \\ p \end{pmatrix} \right\rangle \right| \leq C_\epsilon \left(\|q\|_{H^{1/2}(\mathcal{O})}^2 + \|p\|_{H^{-1/2}(\mathcal{O})}^2 \right), \quad (29)$$

where C_3 and C_ϵ are positive constants and C_ϵ can be made arbitrarily small by taking ϵ small in (25). Indeed, in order to see this, we may first multiply the kernel functions M and $K - M$, respectively, by $\varphi(x)\varphi(y)$ where φ is a smooth function supported in the neighborhood $\tilde{\mathcal{O}}$ of \mathcal{O} and $\varphi \equiv 1$ on \mathcal{O} . The above expressions (28) and (29) will not be affected by this change. We may then localize the kernel functions to $\mathbb{R}^3 \times \mathbb{R}^3$ noting that the Sobolev regularity is preserved. Now we can apply Lemma 4.3 and Corollary 4.4 to derive (28) and (29).

We finally obtain the statement of the theorem from the estimates

$$\begin{aligned}
\frac{C_1}{2} (\|q\|_{H^{1/2}(\mathcal{O})} + \|p\|_{H^{-1/2}(\mathcal{O})}) &\leq (C_1 - C_\epsilon) (\|q\|_{H^{1/2}(\mathcal{O})} + \|p\|_{H^{-1/2}(\mathcal{O})}) \\
&\quad \text{if } \epsilon \text{ is sufficiently small} \\
&\leq \mu_H \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) + \left\langle \begin{pmatrix} q \\ p \end{pmatrix}, (\mathbb{K} - \mathbb{M}) \begin{pmatrix} q \\ p \end{pmatrix} \right\rangle
\end{aligned}$$

$$\begin{aligned}
& \text{by Prop. 4.1 and (29)} \\
&= \mu'_N \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) \\
&\leq (1+C)\mu_N \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) \quad \text{by (27)} \\
&= (1+C) \left(\mu_H \left(\begin{pmatrix} q \\ p \end{pmatrix}, \begin{pmatrix} q \\ p \end{pmatrix} \right) - \left\langle \begin{pmatrix} q \\ p \end{pmatrix}, \mathbb{M} \begin{pmatrix} q \\ p \end{pmatrix} \right\rangle \right) \\
&\leq (1+C)(C_2 + C_3) (\|q\|_{H^{1/2}(\mathcal{O})} + \|p\|_{H^{-1/2}(\mathcal{O})}) \\
&\quad \text{by Prop. 4.1 and (28)}.
\end{aligned}$$

■

Lemma 4.3 *Let $k \in H^{1/2}(\mathbb{R}^n \times \mathbb{R}^n)$. Then the integral operator \mathbb{K} with kernel k induces an operator in $\mathcal{B}(H^{1/2}(\mathbb{R}^n), H^{1/2}(\mathbb{R}^n))$ and $\mathcal{B}(H^{-1/2}(\mathbb{R}^n), H^{-1/2}(\mathbb{R}^n))$. If we even have $k \in H^1(\mathbb{R}^n \times \mathbb{R}^n)$, then \mathbb{K} induces an operator in $\mathcal{B}(H^{-1/2}(\mathbb{R}^n), H^{1/2}(\mathbb{R}^n))$. In both cases, the operator norm of \mathbb{K} can be estimated by the Sobolev norm of k .*

Proof: The boundedness of $\mathbb{K} : H^{\pm 1/2} \rightarrow H^{\pm 1/2}$ is equivalent to the boundedness of $\mathbb{L} := \langle D \rangle^{\pm 1/2} \mathbb{K} \langle D \rangle^{\mp 1/2}$ on $L^2(\mathbb{R}^n)$. (Here $\langle D \rangle^{\pm 1/2} := (1 - \Delta)^{\pm 1/4}$, where Δ is the Euclidean Laplacian.) This in turn will be true, if its integral kernel $l(x, y) := \langle D_x \rangle^{\pm 1/2} \langle D_y \rangle^{\mp 1/2} k(x, y)$ is in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$. In this case

$$\|\mathbb{L}\|_{\mathcal{B}(L^2(\mathbb{R}^n))} \leq \|l\|_{L^2(\mathbb{R}^n \times \mathbb{R}^n)}.$$

We know that $\langle D_x \rangle^{\pm 1/2} \langle D_y \rangle^{\mp 1/2}$ are pseudodifferential operators on $\mathbb{R}^n \times \mathbb{R}^n$ with symbols in $S_{0,0}^{1/2}(\mathbb{R}^{2n} \times \mathbb{R}^{2n})$. By Calderón and Vaillancourt's Theorem (cf. [33, Thm. 7.1.6]), they yield bounded maps $H^{1/2}(\mathbb{R}^n \times \mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n \times \mathbb{R}^n)$. Hence $l \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$ and we obtain the first assertion. For the second assertion we check that $\langle D_x \rangle^{1/2} \langle D_y \rangle^{1/2} k(x, y) \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$. Since the symbol of $\langle D_x \rangle^{1/2} \langle D_y \rangle^{1/2}$ is in $S_{0,0}^1(\mathbb{R}^{2n} \times \mathbb{R}^{2n})$, this holds whenever $k \in H^1$. ■

Corollary 4.4 *If*

$$k = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix}$$

with

$$k_{11} \in L^2(\mathbb{R}^n \times \mathbb{R}^n), \quad k_{12}, k_{21} \in H^{1/2}(\mathbb{R}^n \times \mathbb{R}^n), \quad k_{22} \in H^1(\mathbb{R}^n \times \mathbb{R}^n),$$

then the integral operator \mathbb{K} with kernel k induces a bounded map

$$H^{1/2}(\mathbb{R}^n) \oplus H^{-1/2}(\mathbb{R}^n) \rightarrow H^{-1/2}(\mathbb{R}^n) \oplus H^{1/2}(\mathbb{R}^n).$$

Given $(q, p) \in \mathcal{C}_0^\infty(\mathbb{R}^n) \oplus \mathcal{C}_0^\infty(\mathbb{R}^n)$ we can estimate

$$\left| \left\langle \begin{pmatrix} q \\ p \end{pmatrix}, \mathbb{K} \begin{pmatrix} q \\ p \end{pmatrix} \right\rangle_{L^2 \oplus L^2} \right| \leq \left\| \begin{pmatrix} q \\ p \end{pmatrix} \right\|_{H^{1/2} \oplus H^{-1/2}} \left\| \mathbb{K} \begin{pmatrix} q \\ p \end{pmatrix} \right\|_{H^{-1/2} \oplus H^{1/2}} \leq \|\mathbb{K}\| \left\| \begin{pmatrix} q \\ p \end{pmatrix} \right\|_{H^{1/2} \oplus H^{-1/2}}^2.$$

(Here we used the fact that, for $u \in H^s(\mathbb{R}^n)$ and $v \in H^{-s}(\mathbb{R}^n)$, $\langle u, v \rangle$ can be understood as the extension of the L^2 bilinear form and $|\langle u, v \rangle| \leq \|u\|_{H^s} \|v\|_{H^{-s}}$.)

We now apply Theorem 4.2 to show that adiabatic vacua (of order $N > 3/2$) generate primary representations. The proof is a modification of the corresponding argument for Hadamard states due to Verch [48].

Theorem 4.5 *Let ω_N be an adiabatic vacuum state of order $N > 3/2$ on the Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ of the Klein-Gordon field on (\mathcal{M}, g) and π_{ω_N} its GNS-representation. Then, for any open, relatively compact subset $\mathcal{O} \subset \Sigma$ with smooth boundary, $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ is a factor.*

In the proof of the theorem we will need the following lemma. Recall that the metric \tilde{h} introduced in the proof of Theorem 4.2 differs from h only by a conformal factor which is constant on \mathcal{O} .

Lemma 4.6 $\mathcal{C}_0^\infty(\mathcal{O}) + \mathcal{C}_0^\infty(\Sigma \setminus \overline{\mathcal{O}})$ is dense in $\mathcal{C}_0^\infty(\Sigma)$ w.r.t. the norm of $H^{1/2}(\Sigma, \tilde{h})$ (and hence also w.r.t. the norm of $H^{-1/2}(\Sigma, \tilde{h})$).

Proof: Using a partition of unity we see that the problem is local. We can therefore confine ourselves to a single relatively compact coordinate neighborhood and work on Euclidean space. In view of the fact that \tilde{h} is positive definite, the topology of the Sobolev spaces on Σ locally yields the usual Sobolev topology. The problem therefore reduces to showing that every function in $\mathcal{C}_0^\infty(\mathbb{R}^n)$, $n \in \mathbb{N}$, can be approximated by functions in $\mathcal{C}_0^\infty(\mathbb{R}_+^n) + \mathcal{C}_0^\infty(\mathbb{R}_-^n)$ in the topology of $H^{1/2}(\mathbb{R}^n)$. Following essentially a standard argument [45, 2.9.3] we proceed as follows. We choose a function $\chi \in \mathcal{C}^\infty(\mathbb{R})$ with $\chi(t) = 1$ for $|t| \geq 2$ and $\chi(t) = 0$ for $|t| \leq 1$, $0 \leq \chi \leq 1$. We define $\chi_\epsilon : \mathbb{R}^n \rightarrow \mathbb{R}$ by $\chi_\epsilon(x) := \chi(x_n/\epsilon)$. Given $f \in \mathcal{C}_0^\infty(\mathbb{R}^n)$ we have

$$\begin{aligned} \|f - \chi_\epsilon f\|_{L^2(\mathbb{R}^n)} &\leq C_1 \sqrt{\epsilon} \\ \|f - \chi_\epsilon f\|_{H^1(\mathbb{R}^n)} &\leq \frac{C_2}{\sqrt{\epsilon}}. \end{aligned}$$

Interpolation shows that $\{f - \chi_\epsilon f\}_{0 < \epsilon < 1}$ is bounded in $H^{1/2}(\mathbb{R}^n)$ [45, Thm. 1.9.3]. Since $H^{1/2}$ is a reflexive space, there is a sequence $\epsilon_j \rightarrow 0$ such that $f - \chi_{\epsilon_j} f$ converges weakly [51, Thm. V.2.1]. The limit necessarily is zero, since it is zero in L^2 . According to Mazur's Theorem [51, Thm. V.1.2] there is, for each $\delta > 0$, a finite convex combination $\sum_{j=1}^k \alpha_j (f - \chi_{\epsilon_j} f)$ (with $\alpha_j \geq 0$, $\sum_{j=1}^k \alpha_j = 1$) such that

$$\left\| \sum_{j=1}^k \alpha_j (f - \chi_{\epsilon_j} f) - 0 \right\|_{H^{1/2}} < \delta.$$

Since $\sum \alpha_j \chi_{\epsilon_j} f \in \mathcal{C}_0^\infty(\mathbb{R}_+^n) + \mathcal{C}_0^\infty(\mathbb{R}_-^n)$, the proof is complete. \blacksquare

Proof of Theorem 4.5: Let (k_N, \mathcal{H}_N) be the one-particle Hilbert space structure of ω_N , let

$$k_N(\Gamma(\mathcal{O}))^\vee := \{u \in \mathcal{H}_N; \operatorname{Im} \langle u, v \rangle_{\mathcal{H}_N} = 0 \forall v \in k_N(\Gamma(\mathcal{O}))\} \quad (30)$$

denote the symplectic complement of $k_N(\Gamma(\mathcal{O}))$. It is a closed, real subspace of \mathcal{H}_N . According to results of Araki [1, 34] $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ is a factor iff

$$\overline{k_N(\Gamma(\mathcal{O}))} \cap k_N(\Gamma(\mathcal{O}))^\vee = \{0\}, \quad (31)$$

where the closure is taken w.r.t. the norm in \mathcal{H}_N .

In a first step we prove (31) for the one-particle Hilbert space structure $(\tilde{k}, \tilde{\mathcal{H}})$ of an auxiliary quasifree state on $\mathcal{A}[\Gamma, \tilde{\sigma}]$, where $\tilde{\sigma}$ is the symplectic form w.r.t. the metric \tilde{h} ,

$$\begin{aligned} \tilde{k} : \Gamma &\rightarrow L^2(\Sigma, \tilde{h}) =: \tilde{\mathcal{H}} \\ \begin{pmatrix} q \\ p \end{pmatrix} &\mapsto \frac{1}{\sqrt{2}} (i\langle D \rangle^{1/2} q + \langle D \rangle^{-1/2} p) \end{aligned} \quad (32)$$

(which, in general, induces neither an Hadamard state nor an admissible adiabatic vacuum state). As before, $\langle D \rangle := (1 - \Delta_{\tilde{h}})^{1/2}$. Since $\Delta_{\tilde{h}}$ is essentially selfadjoint on $\mathcal{C}_0^\infty(\Sigma)$, $\sqrt{2}\tilde{k}(\Gamma) = i\langle D \rangle^{1/2}\mathcal{C}_0^\infty(\Sigma) + \langle D \rangle^{-1/2}\mathcal{C}_0^\infty(\Sigma)$ is dense in $L^2(\Sigma, \tilde{h})$ (since $\mathcal{C}_0^\infty(\Sigma)$ is dense in $H^{1/2}(\Sigma)$ as well as in $H^{-1/2}(\Sigma)$), i.e. \tilde{k} describes a pure state.

Note that locally, i.e. on $\Gamma(\mathcal{O})$, the norm given by

$$\tilde{\mu}(F, F) := \langle \tilde{k}F, \tilde{k}F \rangle_{\tilde{\mathcal{H}}} = \frac{1}{2} [\|\langle D \rangle^{1/2} q\|_{\tilde{\mathcal{H}}}^2 + \|\langle D \rangle^{-1/2} p\|_{\tilde{\mathcal{H}}}^2], \quad F := (q, p) \in \Gamma(\mathcal{O}), \quad (33)$$

is independent of the choice of metric and hence equivalent to the norm of $H^{1/2}(\mathcal{O}) \oplus H^{-1/2}(\mathcal{O})$. Also, since the conformal factor f satisfies $f = C > 0$ on $\overline{\mathcal{O}}$, we have

$$\begin{aligned} \tilde{\sigma}(F_1, F_2) &= 2\text{Im}\langle \tilde{k}F_1, \tilde{k}F_2 \rangle_{\tilde{\mathcal{H}}} = \int_{\mathcal{O}} d^3\sigma_{\tilde{h}} (p_1q_2 - q_1p_2) \\ &= C^{3/2} \int_{\mathcal{O}} d^3\sigma_h (p_1q_2 - q_1p_2) = C^{3/2}\sigma(F_1, F_2) \end{aligned}$$

for all $F_i = (q_i, p_i) \in \Gamma(\mathcal{O}), i = 1, 2$.

Define now $\tilde{k}(\Gamma(\mathcal{O}))^\vee := \{u \in \tilde{\mathcal{H}}; \text{Im}\langle u, v \rangle_{\tilde{\mathcal{H}}} = 0 \forall v \in \tilde{k}(\Gamma(\mathcal{O}))\}$ and let $u \in \overline{\tilde{k}(\Gamma(\mathcal{O}))} \cap \tilde{k}(\Gamma(\mathcal{O}))^\vee$. Then $\text{Im}\langle u, \tilde{k}(F) \rangle_{\tilde{\mathcal{H}}} = 0$ for all $F \in \Gamma(\mathcal{O})$ (by the definition of $\tilde{k}(\Gamma(\mathcal{O}))^\vee$) and also $\text{Im}\langle u, \tilde{k}(F) \rangle_{\tilde{\mathcal{H}}} = 0$ for all $F \in \Gamma(\Sigma \setminus \overline{\mathcal{O}})$ (since $\tilde{k}(F) \in \tilde{k}(\Gamma(\mathcal{O}))^\vee$ for $F \in \Gamma(\Sigma \setminus \overline{\mathcal{O}})$). This, together with the density statement of Lemma 4.6, implies that $\text{Im}\langle u, \tilde{k}(F) \rangle_{\tilde{\mathcal{H}}} = 0$ for all $F \in \Gamma$, and, since $\tilde{k}(\Gamma)$ is dense in $\tilde{\mathcal{H}}$, it follows that $u = 0$, i.e. (31) is proven for the auxiliary state given by \tilde{k} on $\mathcal{A}[\Gamma, \tilde{\sigma}]$.

Let us now show (31) for an adiabatic vacuum state $\omega_N, N > 3/2$, on $\mathcal{A}[\Gamma, \sigma]$. Let $u \in \overline{k_N(\Gamma(\mathcal{O}))} \cap k_N(\Gamma(\mathcal{O}))^\vee$, then there is a sequence $\{F_n, n \in \mathbb{N}\} \subset \Gamma(\mathcal{O})$ with $k_N(F_n) \rightarrow u$ in \mathcal{H}_N . Of course, $k_N(F_n)$ is in particular a Cauchy sequence in \mathcal{H}_N , i.e.

$$\mu_N(F_n - F_m, F_n - F_m) = \|k_N(F_n) - k_N(F_m)\|_{\mathcal{H}_N}^2 \rightarrow 0.$$

By Theorem 4.2, the norm given by $\mu_N, N > 3/2$, on $\Gamma(\mathcal{O})$ is equivalent to the norm given by $\tilde{\mu}$, namely that of $H^{1/2}(\mathcal{O}) \oplus H^{-1/2}(\mathcal{O})$. Therefore we also have

$$\|\tilde{k}(F_n) - \tilde{k}(F_m)\|_{\tilde{\mathcal{H}}}^2 = \tilde{\mu}(F_n - F_m, F_n - F_m) \rightarrow 0$$

and it follows that also $\tilde{k}(F_n) \rightarrow v$ in $\tilde{\mathcal{H}}$ for some $v \in \overline{\tilde{k}(\Gamma(\mathcal{O}))}$. For all $G \in \Gamma(\mathcal{O})$ we have the equalities

$$\begin{aligned} 0 &= \text{Im}\langle u, k_N(G) \rangle_{\mathcal{H}_N} = \lim_{n \rightarrow \infty} \text{Im}\langle k_N(F_n), k_N(G) \rangle_{\mathcal{H}_N} \\ &= \frac{1}{2} \lim_{n \rightarrow \infty} \sigma(F_n, G) = \frac{1}{2} C^{-3/2} \lim_{n \rightarrow \infty} \tilde{\sigma}(F_n, G) \\ &= C^{-3/2} \lim_{n \rightarrow \infty} \text{Im}\langle \tilde{k}(F_n), \tilde{k}(G) \rangle_{\tilde{\mathcal{H}}} = C^{-3/2} \text{Im}\langle v, \tilde{k}(G) \rangle_{\tilde{\mathcal{H}}}, \end{aligned}$$

which imply that $v \in \overline{\tilde{k}(\Gamma(\mathcal{O}))} \cap \tilde{k}(\Gamma(\mathcal{O}))^\vee = \{0\}$ and therefore $\tilde{k}(F_n) \rightarrow 0$ in $\tilde{\mathcal{H}}$. Since the norms given by k_N and \tilde{k} are equivalent on $\Gamma(\mathcal{O})$ we also have $u = \lim_{n \rightarrow \infty} k_N(F_n) = 0$ in \mathcal{H}_N , which proves the theorem. \blacksquare

Our main theorem is the following:

Theorem 4.7 *Let ω_N be an adiabatic vacuum state of order N and ω_H an Hadamard state on the Weyl algebra $\mathcal{A}[\Gamma, \sigma]$ of the Klein-Gordon field in the globally hyperbolic spacetime (\mathcal{M}, g) , and let π_{ω_N} and π_{ω_H} be their associated GNS-representations.*

(i) *If $N > 5/2$, then $\pi_{\omega_N} \upharpoonright \mathcal{A}(\mathcal{O})$ and $\pi_{\omega_H} \upharpoonright \mathcal{A}(\mathcal{O})$ are quasiequivalent for every open, relatively compact subset $\mathcal{O} \subset \Sigma$.*

(ii) *If ω_N and ω_H are pure states on a spacetime with compact Cauchy surface and $N > 3/2$, then π_{ω_N} and π_{ω_H} are unitarily equivalent.*

As explained at the beginning of this section it is sufficient to prove the quasiequivalence of the GNS-representations of the partial states $\omega_N \upharpoonright \mathcal{A}(\mathcal{O})$ and $\omega_H \upharpoonright \mathcal{A}(\mathcal{O})$ for part (i) of the theorem, for part (ii) we can take $\mathcal{O} = \Sigma$. To this end we shall use a result of Araki & Yamagami [2]. To state it we first need some notation.

Given a bilinear form μ on a real vector space K we shall denote by $\mu^{\mathbb{C}}$ the extension of μ to the complexification $K^{\mathbb{C}}$ of K (such that it is antilinear in the first argument):

$$\mu^{\mathbb{C}}(F_1 + iF_2, G_1 + iG_2) := \mu(F_1, G_1) + \mu(F_2, G_2) + i\mu(F_1, G_2) - i\mu(F_2, G_1).$$

The theorem of Araki & Yamagami gives necessary and sufficient conditions for the quasiequivalence of two quasifree states ω_{μ_1} and ω_{μ_2} on the Weyl algebra $\mathcal{A}[K, \sigma]$ of a phase space (K, σ) in terms of the complexified data $K^{\mathbb{C}}, \sigma^{\mathbb{C}}$, and $\mu_i^{\mathbb{C}}, i = 1, 2$. Assuming that $\mu_1^{\mathbb{C}}$ and $\mu_2^{\mathbb{C}}$ induce the same topology on $K^{\mathbb{C}}$, denote by $\bar{K}^{\mathbb{C}}$ the completion. Then $\mu_1^{\mathbb{C}}, \mu_2^{\mathbb{C}}$, and $\lambda_1^{\mathbb{C}} := \mu_1^{\mathbb{C}} + \frac{i}{2}\sigma^{\mathbb{C}}, \lambda_2^{\mathbb{C}} := \mu_2^{\mathbb{C}} + \frac{i}{2}\sigma^{\mathbb{C}}$ extend to $\bar{K}^{\mathbb{C}}$ by continuity ($\sigma^{\mathbb{C}}$ extends due to (8)). We define bounded positive selfadjoint operators S_1, S_2 , and S'_2 on $\bar{K}^{\mathbb{C}}$ by

$$\begin{aligned} \lambda_j^{\mathbb{C}}(F, G) &= 2\mu_j^{\mathbb{C}}(F, S_j G), \quad j = 1, 2, \\ \lambda_2^{\mathbb{C}}(F, G) &= 2\mu_1^{\mathbb{C}}(F, S'_2 G), \quad F, G \in \bar{K}^{\mathbb{C}}. \end{aligned} \tag{34}$$

Note that S_j is a projection operator if and only if ω_{μ_j} is a Fock state. The theorem of Araki & Yamagami [2] then states that the corresponding GNS-representations π_{ω_1} and π_{ω_2} are quasiequivalent if and only if both of the following two conditions are satisfied:

(AY1) $\mu_1^{\mathbb{C}}$ and $\mu_2^{\mathbb{C}}$ induce the same topology on $K^{\mathbb{C}}$,

(AY2) $S_1^{1/2} - S_2^{1/2}$ is a Hilbert-Schmidt operator on $(\bar{K}^{\mathbb{C}}, \mu_1^{\mathbb{C}})$.

Proof of Theorem 4.7: (i) We choose $K = \Gamma(\mathcal{O}) = \mathcal{C}_0^\infty(\mathcal{O}) \oplus \mathcal{C}_0^\infty(\mathcal{O})$, σ our real symplectic form (7), μ_H and μ_N the real scalar products on K defining an Hadamard state and an adiabatic vacuum state of order $N > 5/2$, respectively, and check (AY1) and (AY2) for the data $K^{\mathbb{C}}, \sigma^{\mathbb{C}}, \mu_H^{\mathbb{C}}$ and $\mu_N^{\mathbb{C}}$. From Theorem 4.2 we know that the topologies induced by μ_H and μ_N on $\Gamma(\mathcal{O})$ coincide. In view of the fact that

$$\mu_H^{\mathbb{C}}(F_1 + iF_2, F_1 + iF_2) = \mu_H(F_1, F_1) + \mu_H(F_2, F_2), \quad F_1, F_2 \in \Gamma(\mathcal{O}),$$

(and the corresponding relation for μ_N), we see that the topologies coincide also on the complexification. Hence (AY1) holds.

In order to prove (AY2), we first note that the difference $S_H^{1/2} - S_N^{1/2}$ for the operators S_H and S'_N induced by μ_H and μ_N via (34) will be a Hilbert-Schmidt operator provided that $S_H - S'_N$ is of trace class, cf. [40, Lemma 4.1]. By definition,

$$\mu_H^{\mathbb{C}}(F, (S_H - S'_N)G) = \frac{1}{2} (\lambda_H^{\mathbb{C}} - \lambda_N^{\mathbb{C}}) (F, G) = \frac{1}{2} (\mu_H^{\mathbb{C}} - \mu_N^{\mathbb{C}}) (F, G). \quad (35)$$

As in (23), (24), our assumption $N > 5/2$ and Lemma 3.3 imply that there is an integral kernel $M = M(x, y)$ on $\mathcal{O} \times \mathcal{O}$, given by (24) with entries satisfying (20)–(22), such that

$$\frac{1}{2} (\mu_H^{\mathbb{C}} - \mu_N^{\mathbb{C}}) (F, G) = \langle F, \mathbb{M}G \rangle_{L^2(\mathcal{O}) \oplus L^2(\mathcal{O})}, \quad F, G \in \Gamma(\mathcal{O}), \quad (36)$$

where \mathbb{M} is the integral operator with kernel M . We may multiply M by $\varphi(x)\varphi(y)$ where φ is a smooth function supported in a relatively compact neighborhood $\tilde{\mathcal{O}}$ of \mathcal{O} with $\varphi \equiv 1$ on \mathcal{O} . Equality (36) is not affected by this change. Moreover, as we saw in the beginning of this section we may suppose that \mathcal{O} and $\tilde{\mathcal{O}}$ have smooth boundary. Using a partition of unity it is no loss of generality to assume that $\tilde{\mathcal{O}}$ is contained in a single coordinate neighborhood. We then denote by $\mathcal{O}_* \subset \mathbb{R}^3$ the image of \mathcal{O} under the coordinate map. We shall use the notation $\mu_H^{\mathbb{C}}, \mu_N^{\mathbb{C}}$, and M, \mathbb{M} also for the push-forwards of these objects. We note that the closure of $\Gamma(\mathcal{O}_*)$ with respect to the topology of $H^{1/2}(\mathbb{R}^3) \oplus H^{-1/2}(\mathbb{R}^3)$ is $H_0^{1/2}(\overline{\mathcal{O}_*}) \oplus H_0^{-1/2}(\overline{\mathcal{O}_*}) =: \mathcal{H}$, cf. Appendix A for the notation. The dual space \mathcal{H}' w.r.t. the extension of $\langle \cdot, \cdot \rangle_{L^2(\mathcal{O}_*) \oplus L^2(\mathcal{O}_*)}$, denoted by $\langle \cdot, \cdot \rangle$, is $H^{-1/2}(\mathcal{O}_*) \oplus H^{1/2}(\mathcal{O}_*)$. The inner product $\mu_H^{\mathbb{C}}$ extends to \mathcal{H} . By Riesz' theorem, $\mu_H^{\mathbb{C}}$ induces an antilinear isometry $\tilde{\theta} : \mathcal{H} \rightarrow \mathcal{H}'$ by $\langle \tilde{\theta}F, G \rangle = \mu_H^{\mathbb{C}}(F, G)$. Defining instead

$$\langle F, \theta G \rangle = \mu_H^{\mathbb{C}}(F, G) \quad (37)$$

we obtain a linear isometry θ from \mathcal{H} to the space $\tilde{\mathcal{H}}'$ of antilinear functionals on \mathcal{H} . Complex conjugation provides a (real-linear) isometry between \mathcal{H}' and $\tilde{\mathcal{H}}'$, hence $\tilde{\mathcal{H}}' = H^{-1/2}(\mathcal{O}_*) \oplus H^{1/2}(\mathcal{O}_*)$ as a normed space (and hence as a Hilbert space). We deduce from Lemma 4.8 and Corollary 4.9 below, in connection with the continuity of the extension operator $\mathcal{H} \rightarrow$

$H^{1/2}(\mathbb{R}^3) \oplus H^{-1/2}(\mathbb{R}^3)$ and the restriction operator $H^{-1/2}(\mathbb{R}^3) \oplus H^{1/2}(\mathbb{R}^3) \rightarrow H^{-1/2}(\mathcal{O}_*) \oplus H^{1/2}(\mathcal{O}_*)$, that M induces a mapping

$$\mathbb{M} : \mathcal{H} \rightarrow H^{-1/2}(\mathcal{O}_*) \oplus H^{1/2}(\mathcal{O}_*)$$

which is trace class. In particular, for $G \in \mathcal{H}$, $\mathbb{M}G$ defines an element of $\tilde{\mathcal{H}}'$ by $F \mapsto \langle F, \mathbb{M}G \rangle$. Combining (35)–(37), we see that, for $F, G \in \mathcal{H}$,

$$\langle F, \mathbb{M}G \rangle = \langle F, \theta(S_H - S'_N)G \rangle.$$

Hence

$$\theta(S_H - S'_N) = \mathbb{M} \quad \text{in } \mathcal{B}(\mathcal{H}, \tilde{\mathcal{H}}'),$$

so that

$$S_H - S'_N = \theta^{-1}\mathbb{M} \quad \text{in } \mathcal{B}(\mathcal{H}).$$

As a consequence of the fact that $\theta^{-1} : \tilde{\mathcal{H}}' \rightarrow \mathcal{H}$ is an isometry while $\mathbb{M} : \mathcal{H} \rightarrow \tilde{\mathcal{H}}'$ is trace class, this implies that $S_H - S'_N$ is trace class.

(ii) To prove (ii) we apply the technique of Bogoljubov transformations (we follow [35] and [50, p. 68f.]). Assume that Σ is compact and let S_H, S_N , and S'_N be the operators induced by a pure Hadamard state ω_H resp. a pure adiabatic state ω_N of order $N > 3/2$ via (34). As remarked above, S_H and S_N are projection operators on $\bar{K}^{\mathbb{C}}$, the closure of the complexification of $K := \Gamma(\Sigma)$ w.r.t. $\mu_H^{\mathbb{C}}$ or $\mu_N^{\mathbb{C}}$ (since Σ is compact, $\mu_H^{\mathbb{C}}$ and $\mu_N^{\mathbb{C}}$ are equivalent on all of $\Gamma(\Sigma)$, Theorem 4.2). We make a direct sum decomposition of $\bar{K}^{\mathbb{C}}$ into

$$\bar{K}^{\mathbb{C}} = \begin{array}{c} \mathcal{H}_N^+ \\ \oplus \\ \mathcal{H}_N^- \end{array} = \begin{array}{c} \mathcal{H}_H^+ \\ \oplus \\ \mathcal{H}_H^- \end{array} \quad (38)$$

such that $S_{H/N}$ has the eigenvalue 1 on $\mathcal{H}_{H/N}^+$ and 0 on $\mathcal{H}_{H/N}^-$, and the first decomposition is orthogonal w.r.t. $\mu_N^{\mathbb{C}}$, the second w.r.t. $\mu_H^{\mathbb{C}}$. We also denote the corresponding orthogonal projections of $\bar{K}^{\mathbb{C}}$ onto $\mathcal{H}_{H/N}^+$ resp. $\mathcal{H}_{H/N}^-$ by $P_{H/N}^+ := S_{H/N}$ resp. $P_{H/N}^- := 1 - S_{H/N}$. From Eq.s (9) and (34) we obtain for $j \in \{H, N\}$

$$\begin{aligned} 2\mu_j^{\mathbb{C}}(F, S_j G) &= \lambda_j^{\mathbb{C}}(F, G) = \mu_j^{\mathbb{C}}(F, G) - \frac{i}{2}\sigma^{\mathbb{C}}(F, G) \\ \Rightarrow \sigma^{\mathbb{C}}(F, G) &= 2\mu_j^{\mathbb{C}}(F, i(2S_j - 1)G) = 2\mu_j^{\mathbb{C}}(F, J_j G) \end{aligned} \quad (39)$$

where $J_j := i(2S_j - 1)$ is a bounded operator on $\bar{K}^{\mathbb{C}}$ with the properties $J_j^2 = -1$, $J_j^* = -J_j$ (w.r.t. $\mu_j^{\mathbb{C}}$). It has eigenvalue $+i$ on \mathcal{H}_j^+ and $-i$ on \mathcal{H}_j^- and is called the complex structure associated to μ_j . Because of (39) both decompositions in (38) are orthogonal w.r.t. $\sigma^{\mathbb{C}}$. We now define the Bogoljubov transformation

$$\begin{pmatrix} A & C \\ B & D \end{pmatrix} : \begin{array}{c} \mathcal{H}_N^+ \\ \oplus \\ \mathcal{H}_N^- \end{array} \rightarrow \begin{array}{c} \mathcal{H}_H^+ \\ \oplus \\ \mathcal{H}_H^- \end{array} \quad (40)$$

by the bounded operators

$$A := P_H^+|_{\mathcal{H}_N^+}, \quad B := P_H^-|_{\mathcal{H}_N^+}, \quad C := P_H^+|_{\mathcal{H}_N^-}, \quad D := P_H^-|_{\mathcal{H}_N^-}.$$

Taking into account Eq. (39) and the fact that the decomposition (38) is orthogonal w.r.t. $\sigma^{\mathbb{C}}$ we obtain for $F, G \in \mathcal{H}_N^+$

$$\begin{aligned} \mu_N^{\mathbb{C}}(F, G) &= \mu_N^{\mathbb{C}}(F, -iJ_N G) = -\frac{i}{2}\sigma^{\mathbb{C}}(F, G) \\ &= -\frac{i}{2}\sigma^{\mathbb{C}}(P_H^+ F, P_H^+ G) - \frac{i}{2}\sigma^{\mathbb{C}}(P_H^- F, P_H^- G) \\ &= -\frac{i}{2}\sigma^{\mathbb{C}}(AF, AG) - \frac{i}{2}\sigma^{\mathbb{C}}(BF, BG) \\ &= -i\mu_H^{\mathbb{C}}(AF, J_H AG) - i\mu_H^{\mathbb{C}}(BF, J_H BG) \\ &= \mu_H^{\mathbb{C}}(AF, AG) - \mu_H^{\mathbb{C}}(BF, BG), \end{aligned}$$

similarly for $F, G \in \mathcal{H}_N^-$

$$\mu_N^{\mathbb{C}}(F, G) = \mu_H^{\mathbb{C}}(DF, DG) - \mu_H^{\mathbb{C}}(CF, CG),$$

and for $F \in \mathcal{H}_N^+, G \in \mathcal{H}_N^-$

$$\begin{aligned} 0 = \mu_N^{\mathbb{C}}(F, G) &= \mu_N^{\mathbb{C}}(F, iJ_N G) = \frac{i}{2}\sigma^{\mathbb{C}}(F, G) \\ &= \frac{i}{2}\sigma^{\mathbb{C}}(P_H^+ F, P_H^+ G) + \frac{i}{2}\sigma^{\mathbb{C}}(P_H^- F, P_H^- G) \\ &= \frac{i}{2}\sigma^{\mathbb{C}}(AF, CG) + \frac{i}{2}\sigma^{\mathbb{C}}(BF, DG) \\ &= i\mu_H^{\mathbb{C}}(AF, J_H CG) + i\mu_H^{\mathbb{C}}(BF, J_H DG) \\ &= -\mu_H^{\mathbb{C}}(AF, CG) + \mu_H^{\mathbb{C}}(BF, DG), \end{aligned}$$

hence

$$\begin{aligned} A^*A - B^*B &= 1 \quad \text{in } \mathcal{B}(\mathcal{H}_N^+, \mathcal{H}_N^+) \\ D^*D - C^*C &= 1 \quad \text{in } \mathcal{B}(\mathcal{H}_N^-, \mathcal{H}_N^-) \\ B^*D - A^*C &= 0 \quad \text{in } \mathcal{B}(\mathcal{H}_N^-, \mathcal{H}_N^+). \end{aligned} \tag{41}$$

In a completely analogous way we can define the inverse Bogoljubov transformation

$$\begin{pmatrix} \tilde{A} & \tilde{C} \\ \tilde{B} & \tilde{D} \end{pmatrix} : \begin{array}{cc} \mathcal{H}_H^+ & \mathcal{H}_N^+ \\ \oplus & \rightarrow \oplus \\ \mathcal{H}_H^- & \mathcal{H}_N^- \end{array} \tag{42}$$

by

$$\tilde{A} := P_N^+|_{\mathcal{H}_H^+}, \quad \tilde{B} := P_N^-|_{\mathcal{H}_H^+}, \quad \tilde{C} := P_N^+|_{\mathcal{H}_H^-}, \quad \tilde{D} := P_N^-|_{\mathcal{H}_H^-}.$$

These operators satisfy relations analogous to (41). Moreover, for $F \in \mathcal{H}_N^+, G \in \mathcal{H}_H^+$

$$\begin{aligned}\mu_N^{\mathbb{C}}(F, \tilde{A}G) &= \mu_N^{\mathbb{C}}(F, -iJ_N\tilde{A}G) = -\frac{i}{2}\sigma^{\mathbb{C}}(F, \tilde{A}G) = -\frac{i}{2}\sigma^{\mathbb{C}}(F, P_N^+G) \\ &= -\frac{i}{2}\sigma^{\mathbb{C}}(F, G) = -\frac{i}{2}\sigma^{\mathbb{C}}(P_H^+F, G) = -i\mu_H^{\mathbb{C}}(AF, J_HG) \\ &= \mu_H^{\mathbb{C}}(AF, G),\end{aligned}$$

$$\begin{aligned}\text{i.e. } \tilde{A} &= A^* : \mathcal{H}_H^+ \rightarrow \mathcal{H}_N^+ \\ \text{and similarly } \tilde{B} &= -C^* : \mathcal{H}_H^+ \rightarrow \mathcal{H}_N^- \\ \tilde{C} &= -B^* : \mathcal{H}_H^- \rightarrow \mathcal{H}_N^+ \\ \tilde{D} &= D^* : \mathcal{H}_H^- \rightarrow \mathcal{H}_N^-.\end{aligned}\tag{43}$$

From (41) and (43) one easily finds that

$$\begin{aligned}AA^* - CC^* &= 1 \quad \text{in } \mathcal{B}(\mathcal{H}_H^+, \mathcal{H}_H^+) \\ DD^* - BB^* &= 1 \quad \text{in } \mathcal{B}(\mathcal{H}_H^-, \mathcal{H}_H^-) \\ AB^* - CD^* &= 0 \quad \text{in } \mathcal{B}(\mathcal{H}_H^-, \mathcal{H}_H^+)\end{aligned}\tag{44}$$

and that (42) is the inverse of (40). Moreover, A is invertible with bounded inverse: It follows from the first Eq.s in (41) and (44) that $A^*A \geq 1$ on \mathcal{H}_N^+ and $AA^* \geq 1$ on \mathcal{H}_H^+ , hence A and A^* are injective. Since $\{0\} = \text{Ker}(A^*) = \text{Ran}(A)^\perp$, A has dense range in \mathcal{H}_H^+ . For $F = AG \in \text{Ran}(A)$ we have $\|A^{-1}F\|_{\mathcal{H}_N^+}^2 = \|G\|_{\mathcal{H}_N^+}^2 \leq \langle G, A^*AG \rangle_{\mathcal{H}_N^+} = \|AG\|_{\mathcal{H}_H^+}^2 = \|F\|_{\mathcal{H}_H^+}^2$, i.e. A^{-1} is bounded and can be defined on all of \mathcal{H}_H^+ .

We are now prepared to show that $S_H^{1/2} - S_N'^{1/2}$ is a Hilbert-Schmidt operator on $(\bar{K}^{\mathbb{C}}, \mu_H^{\mathbb{C}})$: We write $F \in \bar{K}^{\mathbb{C}}$ as a column vector w.r.t. the decomposition of $\bar{K}^{\mathbb{C}}$ w.r.t. $\mu_H^{\mathbb{C}}$:

$$F = \begin{pmatrix} P_H^+F \\ P_H^-F \end{pmatrix} =: \begin{pmatrix} F^+ \\ F^- \end{pmatrix} \in \begin{matrix} \mathcal{H}_H^+ \\ \oplus \\ \mathcal{H}_H^- \end{matrix}.$$

Then

$$S_H F = P_H^+ F = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} F^+ \\ F^- \end{pmatrix}.\tag{45}$$

For S_N' we get by the basis transformation (42) for all $F, G \in \bar{K}^{\mathbb{C}}$

$$\begin{aligned}\mu_H^{\mathbb{C}}(G, S_N'F) &= \frac{1}{2}\lambda_N^{\mathbb{C}}(G, F) = \mu_N^{\mathbb{C}}(G, S_N F) \\ &= \mu_N^{\mathbb{C}}\left(\begin{pmatrix} P_N^+G \\ P_N^-G \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} P_N^+F \\ P_N^-F \end{pmatrix}\right) \\ &= \mu_N^{\mathbb{C}}\left(\begin{pmatrix} \tilde{A} & \tilde{C} \\ \tilde{B} & \tilde{D} \end{pmatrix} \begin{pmatrix} P_H^+G \\ P_H^-G \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{A} & \tilde{C} \\ \tilde{B} & \tilde{D} \end{pmatrix} \begin{pmatrix} P_H^+F \\ P_H^-F \end{pmatrix}\right) \\ &= \mu_H^{\mathbb{C}}\left(\begin{pmatrix} G^+ \\ G^- \end{pmatrix}, \begin{pmatrix} \tilde{A}^* & \tilde{B}^* \\ \tilde{C}^* & \tilde{D}^* \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{A} & \tilde{C} \\ \tilde{B} & \tilde{D} \end{pmatrix} \begin{pmatrix} F^+ \\ F^- \end{pmatrix}\right),\end{aligned}$$

and hence, utilizing (43),

$$\begin{aligned} S'_N \begin{pmatrix} F^+ \\ F^- \end{pmatrix} &= \begin{pmatrix} A & -C \\ -B & D \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} A^* & -B^* \\ -C^* & D^* \end{pmatrix} \begin{pmatrix} F^+ \\ F^- \end{pmatrix} \\ &= \begin{pmatrix} AA^* & -AB^* \\ -BA^* & BB^* \end{pmatrix} \begin{pmatrix} F^+ \\ F^- \end{pmatrix}. \end{aligned} \quad (46)$$

From (45) and (46) we have now on $\mathcal{H}_H^+ \oplus \mathcal{H}_H^-$

$$\begin{aligned} S_H^{1/2} - S'_N{}^{1/2} &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}^{1/2} - \begin{pmatrix} AA^* & -AB^* \\ -BA^* & BB^* \end{pmatrix}^{1/2} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} AZ^{-1/2}A^* & -AZ^{-1/2}B^* \\ -BZ^{-1/2}A^* & BZ^{-1/2}B^* \end{pmatrix}, \end{aligned} \quad (47)$$

where $Z := A^*A + B^*B = 1 + 2B^*B$ is a bounded selfadjoint positive operator on \mathcal{H}_N^+ , which has a bounded inverse due to the fact that $Z \geq 1$. In Lemma 4.11 below we will show that (47) is a Hilbert-Schmidt operator on $\mathcal{H}_H^+ \oplus \mathcal{H}_H^-$ if and only if the operator

$$Y := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} AA^* & -AB^* \\ -BA^* & BB^* \end{pmatrix}$$

is Hilbert-Schmidt. From (46) and (34) we see that

$$\begin{aligned} \mu_H^{\mathbb{C}}(G, YF) &= \mu_H^{\mathbb{C}}(G, (S_H - S'_N)F) = \frac{1}{2} (\lambda_H^{\mathbb{C}}(G, F) - \lambda_N^{\mathbb{C}}(G, F)) \\ &= \frac{1}{2} (\mu_H^{\mathbb{C}}(G, F) - \mu_N^{\mathbb{C}}(G, F)). \end{aligned}$$

Now we argue as in the proof of part (i): $\mu_H^{\mathbb{C}} - \mu_N^{\mathbb{C}}$ is given by an integral operator \mathbb{M} with kernel M , where M has the form (24) with entries satisfying (20)–(22). Using a partition of unity we can transfer the problem to \mathbb{R}^n with the Sobolev regularity of the entries preserved. For $N > 3/2$ the conditions in Remark 4.10 are satisfied. Hence \mathbb{M} and also Y are Hilbert-Schmidt operators, i.e. ω_H and ω_N are quasiequivalent on $\mathcal{A}[\Gamma, \sigma]$, which, in turn, is equivalent to the unitary equivalence of the representations π_{ω_H} and π_{ω_N} , if ω_H and ω_N are pure states. \blacksquare

Lemma 4.8 *Let $M \in H_{comp}^s(\mathbb{R}^n \times \mathbb{R}^n)$, $s \geq 0$, and consider the integral operator \mathbb{M} with kernel M , defined by*

$$(\mathbb{M}u)(x) = \int M(x, y)u(y) dy, \quad u \in \mathcal{C}_0^\infty(\mathbb{R}^n).$$

If $s > \frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}$, and $\frac{n}{2} + 1$, respectively, then \mathbb{M} yields trace class operators in

$$\mathcal{B}(H^{1/2}(\mathbb{R}^n), H^{-1/2}(\mathbb{R}^n)), \mathcal{B}(H^{-1/2}(\mathbb{R}^n)), \mathcal{B}(H^{1/2}(\mathbb{R}^n)), \mathcal{B}(H^{-1/2}(\mathbb{R}^n), H^{1/2}(\mathbb{R}^n)),$$

respectively.

Proof: For the first case, $s > \frac{n-1}{2}$, write

$$\mathbb{M} = \left(\langle D \rangle^{-s-\frac{1}{2}} \langle x \rangle^{-s-\frac{1}{2}} \right) \left(\langle x \rangle^{s+\frac{1}{2}} \langle D \rangle^{s+\frac{1}{2}} \mathbb{M} \right)$$

where $\langle x \rangle^s$ is the operator of multiplication by $\langle x \rangle^s$ and $\langle D \rangle^s = op(\langle \xi \rangle^s)$ w.r.t. the flat Euclidean metric of \mathbb{R}^n . The first factor is known to be a Hilbert-Schmidt operator on $H^{-1/2}(\mathbb{R}^n)$. Since M has compact support, it is sufficient to check the Hilbert-Schmidt property of $\langle D \rangle^{s+\frac{1}{2}} \mathbb{M}$ in $\mathcal{B}(H^{1/2}(\mathbb{R}^n), H^{-1/2}(\mathbb{R}^n))$ or, equivalently, of $\langle D \rangle^s \mathbb{M} \langle D \rangle^{-1/2}$ on $L^2(\mathbb{R}^n)$. This operator, however, has the integral kernel $\langle D_x \rangle^s \langle D_y \rangle^{-1/2} M(x, y)$. We may consider $\langle D_x \rangle^s$ as the pseudodifferential operator $\langle D_x \rangle^s \otimes I$ on $\mathbb{R}^n \times \mathbb{R}^n$ with a symbol in the class $S_{0,0}^s(\mathbb{R}^{2n} \times \mathbb{R}^{2n})$ and $\langle D_y \rangle^{-1/2}$ as the pseudodifferential operator $I \otimes \langle D_y \rangle^{-1/2}$ on $\mathbb{R}^n \times \mathbb{R}^n$ with symbol in $S_{0,0}^0(\mathbb{R}^{2n} \times \mathbb{R}^{2n})$. By Calderón and Vaillancourt's Theorem, $\langle D_x \rangle^s \langle D_y \rangle^{-1/2}$ maps $H^s(\mathbb{R}^n \times \mathbb{R}^n)$ to $L^2(\mathbb{R}^n \times \mathbb{R}^n)$, hence $\langle D \rangle^s \mathbb{M} \langle D \rangle^{-1/2}$ is an integral operator with a square integrable kernel, hence Hilbert-Schmidt, and \mathbb{M} is the composition of two Hilbert-Schmidt operators, hence trace class.

The proofs of the other cases are similar. ■

Corollary 4.9 *It is well-known that the operator*

$$\mathbb{M} = \begin{pmatrix} \mathbb{M}_{11} & \mathbb{M}_{12} \\ \mathbb{M}_{21} & \mathbb{M}_{22} \end{pmatrix} : \begin{array}{ccc} H^{1/2}(\mathbb{R}^n) & & H^{-1/2}(\mathbb{R}^n) \\ & \oplus & \rightarrow \oplus \\ H^{-1/2}(\mathbb{R}^n) & & H^{1/2}(\mathbb{R}^n) \end{array}$$

is trace class if and only if each of the entries \mathbb{M}_{ij} of the matrix is a trace class operator between the respective spaces, cf. e.g. [42, Sect. 4.1.1.2, Lemma 2]. Denoting by M_{ij} the integral kernel of \mathbb{M}_{ij} , \mathbb{M} will be trace class if

$$\begin{aligned} M_{11} &\in H^s(\mathbb{R}^n \times \mathbb{R}^n), & s > \frac{n-1}{2} \\ M_{12} &\in H^s(\mathbb{R}^n \times \mathbb{R}^n), & s > \frac{n}{2} \\ M_{21} &\in H^s(\mathbb{R}^n \times \mathbb{R}^n), & s > \frac{n+1}{2} \\ M_{22} &\in H^s(\mathbb{R}^n \times \mathbb{R}^n), & s > \frac{n}{2} + 1. \end{aligned}$$

Remark 4.10 *In the situation of Corollary 4.9, \mathbb{M} will be a Hilbert-Schmidt operator if each of its entries has this property. Using the fact that an integral operator on $L^2(\mathbb{R}^n)$ is Hilbert-Schmidt if its kernel is in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$, we easily see that it is sufficient for the Hilbert-Schmidt property of \mathbb{M} that*

$$\begin{aligned} M_{11} &\in L^2(\mathbb{R}^n \times \mathbb{R}^n) \\ M_{12}, M_{21} &\in H^{1/2}(\mathbb{R}^n \times \mathbb{R}^n) \\ M_{22} &\in H^1(\mathbb{R}^n \times \mathbb{R}^n). \end{aligned}$$

Lemma 4.11 *In the notation of above, the following statements are equivalent:*

(i) *The operator*

$$X := \begin{pmatrix} 1 - AZ^{-1/2}A^* & AZ^{-1/2}B^* \\ BZ^{-1/2}A^* & -BZ^{-1/2}B^* \end{pmatrix} : \begin{array}{ccc} \mathcal{H}_H^+ & & \mathcal{H}_H^+ \\ \oplus & \rightarrow & \oplus \\ \mathcal{H}_H^- & & \mathcal{H}_H^- \end{array}$$

is Hilbert-Schmidt.

(ii) *The operator*

$$Y := \begin{pmatrix} 1 - AA^* & AB^* \\ BA^* & -BB^* \end{pmatrix} : \begin{array}{ccc} \mathcal{H}_H^+ & & \mathcal{H}_H^+ \\ \oplus & \rightarrow & \oplus \\ \mathcal{H}_H^- & & \mathcal{H}_H^- \end{array}$$

is Hilbert-Schmidt.

(iii) *The operator $BB^* : \mathcal{H}_H^- \rightarrow \mathcal{H}_H^-$ is of trace class.*

Proof: Using again the fact that a 2×2 -matrix of operators is trace class if and only if each of its entries is a trace class operator [42, Sec. 4.1.1.2, Lemma 2] it is sufficient to show the equivalence of the following statements:

(i) Each of the entries of the operator

$$X^*X = \begin{pmatrix} 1 - A(2Z^{-1/2} - 1)A^* & A(Z^{-1/2} - 1)B^* \\ B(Z^{-1/2} - 1)A^* & BB^* \end{pmatrix} : \begin{array}{ccc} \mathcal{H}_H^+ & & \mathcal{H}_H^+ \\ \oplus & \rightarrow & \oplus \\ \mathcal{H}_H^- & & \mathcal{H}_H^- \end{array}$$

is trace class.

(ii) Each of the entries of the operator

$$Y^*Y = \begin{pmatrix} 1 - A(2 - Z)A^* & A(1 - Z)B^* \\ B(1 - Z)A^* & BZB^* \end{pmatrix} : \begin{array}{ccc} \mathcal{H}_H^+ & & \mathcal{H}_H^+ \\ \oplus & \rightarrow & \oplus \\ \mathcal{H}_H^- & & \mathcal{H}_H^- \end{array}$$

is trace class.

(iii) $BB^* : \mathcal{H}_H^- \rightarrow \mathcal{H}_H^-$ is trace class.

Remember that a compact operator $T : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ acting between two (possibly different) Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 is said to be trace class, $T \in \mathcal{B}_1(\mathcal{H}_1, \mathcal{H}_2)$, if it has finite trace norm $\|T\|_1 := \sum_{i=1}^{\infty} s_i < \infty$, where s_i are the eigenvalues of $|T| := (T^*T)^{1/2}$ on \mathcal{H}_1 .

Note first, that $BB^* \in \mathcal{B}_1(\mathcal{H}_H^-, \mathcal{H}_H^-) \Leftrightarrow B : \mathcal{H}_N^+ \rightarrow \mathcal{H}_H^-$ is Hilbert-Schmidt $\Leftrightarrow B^* : \mathcal{H}_H^- \rightarrow \mathcal{H}_N^+$ is Hilbert-Schmidt $\Leftrightarrow B^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+)$.

Since $Z := 1 + 2B^*B : \mathcal{H}_N^+ \rightarrow \mathcal{H}_N^+$ is a bounded operator with bounded inverse we have

$$B^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \Leftrightarrow ZB^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \Leftrightarrow BZB^* \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+)$$

which proves the assertion for the 22-components of X^*X and Y^*Y .

For the 12-components we note that

$$-2B^*B = 1 - Z = (Z^{-1/2} - 1)(Z^{1/2} + Z) \quad (48)$$

where $Z^{1/2} + Z$ is a bounded operator on \mathcal{H}_N^+ with bounded inverse. As shown after Eq. (44), also $A : \mathcal{H}_N^+ \rightarrow \mathcal{H}_H^+$ is a bounded operator with bounded inverse, therefore

$$\begin{aligned} B^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) &\Leftrightarrow A(1 - Z) = -2AB^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_H^+) \\ &\begin{cases} \Rightarrow A(1 - Z)B^* \in \mathcal{B}_1(\mathcal{H}_H^-, \mathcal{H}_H^+) \\ \Rightarrow A(Z^{-1/2} - 1)B^* = A(1 - Z)(Z^{1/2} + Z)^{-1}B^* \in \mathcal{B}_1(\mathcal{H}_H^-, \mathcal{H}_H^+). \end{cases} \end{aligned}$$

The argument for the 21-component is analogous.

As for the 11-component of Y^*Y we note, using the invertibility of A , the identity $Z = 1 + 2B^*B$, and (41), that

$$\begin{aligned} 1 - A(2 - Z)A^* \in \mathcal{B}_1(\mathcal{H}_H^+, \mathcal{H}_H^+) &\Leftrightarrow A^*A - A^*A(2 - Z)A^*A \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \\ &\Leftrightarrow (1 + B^*B)B^*B(1 + 2B^*B) \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \Leftrightarrow B^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+). \end{aligned}$$

Similarly, using $A^*A = 1 + B^*B = \frac{1}{2}(1 + Z)$, we rewrite the 11-component of X^*X in terms of Z and obtain

$$\begin{aligned} 1 - A(2Z^{-1/2} - 1)A^* \in \mathcal{B}_1(\mathcal{H}_H^+, \mathcal{H}_H^+) &\Leftrightarrow A^*A - A^*A(2Z^{-1/2} - 1)A^*A \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \\ &\Leftrightarrow (1 + Z)(1 - Z^{-1/2})(2 - Z^{1/2} + Z) \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+). \end{aligned} \quad (49)$$

Taking into account (48) and the identity

$$(2 - Z^{1/2} + Z)(Z^{1/2} + Z + 2) = 4 + 3Z + Z^2,$$

where both $Z^{1/2} + Z + 2$ and $4 + 3Z + Z^2$ are bounded operators with bounded inverse, we note that (49) is equivalent to

$$\begin{aligned} (1 + Z)(Z - 1)(4 + 3Z + Z^2) \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \\ \Leftrightarrow Z - 1 \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+) \Leftrightarrow B^*B \in \mathcal{B}_1(\mathcal{H}_N^+, \mathcal{H}_N^+). \end{aligned}$$

This finishes the proof. ■

Theorem 4.5 and Theorem 4.7 imply that, for $N > 5/2$, $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ and $\pi_{\omega_H}(\mathcal{A}(\mathcal{O}))''$, and, if Σ is compact, for $N > 3/2$, $\pi_{\omega_N}(\mathcal{A}[\Gamma, \sigma])''$ and $\pi_{\omega_H}(\mathcal{A}[\Gamma, \sigma])''$ are isomorphic von Neumann factors. Therefore it follows from the corresponding results for Hadamard representations due to Verch [49, Thm. 3.6] that $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ is isomorphic to the unique hyperfinite type III_1 factor if \mathcal{O}^c is non-empty, and is a type I_∞ factor if $\mathcal{O}^c = \emptyset$ (i.e. $\Sigma = \mathcal{O}$ is a compact Cauchy surface).

Our Theorem 4.7 is the analogue of Theorem 3.3 of Lüders & Roberts [35] extended to our definition of adiabatic states on arbitrary curved spacetime manifolds. The loss of order $3/2 + \epsilon$ in the compact case and $1/2 + \epsilon$ in the non-compact case ($\epsilon > 0$ arbitrary) compared to their result is probably due to the fact that we use the regularity of $\Lambda_H - \Lambda_N$ rather generously in the part of the proof of Theorem 4.2 between Eq.s (20) and (25).

4.2 Local definiteness and Haag duality

The next property of adiabatic vacua we check is that of local definiteness. It says that any two adiabatic vacua (of order $> 5/2$) get indistinguishable upon measurements in smaller and smaller spacetime regions. In a first step let us show that in the representation π_{ω_N} generated by an adiabatic vacuum state ω_N (of order $N > 3/2$) there are no nontrivial observables which are localized at a single point, more precisely:

Theorem 4.12 *Let $x \in \Sigma$. Then, for $N > 3/2$,*

$$\bigcap_{\mathcal{O} \ni x} \pi_{\omega_N}(\mathcal{A}(\mathcal{O}))'' = \mathbb{C}\mathbf{1},$$

where the intersection is taken over all open bounded subsets $\mathcal{O} \subset \Sigma$.

Before we prove the theorem let us recall how this, combined with Theorem 4.7, implies the property of local definiteness:

Corollary 4.13 *Let ω_N be an adiabatic vacuum state of order $N > 5/2$ and ω_H an Hadamard state. Let \mathcal{O}_n , $n \in \mathbb{N}_0$, be a sequence of open bounded subsets of Σ shrinking to a point $x \in \Sigma$, i.e. $\mathcal{O}_{n+1} \subset \mathcal{O}_n$ and $\bigcap_{n \in \mathbb{N}_0} \mathcal{O}_n = \{x\}$. Then*

$$\|(\omega_N - \omega_H)|_{\mathcal{A}(\mathcal{O}_n)}\| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Proof: Let $(\pi_{\omega_N}, \mathcal{H}_{\omega_N}, \Omega_{\omega_N})$ be the GNS-triple generated by ω_N , and let $\mathcal{R}_N(\mathcal{O}_n) := \pi_{\omega_N}(\mathcal{A}(\mathcal{O}_n))''$ be the corresponding von Neumann algebras associated to the regions $\mathcal{O}_n \subset \Sigma$. Due to Theorem 4.7 and the remarks at the beginning of Section 4.1 $\pi_{(\omega_H|_{\mathcal{A}(\mathcal{O}_0)})}$ is quasiequivalent to $\pi_{\omega_N}|_{\mathcal{A}(\mathcal{O}_0)}$. This implies [6, Thm. 2.4.21] that $\omega_H|_{\mathcal{A}(\mathcal{O}_0)}$ can be represented in \mathcal{H}_{ω_N} as a density matrix, i.e. there is a sequence $\psi_m \in \mathcal{H}_{\omega_N}$ with $\sum_m \|\psi_m\|^2 = 1$ such that $\omega_H(A) = \sum_m \langle \psi_m, A\psi_m \rangle$ for all $A \in \mathcal{A}(\mathcal{O}_0)$.

Let now $A_n \in \mathcal{R}_N(\mathcal{O}_n) \subset \mathcal{R}_N(\mathcal{O}_0)$ be a sequence of observables with $\|A_n\| = 1$. From Theorem 4.12 it follows that $A_n \rightarrow c\mathbf{1}$ in the topology of $\mathcal{R}_N(\mathcal{O}_0)$ for some $c \in \mathbb{C}$. In particular, $A_n \rightarrow c\mathbf{1}$ in the weak topology, thus

$$|\langle \Omega_{\omega_N}, (A_n - c\mathbf{1})\Omega_{\omega_N} \rangle| \rightarrow 0 \quad \text{as } n \rightarrow \infty,$$

and $A_n \rightarrow c\mathbf{1}$ in the σ -weak topology, thus

$$\sum_m |\langle \psi_m, (A_n - c\mathbf{1})\psi_m \rangle| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

From this we can now conclude

$$\begin{aligned} |(\omega_N - \omega_H)(A_n)| &= |\langle \Omega_{\omega_N}, A_n \Omega_{\omega_N} \rangle - \sum_m \langle \psi_m, A_n \psi_m \rangle| \\ &= |\langle \Omega_{\omega_N}, (A_n - c\mathbf{1})\Omega_{\omega_N} \rangle - \sum_m \langle \psi_m, (A_n - c\mathbf{1})\psi_m \rangle| \\ &\leq |\langle \Omega_{\omega_N}, (A_n - c\mathbf{1})\Omega_{\omega_N} \rangle| + \sum_m |\langle \psi_m, (A_n - c\mathbf{1})\psi_m \rangle| \\ &\rightarrow 0 \quad \text{as } n \rightarrow \infty, \end{aligned} \tag{50}$$

i.e. $(\omega_N - \omega_H)(A_n)$ converges to 0 pointwise for each sequence A_n . To show the uniform convergence we note that due to $\mathcal{A}(\mathcal{O}_{n+1}) \subset \mathcal{A}(\mathcal{O}_n)$

$$r_n := \sup\{ |(\omega_N - \omega_H)(A)|; A \in \mathcal{A}(\mathcal{O}_n), \|A\| = 1 \}$$

is a bounded monotonically decreasing sequence in $n \in \mathbb{N}_0$ with values in \mathbb{R}_0^+ . Hence $r_n \rightarrow r$ for some $r \in \mathbb{R}_0^+$. To show that $r = 0$ let $\epsilon > 0$. For all $n \in \mathbb{N}_0$ there is an $A_n \in \mathcal{A}(\mathcal{O}_n)$ with $\|A_n\| = 1$ such that

$$0 \leq r_n - |(\omega_N - \omega_H)(A_n)| \leq \epsilon.$$

Furthermore, due to (50) there is an $n_o \in \mathbb{N}_0$ such that for all $n \geq n_o$

$$|(\omega_N - \omega_H)(A_n)| \leq \epsilon.$$

From these inequalities we obtain for $n \geq n_o$

$$0 \leq r \leq r_n \leq \epsilon + |(\omega_N - \omega_H)(A_n)| \leq 2\epsilon$$

and hence $r = 0$. This proves the assertion. ■

To prove Theorem 4.12 we show an even stronger statement, namely

$$\bigcap_{\mathcal{O} \supset S} \pi_{\omega_N}(\mathcal{A}(\mathcal{O}))'' = \mathbf{C1} \tag{51}$$

for any smooth 2-dim. closed submanifold S of Σ . The statement of Theorem 4.12 then follows if we choose $x \in S$. In the proof we will need the following lemma:

Lemma 4.14

$$\bigcap_{\mathcal{O} \supset S} \overline{\mathcal{C}_0^\infty(\mathcal{O})} = \{0\},$$

where the closure is taken w.r.t. the norm of $H^{-1/2}(\Sigma)$ (and hence it also holds w.r.t. the norm of $H^{1/2}(\Sigma)$).

Note that we can confine the intersection to all sets \mathcal{O} contained in a suitable compact subset of Σ . Hence we can assume that (Σ, h) is a complete Riemannian manifold (otherwise we modify h as in the proof of Theorem 4.2), so that $H^{\pm 1/2}(\Sigma)$ is well-defined.

Proof of Lemma 4.14: The problem is local, so it suffices to consider the case $\Sigma = \mathbb{R}^n$, $S = \mathbb{R}^{n-1} \times \{0\}$. Suppose the above intersection contains some $f \in H^{-1/2}(\mathbb{R}^n)$, say $\|f\|_{H^{-1/2}} = 1$. Fix $0 < \epsilon < 1/2$. Since

$$\|f\|_{H^{-1/2}} = \sup\{|f(F)|; F \in H^{1/2}, \|F\|_{H^{1/2}} = 1\}$$

we find some $F \in H^{1/2}(\mathbb{R}^n)$ such that $\|F\|_{H^{1/2}} = 1$ and $f(F) > 1 - \epsilon$. According to Lemma 4.6 there exists an $F_0 \in \mathcal{C}_0^\infty(\mathbb{R}^n \setminus (\mathbb{R}^{n-1} \times \{0\}))$ such that $\|F - F_0\|_{H^{1/2}} < \epsilon$ and therefore

$f(F_0) = f(F) + f(F_0 - F) > 1 - 2\epsilon$. Clearly there is a $\delta > 0$ such that $|x_n| > 2\delta$ for each $x = (x', x_n) \in \text{supp } F_0$.

On the other hand, $f \in \overline{\mathcal{C}_0^\infty(\mathbb{R}^{n-1} \times (-\delta, \delta))}^{H^{-1/2}}$, hence $\text{supp } f \subset \mathbb{R}^{n-1} \times [-\delta, \delta]$ (in order to see this, use the fact that the closure of $\mathcal{C}_0^\infty(\mathbb{R}_+^n)$ in the topology of $H^s(\mathbb{R}^n)$ is equal to $\{u \in H^s(\mathbb{R}^n); \text{supp } u \subset \overline{\mathbb{R}_+^n}\}$ for $s \in \mathbb{R}$, cf. [45, 2.10.3]). Denoting by χ_δ a smooth function, equal to 1 on $\mathbb{R}^{n-1} \times [-\delta, \delta]$ and vanishing outside $\mathbb{R}^{n-1} \times (-2\delta, 2\delta)$, we have $f = \chi_\delta f$ and therefore

$$1 - 2\epsilon < f(F_0) = (\chi_\delta f)(F_0) = f(\chi_\delta F_0) = f(0) = 0,$$

a contradiction. ■

Proof of Theorem 4.12: Let (k_N, \mathcal{H}_N) be the one-particle Hilbert space structure of ω_N . According to results of Araki [1, 34] (51) holds iff

$$\bigcap_{\mathcal{O} \supset S} \overline{k_N(\Gamma(\mathcal{O}))} = \{0\}, \quad (52)$$

where the closure is taken w.r.t. the norm in \mathcal{H}_N .

As in the proof of Theorem 4.5, let us define a one-particle Hilbert space structure $(\tilde{k}, \tilde{\mathcal{H}})$ of an auxiliary pure quasifree state on $\mathcal{A}[\Gamma, \sigma]$ by

$$\begin{aligned} \tilde{k} : \Gamma &\rightarrow L^2(\Sigma, h) =: \tilde{\mathcal{H}} \\ \begin{pmatrix} q \\ p \end{pmatrix} &\mapsto \frac{1}{\sqrt{2}} (i\langle D \rangle^{1/2} q + \langle D \rangle^{-1/2} p); \end{aligned}$$

as before, we may change h near infinity to obtain completeness. Note that the norm given by

$$\tilde{\mu}(F, F) := \langle \tilde{k}F, \tilde{k}F \rangle_{\tilde{\mathcal{H}}} = \frac{1}{2} [\|\langle D \rangle^{1/2} q\|_{L^2}^2 + \|\langle D \rangle^{-1/2} p\|_{L^2}^2], \quad F := (q, p) \in \Gamma,$$

is equivalent to the norm of $H^{1/2}(\Sigma) \oplus H^{-1/2}(\Sigma)$.

Let $u \in \overline{k_N(\Gamma(\mathcal{O}))}$ for all $\mathcal{O} \supset S$. Thus for every \mathcal{O} there is a sequence $\{F_n^\mathcal{O}, n \in \mathbb{N}\} \subset \Gamma(\mathcal{O})$ with $k_N(F_n^\mathcal{O}) \rightarrow u$ in \mathcal{H}_N . By Theorem 4.2 the norm given by μ_N , $N > 3/2$, on $\Gamma(\mathcal{O})$ is equivalent to the norm given by $\tilde{\mu}$, namely that of $H^{1/2}(\mathcal{O}) \oplus H^{-1/2}(\mathcal{O})$. Therefore it follows that also $\tilde{k}(F_n^\mathcal{O}) \rightarrow v^\mathcal{O}$ in $\tilde{\mathcal{H}}$ for some $v^\mathcal{O} \in \overline{\tilde{k}(\Gamma(\mathcal{O}))}$. Moreover, $v^\mathcal{O}$ must be independent of \mathcal{O} : To see this, suppose that \mathcal{O}_1 and \mathcal{O}_2 are contained in a common open, bounded set $\tilde{\mathcal{O}} \subset \Sigma$, and let $\epsilon > 0$. Then there is an $n \in \mathbb{N}$ such that

$$\begin{aligned} \|v^{\mathcal{O}_1} - v^{\mathcal{O}_2}\|_{\tilde{\mathcal{H}}} &\leq \|v^{\mathcal{O}_1} - \tilde{k}(F_n^{\mathcal{O}_1})\|_{\tilde{\mathcal{H}}} + \|\tilde{k}(F_n^{\mathcal{O}_1}) - \tilde{k}(F_n^{\mathcal{O}_2})\|_{\tilde{\mathcal{H}}} + \|\tilde{k}(F_n^{\mathcal{O}_2}) - v^{\mathcal{O}_2}\|_{\tilde{\mathcal{H}}} \\ &\leq 2\epsilon + \|\tilde{k}(F_n^{\mathcal{O}_1} - F_n^{\mathcal{O}_2})\|_{\tilde{\mathcal{H}}} = 2\epsilon + \tilde{\mu}(F_n^{\mathcal{O}_1} - F_n^{\mathcal{O}_2}, F_n^{\mathcal{O}_1} - F_n^{\mathcal{O}_2})^{1/2} \\ &\leq 2\epsilon + C(\tilde{\mathcal{O}}) \mu_N(F_n^{\mathcal{O}_1} - F_n^{\mathcal{O}_2}, F_n^{\mathcal{O}_1} - F_n^{\mathcal{O}_2})^{1/2} \\ &= 2\epsilon + C(\tilde{\mathcal{O}}) \|k_N(F_n^{\mathcal{O}_1}) - k_N(F_n^{\mathcal{O}_2})\|_{\mathcal{H}_N} \\ &\leq 2\epsilon + C(\tilde{\mathcal{O}}) (\|k_N(F_n^{\mathcal{O}_1}) - u\|_{\mathcal{H}_N} + \|u - k_N(F_n^{\mathcal{O}_2})\|_{\mathcal{H}_N}) \\ &\leq 2\epsilon(1 + C(\tilde{\mathcal{O}})), \end{aligned}$$

hence $v^{\mathcal{O}_1} = v^{\mathcal{O}_2}$, and we denote this unique element of $\tilde{\mathcal{H}}$ by v .

Since $v \in \bigcap_{\mathcal{O} \supset S} \overline{\tilde{k}(\Gamma(\mathcal{O}))}^{\tilde{\mathcal{H}}}$ it follows from Lemma 4.14 that $v = 0$ and therefore $\tilde{k}(F_n^{\mathcal{O}}) \rightarrow 0$ in $\tilde{\mathcal{H}}$. Since the norms given by k_N and \tilde{k} are equivalent on $\Gamma(\mathcal{O})$ we also have $k_N(F_n^{\mathcal{O}}) \rightarrow 0$ in \mathcal{H}_N and thus $u = \lim_{n \rightarrow \infty} k_N(F_n^{\mathcal{O}}) = 0$, which proves the theorem. \blacksquare

In the following theorem we show that the observable algebras $\mathcal{R}_N(\mathcal{O}) := \pi_{\omega_N}(\mathcal{A}(\mathcal{O}))''$ generated by adiabatic vacuum states (of order $N > 3/2$) satisfy a certain maximality property, called Haag duality. Due to the locality requirement it is clear that all observables localized in spacelike separated regions of spacetime commute. If \mathcal{O} is some open, relatively compact subset of the Cauchy surface Σ with smooth boundary, this means that

$$\mathcal{R}_N(\mathcal{O}^c) \subset \mathcal{R}_N(\mathcal{O})', \quad (53)$$

where $\mathcal{O}^c := \Sigma \setminus \overline{\mathcal{O}}$ and

$$\mathcal{R}_N(\mathcal{O}^c) := \left(\bigcup_{\overline{\mathcal{O}_1} \subset \mathcal{O}^c} \pi_{\omega_N}(\mathcal{A}(\mathcal{O}_1)) \right)'' \quad (54)$$

is the von Neumann algebra generated by all $\pi_{\omega_N}(\mathcal{A}(\mathcal{O}_1))$ with \mathcal{O}_1 bounded and $\overline{\mathcal{O}_1} \subset \mathcal{O}^c$. One says that Haag duality holds for the net of von Neumann algebras generated by a pure state if (53) is even an equality. For mixed states (i.e. reducible GNS-representations) this can certainly not be true, because in this case, by Schur's lemma [6, Prop. 2.3.8], there is a set \mathcal{S} of non-trivial operators commuting with the representation π_{ω_N} , i.e.

$$\mathcal{S} \subset \mathcal{R}_N(\mathcal{O})' \cap \mathcal{R}_N(\mathcal{O}^c)'. \quad (55)$$

If equality held in (53) then the right hand side of (55) would be equal to $\mathcal{R}_N(\mathcal{O})' \cap \mathcal{R}_N(\mathcal{O})$, i.e. to the centre of $\mathcal{R}_N(\mathcal{O})$, which, however, is trivial due to the local primarity (Theorem 4.5) of the representation π_{ω_N} , hence $\mathcal{S} \subset \mathbb{C}\mathbf{1}$, a contradiction. Therefore, in the reducible case one has to take the intersection with $\mathcal{R}_N := \pi_{\omega_N}(\mathcal{A}[\Gamma, \sigma])''$ on the right hand side of (53) to get equality¹ (in the irreducible case, again by Schur's lemma, $\pi_{\omega_N}(\mathcal{A})' = \mathbb{C}\mathbf{1} \Rightarrow \pi_{\omega_N}(\mathcal{A})'' = \mathcal{B}(\mathcal{H}_{\omega_N})$, hence the intersection with \mathcal{R}_N is redundant). Haag duality is an important assumption in the theory of superselection sectors [21] and has therefore been checked in many models of physical interest. For our situation at hand, Haag duality has been shown by Lüders & Roberts [35] to hold for the GNS-representations of adiabatic vacua on Robertson-Walker spacetimes and by Verch [47, 49] for those of Hadamard Fock states. He also noticed that it extends to all Fock states that are locally quasiequivalent to Hadamard states, hence, by our Theorem 4.7, to pure adiabatic states of order $N > 5/2$. Nevertheless, we present an independent proof of Haag duality for adiabatic states that does not rely on quasiequivalence but only on Theorem 4.2 and also holds for mixed states.

¹We are grateful to Fernando Lledó for pointing out to us this generalization of Haag duality and discussion about this topic.

Theorem 4.15 *Let ω_N be an adiabatic state of order $N > 3/2$.*

Then, for any open, relatively compact subset $\mathcal{O} \subset \Sigma$ with smooth boundary,

$$\mathcal{R}_N(\mathcal{O}^c) = \mathcal{R}_N(\mathcal{O})' \cap \mathcal{R}_N,$$

where $\mathcal{O}^c := \Sigma \setminus \overline{\mathcal{O}}$ and $\mathcal{R}_N(\mathcal{O}^c)$ is defined by (54).

Proof: Denoting again by (k_N, \mathcal{H}_N) the one-particle Hilbert space structure of ω_N , it follows from results of Araki [1, 34] that the assertion is equivalent to the statement

$$\overline{k_N(\Gamma(\mathcal{O}^c))} = k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)},$$

where the closure has to be taken w.r.t. \mathcal{H}_N and $k_N(\Gamma(\mathcal{O}))^\vee$ was defined in Eq. (30). Since

$$k_N(\Gamma(\mathcal{O}^c)) \subset k_N(\Gamma(\mathcal{O}))^\vee \cap k_N(\Gamma)$$

(due to the locality of σ , compare (53) above), we only have to show that $k_N(\Gamma(\mathcal{O}^c))$ is dense in $k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)}$. This in turn is the case iff

$$k_N(\Gamma(\mathcal{O})) + k_N(\Gamma(\mathcal{O}^c)) \text{ is dense in } \overline{k_N(\Gamma)} \quad (56)$$

(for the convenience of the reader, the argument will be given in Lemma 4.16 below). (56) will follow if we show that every element $u = k_N(F) \in k_N(\Gamma)$, $F = (q, p) \in \Gamma$, can be approximated by a sequence in $k_N(\Gamma(\mathcal{O})) + k_N(\Gamma(\mathcal{O}^c))$.

To this end we fix a bounded open set $\mathcal{O}_0 \subset \Sigma$ with smooth boundary such that $\text{supp } p$ and $\text{supp } q \subset \mathcal{O}_0$. According to Lemma 4.6 we find sequences $\{q_n\}, \{p_n\} \subset \mathcal{C}_0^\infty(\mathcal{O})$, $\{q_n^c\}, \{p_n^c\} \subset \mathcal{C}_0^\infty(\mathcal{O}^c)$ such that

$$q - (q_n + q_n^c) \rightarrow 0 \text{ in } H^{1/2}(\mathcal{O}_0) \quad (57)$$

$$p - (p_n + p_n^c) \rightarrow 0 \text{ in } H^{-1/2}(\mathcal{O}_0). \quad (58)$$

Note that it is no restriction to ask that the supports of all functions are contained in \mathcal{O}_0 . Let us denote by $(\tilde{k}, \tilde{\mathcal{H}})$ the one-particle Hilbert space structure introduced in (32) with the real scalar product $\tilde{\mu}$ given by (33). The relations (57) and (58) imply that

$$\Gamma(\mathcal{O}_0) \ni F_n := (q - (q_n + q_n^c), p - (p_n + p_n^c)) \rightarrow 0$$

with respect to the norm induced by $\tilde{\mu}$. According to Theorem 4.2 it also tends to zero with respect to the norm induced by μ_N , in other words

$$k_N(F_n) \rightarrow 0 \text{ in } \mathcal{H}_N.$$

This completes the argument. ■

Lemma 4.16

$$k_N(\Gamma(\mathcal{O})) + k_N(\Gamma(\mathcal{O}^c)) \text{ is dense in } \overline{k_N(\Gamma)} \Leftrightarrow k_N(\Gamma(\mathcal{O}^c)) \text{ is dense in } k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)}.$$

Proof: \Rightarrow . Let $u \in k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)}$, and choose $v_n \in k_N(\Gamma(\mathcal{O})), w_n \in k_N(\Gamma(\mathcal{O}^c))$ such that

$$v_n + w_n \rightarrow u \text{ in } \mathcal{H}_N. \quad (59)$$

In view of the fact that $k_N(\Gamma(\mathcal{O}^c)) \subset k_N(\Gamma(\mathcal{O}))^\vee$ we have

$$\overline{k_N(\Gamma(\mathcal{O}))} \cap \overline{k_N(\Gamma(\mathcal{O}^c))} \subset \overline{k_N(\Gamma(\mathcal{O}))} \cap k_N(\Gamma(\mathcal{O}))^\vee = \{0\}.$$

Indeed, the last equality is a consequence of Theorem 4.5, cf. (31). We can therefore define a continuous map

$$\begin{aligned} \pi : \overline{k_N(\Gamma(\mathcal{O}))} \oplus \overline{k_N(\Gamma(\mathcal{O}^c))} &\rightarrow \mathcal{H}_N \\ v \oplus w &\mapsto v. \end{aligned}$$

Now (59) implies that $\{v_n + w_n\}$ is a Cauchy sequence in \mathcal{H}_N , hence so are $\{v_n\} = \{\pi(v_n + w_n)\}$ and $\{w_n\}$. Let $v_0 := \lim v_n \in \overline{k_N(\Gamma(\mathcal{O}))}, w_0 := \lim w_n \in \overline{k_N(\Gamma(\mathcal{O}^c))}$. By (59),

$$u - w_0 = v_0 \in k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma(\mathcal{O}))} = \{0\}.$$

Therefore $u = w_0 \in \overline{k_N(\Gamma(\mathcal{O}^c))}$.

\Leftarrow . Denoting by \perp the orthogonal complement in $\overline{k_N(\Gamma)}$, we clearly have from the definition (30) of \vee that $k_N(\Gamma(\mathcal{O}))^\perp \subset k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)}$. Since $\overline{k_N(\Gamma(\mathcal{O}))} + k_N(\Gamma(\mathcal{O}))^\perp = \overline{k_N(\Gamma)}$ it follows that $k_N(\Gamma(\mathcal{O})) + \left(k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)}\right)$ is dense in $\overline{k_N(\Gamma)}$. From the assumption that $k_N(\Gamma(\mathcal{O}^c))$ is dense in $k_N(\Gamma(\mathcal{O}))^\vee \cap \overline{k_N(\Gamma)}$ the assertion follows. \blacksquare

5 Construction of adiabatic vacuum states

The existence of Hadamard states on arbitrary globally hyperbolic spacetimes has been proven by Fulling, Narcowich & Wald [19] using an elegant deformation argument. Presumably, the existence of adiabatic vacuum states could be shown in a similar way employing the propagation of the Sobolev wavefront set, Proposition B.4. Instead of a mere existence argument, however, we prefer to explicitly construct a large class of adiabatic vacuum states as it is indispensable for the extraction of concrete information in physically relevant situations to have available a detailed construction of the solutions of the theory.

In Section 5.1 we first present a parametrization of quasifree states in terms of two operators R and J acting on the L^2 -Hilbert space w.r.t. a Cauchy surface Σ , Theorem 5.1. The main technical result is Theorem 5.3 which gives a sufficient condition on R and J such that the associated quasifree states are adiabatic of a certain order. In Section 5.2 we construct operators R and J satisfying the above assumptions, Theorem 5.10.

5.1 Criteria for initial data of adiabatic vacuum states

We recall the following theorem from [31, Thm. 3.11]:

Theorem 5.1 *Let (\mathcal{M}, g) be a globally hyperbolic spacetime with Cauchy surface Σ . Let J, R be operators on $L^2(\Sigma, d^3\sigma)$ satisfying the following conditions:*

- (i) $\mathcal{C}_0^\infty(\Sigma) \subset \text{dom}(J)$,
- (ii) J and R map $\mathcal{C}_0^\infty(\Sigma, \mathbb{R})$ to $L^2_{\mathbb{R}}(\Sigma, d^3\sigma)$,
- (iii) J is selfadjoint and positive with bounded inverse,
- (iv) R is bounded and selfadjoint.

Then

$$\begin{aligned} k : \Gamma &\rightarrow \mathcal{H} := \overline{k(\Gamma)} \subset L^2(\Sigma, d^3\sigma) \\ (q, p) &\mapsto (2J)^{-1/2} [(R - iJ)q - p] \end{aligned} \quad (60)$$

is the one-particle Hilbert space structure of a pure quasifree state.

Note that we can define the inverse square root by

$$(2J)^{-1/2} = \frac{1}{\pi} \int_0^\infty \lambda^{-1/2} (\lambda + 2J)^{-1} d\lambda. \quad (61)$$

The integral converges since $\lambda + 2J \geq \lambda$ and hence $(\lambda + 2J)^{-1} \leq \lambda^{-1}$ for $\lambda \geq 0$. Therefore $(2J)^{-1/2}$ is a bounded operator on $L^2(\Sigma, d^3\sigma)$. Moreover, $(2J)^{-1/2}$ maps $L^2_{\mathbb{R}}(\Sigma, d^3\sigma)$ to itself since $\lambda + 2J$ and therefore $(\lambda + 2J)^{-1}$ commutes with complex conjugation ($\lambda \geq 0$).

Proof: A short computation shows that for $F_j = (q_j, p_j) \in \Gamma$, $j = 1, 2$, we have

$$\sigma(F_1, F_2) = -\langle q_1, p_2 \rangle + \langle p_1, q_2 \rangle = 2\text{Im} \langle kF_1, kF_2 \rangle.$$

Here, $\langle \cdot, \cdot \rangle$ is the scalar product of $L^2(\Sigma, d^3\sigma)$. We then let

$$\mu(F_1, F_2) := \text{Re} \langle kF_1, kF_2 \rangle.$$

We note that

$$\begin{aligned} |\sigma(F_1, F_2)|^2 &\leq 4|\langle kF_1, kF_2 \rangle|^2 \leq 4\langle kF_1, kF_1 \rangle \langle kF_2, kF_2 \rangle \\ &= 4\mu(F_1, F_1)\mu(F_2, F_2); \end{aligned}$$

hence k defines the one-particle Hilbert space structure of a quasifree state with real scalar product μ (Definition 2.3) and one-particle Hilbert space $\mathcal{H} = \overline{k\Gamma} + ik\Gamma$ (Proposition 2.4).

Let us next show that the state is pure, i.e. $k\Gamma$ is dense in \mathcal{H} (see Proposition 2.4). We apply a criterion by Araki & Yamagami [2] and check that the operator $S : \Gamma \rightarrow L^2(\Sigma, d^3\sigma) \oplus L^2(\Sigma, d^3\sigma)$ defined by $\langle kF_1, kF_2 \rangle = 2\mu(F_1, SF_2)$ is a projection (cf. Eq. (34)). Indeed, this relation implies that

$$S = \frac{1}{2} \begin{pmatrix} iJ^{-1}R + \mathbf{1} & -iJ^{-1} \\ iRJ^{-1}R + iJ & -iRJ^{-1} + \mathbf{1} \end{pmatrix}.$$

Therefore $S^2 = S$, and the proof is complete. ■

The distinguished parametrices of the Klein-Gordon operator

In the following we shall use the calculus of Fourier integral operators of Duistermaat & Hörmander [16] in order to analyze the wavefront set of certain bilinear forms related to fundamental solutions of the Klein-Gordon operator $P = \square_g + m^2$. We recall from [16, Thm. 6.5.3] that P on a globally hyperbolic spacetime (which is known to be pseudo-convex w.r.t. P , see [41]) has $2^2 = 4$ orientations $C \setminus \text{diag}(C) = C_\nu^1 \dot{\cup} C_\nu^2$ of the bicharacteristic relation C , Eq. (15). Here, ν is one of the four sets $\{\emptyset, N_+, N_-, N_+ \cup N_-\}$ of components of the lightcone $N := \text{char } P$, with $N_\pm := N \cap \{\xi_0 \gtrless 0\}$. $C_\nu^{1(2)}$ are the subsets of the bicharacteristic relation which are denoted by $C_\nu^{+(-)}$ in [16]. Associated to these orientations there are four pairs E_ν^1, E_ν^2 of distinguished parametrices with

$$WF'(E_\nu^1) = \Delta^* \cup C_\nu^1, \quad WF'(E_\nu^2) = \Delta^* \cup C_\nu^2$$

where Δ^* is the diagonal in $(T^*X \setminus 0) \times (T^*X \setminus 0)$. Moreover, Duistermaat & Hörmander show that every parametrix E with $WF'(E)$ contained in $\Delta^* \cup C_\nu^1$ resp. $\Delta^* \cup C_\nu^2$ must be equal to E_ν^1 resp. E_ν^2 modulo \mathcal{C}^∞ . In addition,

$$E_\nu^1 - E_\nu^2 \in I^{1/2-2}(\mathcal{M} \times \mathcal{M}, C')$$

and $E_\nu^1 - E_\nu^2$ is noncharacteristic at every point of C' . Here, $I^\mu(X, \Lambda)$ denotes the space of Lagrangean distributions of order μ over the manifold X associated to the Lagrangean submanifold $\Lambda \subset T^*X \setminus 0$, cf. [28, Def. 25.1.1].

We shall need three particular parametrices: For the forward light cone N_+ we obtain $E_{N_+}^1 = E^R \pmod{\mathcal{C}^\infty}$, the retarded Green's function, for the backward light cone N_- we have the advanced Green's function $E_{N_-}^1 = E^A \pmod{\mathcal{C}^\infty}$ while $E_{N_+ \cup N_-}^1$ is the so-called Feynman parametrix $E^F \pmod{\mathcal{C}^\infty}$. We deduce that $E_{N_+}^1 = E_{N_-}^2 \pmod{\mathcal{C}^\infty}$, in particular

$$E = E^R - E^A \in I^{-3/2}(\mathcal{M} \times \mathcal{M}, C').$$

We next write $E = E^+ + E^-$ with $E^+ := E^F - E^A, E^- := E^R - E^F$. We deduce from [16, Thm. 6.5.7] that

$$E^- = E^R - E^F = E_{N_+}^1 - E_{N_+ \cup N_-}^1 \in I^{-3/2}(\mathcal{M} \times \mathcal{M}, (C^-)') \quad (62)$$

$$E^+ = E^F - E^A = E_{N_+ \cup N_-}^1 - E_{N_-}^1 \in I^{-3/2}(\mathcal{M} \times \mathcal{M}, (C^+)') \quad (63)$$

where $C^+ = C \cap (N_+ \times N_+)$, $C^- = C \cap (N_- \times N_-)$ as in Eq. (16).

It follows from [41, Thm. 5.1] that the two-point function Λ_H of every Hadamard state coincides with $iE^+ \pmod{\mathcal{C}^\infty}$. (We define the physical Feynman propagator by $F(x, y) := -i\langle T\Phi(x)\Phi(y) \rangle$, i.e. $-i \times$ the expectation value of the time ordered product of two field operators. From this choice it follows that $iF = \Lambda_H + iE^A$ and hence $F = E^F \pmod{\mathcal{C}^\infty}$ and $\Lambda_H = iE^+ \pmod{\mathcal{C}^\infty}$.)

Lemma 5.2 *For every Hadamard state Λ_H we have*

$$WF'^s(\Lambda_H) = WF'^s(E^+) = \begin{cases} \emptyset, & s < -\frac{1}{2} \\ C^+, & s \geq -\frac{1}{2} \end{cases}.$$

Proof: The statement for $s < -1/2$ follows from Eq. (63) and Proposition B.10. For $s \geq -1/2$ we rely on [16, Section 6]. According to [16, Eq. (6.6.1)]

$$E_{N_+ \cup N_-}^1 + E_\emptyset^1 = E_{N_+}^1 + E_{N_-}^1 \text{ mod } \mathcal{C}^\infty,$$

so that, in the notation of [16, Eq. (6.6.3)],

$$E^+ = E_{N_+}^1 - E_\emptyset^1 = S_{N_+}.$$

The symbol of S_{N_+} is computed in [16, Thm. 6.6.1]. It is non-zero on the diagonal Δ_N in $N \times N$. Moreover, it satisfies a homogenous first order ODE along the bicharacteristics of P in each pair of variables, so that it is non-zero everywhere on C^+ . Hence E^+ is non-characteristic at every point of C^+ . Now Proposition B.10 gives the assertion. \blacksquare

We fix a normal coordinate t which allows us to identify a neighborhood of Σ in \mathcal{M} with $(-T, T) \times \Sigma =: \mathcal{M}_T$. We assume that $R_l = \{R_l(t); -T < t < T\}$ and $J_l = \{J_l(t); -T < t < T\}, l = 1, 2$, are smooth families of properly supported pseudodifferential operators on Σ with local symbols $r_l = r_l(t) \in \mathcal{C}^\infty((-T, T), S^0(\Sigma \times \mathbb{R}^3))$ and $j_l = j_l(t) \in \mathcal{C}^\infty((-T, T), S^1(\Sigma \times \mathbb{R}^3))$. Moreover, let $H = \{H(t); -T < t < T\}$ be a smooth family of properly supported pseudodifferential operators of order -1 on Σ . We can then also view R_l, J_l , and H as operators on, say, $\mathcal{C}_0^\infty((-T, T) \times \Sigma)$.

Theorem 5.3 *Let R_l, J_l , and H be as above, and let Q_l be a properly supported first order pseudodifferential operator on $(-T, T) \times \Sigma$ such that*

$$Q_l(R_l - iJ_l - \partial_t)E^- = S_l^{(N)}E^-, \quad l = 1, 2, \quad (64)$$

with $S_l^{(N)} = S_l^{(N)}(t) \in \mathcal{C}^\infty((-T, T), L^{-N}(\Sigma))$ a smooth family of properly supported pseudodifferential operators on Σ of order $-N$. Moreover, we assume that Q_l has a real-valued principal symbol such that

$$\text{char } Q_l \cap N_- = \emptyset.$$

Then the distribution $D_N \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$, defined by

$$D_N(f_1, f_2) = \langle [(R_1 - iJ_1)\rho_0 - \rho_1] E f_1, H [(R_2 - iJ_2)\rho_0 - \rho_1] E f_2 \rangle$$

satisfies the relation

$$WF^{s'}(D_N) \subset \begin{cases} \emptyset, & s < -1/2 \\ C^+, & -1/2 \leq s < N + 3/2. \end{cases} \quad (65)$$

Note that D_N will in general not be a two-point function unless $R_1 = R_2$ and $J_1 = J_2 = H^{-1}$ are selfadjoint and J is positive (compare Theorem 5.1).

Proof: Since ρ_0 commutes with R_l, J_l and H we have

$$D_N(f_1, f_2) = \langle \rho_0 [R_1 - iJ_1 - \partial_t] E f_1, \rho_0 H [R_2 - iJ_2 - \partial_t] E f_2 \rangle. \quad (66)$$

Denoting by K_1 and K_2 the distributional kernels of $(R_1 - iJ_1 - \partial_t)E$ and $H(R_2 - iJ_2 - \partial_t)E$, respectively, we see that

$$D_N = (\rho_0 K_1)^*(\rho_0 K_2).$$

We shall apply the calculus of Fourier integral operators in order to analyze the composition $(\rho_0 K_1)^*(\rho_0 K_2)$. The following lemma is similar in spirit to [28, Thm. 25.2.4].

Lemma 5.4 *Let $X \subset \mathbb{R}^{n_1}, Y \subset \mathbb{R}^{n_2}$ be open sets and $A \in L^k(X)$ be a properly supported pseudodifferential operator with symbol $a(x, \xi)$. Assume that C is a homogeneous canonical relation from $T^*Y \setminus 0$ to $T^*X \setminus 0$ and that $a(x, \xi)$ vanishes on a conic neighborhood of the projection of C in $T^*X \setminus 0$. If $B \in I^m(X \times Y, C')$ then*

$$AB \in I^{-\infty}(X \times Y, C').$$

Proof: The problem is microlocal, so we may assume that B has the form

$$Bu(x) = \int e^{i\phi(x,y,\xi)} b(x, y, \xi) u(y) dy d^N \xi,$$

where ϕ is a non-degenerate phase function on $X \times Y \times (\mathbb{R}^N \setminus \{0\})$ and $b \in S^{m+(n_1+n_2-2N)/4}(X \times Y \times \mathbb{R}^N)$ an amplitude. We know that $C = T_\phi(C_\phi)$, where

$$C_\phi := \{(x, y, \xi) \in X \times Y \times (\mathbb{R}^N \setminus \{0\}); d_\xi \phi(x, y, \xi) = 0\},$$

and T_ϕ is the map

$$\begin{aligned} T_\phi : X \times Y \times (\mathbb{R}^N \setminus \{0\}) &\rightarrow T^*(X \times Y) \setminus 0 \\ (x, y, \xi) &\mapsto (x, d_x \phi; y, d_y \phi). \end{aligned}$$

We recall that $\text{ess supp } b$ is the smallest closed conic subset of $X \times Y \times (\mathbb{R}^N \setminus \{0\})$ outside of which b is of class $S^{-\infty}$ and that the wavefront set of the kernel of B is contained in the set

$$T_\phi(C_\phi \cap \text{ess supp } b),$$

cf. [15, Thm. 2.2.2]. Hence we may assume that b vanishes outside a conic neighborhood \mathcal{N} of C_ϕ in $X \times Y \times \mathbb{R}^N$. In fact we can choose this neighborhood so small that $a(x, \xi') = 0$ whenever (x, ξ') lies in the projection of $T_\phi(\mathcal{N}) \subset T^*X \times T^*Y$ onto the first component (we call this projection π_1). Then

$$ABu(x) = \int e^{i\phi(x,y,\xi)} c(x, y, \xi) u(y) dy d^N \xi$$

where

$$c(x, y, \xi) = e^{-i\phi(x,y,\xi)} A(b(\cdot, y, \xi)) e^{i\phi(\cdot, y, \xi)}.$$

According to [44, Ch. VIII, Eq. (7.8)], c has the asymptotic expansion

$$c(x, y, \xi) \sim \sum_{\substack{\alpha \geq 0 \\ \beta \leq \alpha}} D_\xi^\alpha a(x, d_x \phi(x, y, \xi)) D_x^\beta b(x, y, \xi) \psi_{\alpha\beta}(x, y, \xi) \quad (67)$$

where $\psi_{\alpha\beta}$ is a polynomial in ξ of degree $\leq |\alpha - \beta|/2$. Now from our assumptions on a and b it follows that in Eq. (67)

$$\begin{aligned} b(x, y, \xi) &= 0 \quad \text{if } (x, y, \xi) \notin \mathcal{N} \\ a(x, \xi') &= 0 \quad \text{if } (x, \xi') \in \pi_1 T_\phi(\mathcal{N}) \quad \Rightarrow \quad a(x, d_x \phi(x, y, \xi)) = 0 \quad \text{if } (x, y, \xi) \in \mathcal{N}, \end{aligned}$$

and hence $c \sim 0$. This proves that $AB \in I^{-\infty}(X \times Y, C')$. \blacksquare

Lemma 5.5 *Let $A \in \mathcal{C}^\infty((-T, T), L^k(\Sigma))$ be properly supported and $B \in I^m(\mathcal{M} \times \mathcal{M}, (C^\pm)')$. Then*

$$AB \in I^{m+k}(\mathcal{M}_T \times \mathcal{M}, (C^\pm)').$$

Proof: Choosing local coordinates and a partition of unity we may assume that $\mathcal{M} = \mathbb{R}^4$, $\Sigma = \mathbb{R}^3 \cong \mathbb{R}^3 \times \{0\} \subset \mathbb{R}^4$ and that A is supported in a compact set. We let $X = \text{op } \chi$ where $\chi = \chi(\tau, \xi) \in \mathcal{C}^\infty(\mathbb{R}^4)$ vanishes near $(\tau, \xi) = 0$ and is homogeneous of degree 0 for $|(\tau, \xi)| \geq 1$ with $\chi(\tau, \xi) = 1$ for (τ, ξ) in a conic neighborhood of $\{\xi = 0\}$, and $\chi(\tau, \xi) = 0$ for (τ, ξ) outside a larger conic neighborhood of $\{\xi = 0\}$, such that, in particular, $\chi(\tau, \xi) = 0$ in a neighborhood of $\pi_1(C^\pm)$ (by π_1 we denote the projection onto the first component in $T^*\mathcal{M} \times T^*\mathcal{M}$, i.e. $\pi_1(x, \xi; y, \eta) := (x, \xi)$). We have

$$AB = AXB + A(1 - X)B.$$

Denoting by $a(t, \mathbf{x}, \xi)$ the local symbol of A , the operator $A(1 - X)$ has the symbol

$$a(t, \mathbf{x}, \xi)(1 - \chi(\tau, \xi)) \in S^k(\mathbb{R}^4 \times \mathbb{R}^4).$$

(Here we have used the fact that $(1 - \chi(\tau, \xi))$ is non-zero only in the area where $\langle \tau \rangle$ can be estimated by $\langle \xi \rangle$.) Hence $A(1 - X)$ is a properly supported pseudodifferential operator of order k on \mathcal{M}_T . We may apply [28, Thm. 25.2.3] with excess equal to zero and obtain that $A(1 - X)B \in I^{m+k}(\mathcal{M}_T \times \mathcal{M}, (C^\pm)').$

On the other hand, X is a pseudodifferential operator with symbol vanishing in a neighborhood of $\pi_1(C^\pm)$. According to Lemma 5.4, $XB \in I^{-\infty}(\mathcal{M} \times \mathcal{M}, (C^\pm)').$ Hence XB is an integral operator with a smooth kernel on $\mathcal{M} \times \mathcal{M}$, and so is AXB , since A is continuous on $\mathcal{C}^\infty(\mathcal{M})$. \blacksquare

Lemma 5.6 (i) $(R_l - iJ_l - \partial_t)E^+ \in I^{-1/2}(\mathcal{M}_T \times \mathcal{M}, (C^+)')$, $l = 1, 2$;
(ii) $H(R_2 - iJ_2 - \partial_t)E^+ \in I^{-3/2}(\mathcal{M}_T \times \mathcal{M}, (C^+)')$;
(iii) $(R_l - iJ_l - \partial_t)E^- \in I^{-N-5/2}(\mathcal{M}_T \times \mathcal{M}, (C^-)'),$ $l = 1, 2$;
(iv) $H(R_2 - iJ_2 - \partial_t)E^- \in I^{-N-7/2}(\mathcal{M}_T \times \mathcal{M}, (C^-)').$

Proof: (i) It follows from (63) and Lemma 5.5 that $(R_l - iJ_l)E^+ \in I^{-1/2}(\mathcal{M}_T \times \mathcal{M}, (C^+)')$. Since ∂_t is a differential operator, the assumptions of the composition theorem for Fourier integral operators [28, Thm. 25.2.3] are met with excess equal to zero, and we conclude from

(63) that also $\partial_t E^+ \in I^{-1/2}(\mathcal{M}_T \times \mathcal{M}, (C^+)')$.

Since, by assumption, $H \in \mathcal{C}^\infty((-T, T), L^{-1}(\Sigma))$ is properly supported we also obtain (ii).

(iii) We know from (64) that

$$Q_l(R_l - iJ_l - \partial_t)E^- = S_l^{(N)}E^-. \quad (68)$$

Applying Lemma 5.5 and (62), the right hand side is an element of $I^{-3/2-N}(\mathcal{M}_T \times \mathcal{M}, (C^-)')$ (note that $S_l^{(N)}$ is properly supported). We next observe that the question is local, so that we can focus on a small neighborhood U of a point $x_0 \in \mathcal{M}$. Here, we write $Q_l = Q_l^{(1)} + Q_l^{(2)}$ as a sum of two pseudodifferential operators, where $Q_l^{(1)}$ is elliptic, and the essential support of $Q_l^{(2)}$ is contained in the complement of N_- . To this end choose a real-valued function $\chi \in \mathcal{C}^\infty(T^*U)$ with the following properties:

(α) $\chi(x, \xi) = 0$ for small $|\xi|$,

(β) χ is homogeneous of degree 1 for $|\xi| \geq 1$,

(γ) $\chi(x, \xi) \equiv 0$ on a conic neighborhood of N_- ,

(δ) $\chi(x, \xi) \equiv |\xi|$ on a neighborhood of $\text{char } Q_l \cap \{|\xi| \geq 1\}$.

We denote the local symbol of Q_l by q_l and let

$$Q_l^{(1)} := \text{op}(q_l(x, \xi) + i\chi(x, \xi)), \quad Q_l^{(2)} := \text{op}(-i\chi(x, \xi)).$$

By the Lemmata 5.4 and 5.5 we have

$$Q_l^{(2)}(R_l - iJ_l - \partial_t)E^- \in I^{-\infty}(\mathcal{M}_T \times \mathcal{M}, (C^-)').$$

Moreover, $Q_l^{(1)}$ is elliptic of order 1, since q_l is real-valued and $\chi(x, \xi) = |\xi|$ on $\text{char } Q_l$. We conclude from (68) that

$$Q_l^{(1)}(R_l - iJ_l - \partial_t)E^- \in I^{-3/2-N}(\mathcal{M}_T \times \mathcal{M}, (C^-)').$$

Multiplication by a parametrix to $Q_l^{(1)}$ shows that

$$(R_l - iJ_l - \partial_t)E^- \in I^{-5/2-N}(\mathcal{M}_T \times \mathcal{M}, (C^-)').$$

(iv) follows from (iii) and Lemma 5.5. ■

We next analyze the effect of the restriction operator ρ_0 . We recall from [15, p. 113] that

$$\rho_0 \in I^{1/4}(\Sigma \times \mathcal{M}, R'_0) \quad (69)$$

where

$$R_0 := \{(x_o, \xi_o; x, \xi) \in (T^*\Sigma \times T^*\mathcal{M}) \setminus 0; x_o = x, \xi_o = \xi|_{T_{x_o}\Sigma}\}.$$

Lemma 5.7

$$\begin{aligned} \rho_0 H(R_2 - iJ_2 - \partial_t)E^- &\in I^{-N-13/4}(\Sigma \times \mathcal{M}, (R_0 \circ C^-)') \\ \rho_0(R_1 - iJ_1 - \partial_t)E^- &\in I^{-N-9/4}(\Sigma \times \mathcal{M}, (R_0 \circ C^-)') \\ \rho_0(R_1 - iJ_1 - \partial_t)E^+ &\in I^{-1/4}(\Sigma \times \mathcal{M}, (R_0 \circ C^+)') \\ \rho_0 H(R_2 - iJ_2 - \partial_t)E^+ &\in I^{-5/4}(\Sigma \times \mathcal{M}, (R_0 \circ C^+)'). \end{aligned}$$

Proof: All these statements follow from (69), Lemma 5.6 and the composition formula for Fourier integral operators [28, Thm. 25.2.3], provided that the compositions $R_0 \circ C^-$ and $R_0 \circ C^+$ of the canonical relations are clean, proper and connected with excess zero (cf. [27, C.3] and [28, p. 18] for notation). We note that

$$\begin{aligned} & (R_0 \times C^+) \cap (T^*\Sigma \times \text{diag}(T^*\mathcal{M}) \times T^*\mathcal{M}) \\ &= \{(x_o, \xi_o; x, \xi; x, \xi; y, \eta); x = x_o, \xi_o = \xi|_{T_{x_o}\Sigma}, (x, \xi; y, \eta) \in C^+\}. \end{aligned} \quad (70)$$

Given $(x_o, \xi_o) \in T^*\Sigma \setminus 0$ there is precisely one $(x, \xi) \in N_+$ such that $x = x_o$ and $\xi|_{T_{x_o}\Sigma} = \xi_o$; given $(x, \xi) \in N_+$ there is a 1-parameter family of (y, η) such that $(x, \xi; y, \eta) \in C^+$. We deduce that

$$\begin{aligned} & \text{codim}(R_0 \times C^+) + \text{codim}(T^*\Sigma \times \text{diag}(T^*\mathcal{M}) \times T^*\mathcal{M}) \\ &= 6 \dim \mathcal{M} - 1 = \text{codim}(R_0 \times C^+) \cap (T^*\Sigma \times \text{diag}(T^*\mathcal{M}) \times T^*\mathcal{M}); \end{aligned}$$

here the codimension is taken in $T^*\Sigma \times (T^*\mathcal{M})^3$. Hence the excess of the intersection, i.e. the difference of the left and the right hand side, is zero. In particular, the intersection is transversal, hence clean. Moreover, the fact that in (70) the (x, ξ) is uniquely determined as soon as (x_o, ξ_o) and (y, η) are given shows that the associated map

$$(x_o, \xi_o; x, \xi; x, \xi; y, \eta) \mapsto (x_o, \xi_o; y, \eta)$$

is proper (i.e. the pre-image of a compact set is compact). Indeed, the pre-image of a closed and bounded set is trivially closed; it is bounded, because $|\xi| \leq C|\xi_o|$ for some constant C . Finally, the pre-image of a single point $(x_o, \xi_o; y, \eta)$ is again a single point, in particular a connected set.

An analogous argument applies to $R_0 \circ C^-$. ■

Lemma 5.8 (i) $(\rho_0(R_1 - iJ_1 - \partial_t)E^-)^*(\rho_0H(R_2 - iJ_2 - \partial_t)E^-) \in I^{-2N-11/2}(\mathcal{M} \times \mathcal{M}, (C^-)'),$
(ii) $(\rho_0(R_1 - iJ_1 - \partial_t)E^+)^*(\rho_0H(R_2 - iJ_2 - \partial_t)E^+) \in I^{-3/2}(\mathcal{M} \times \mathcal{M}, (C^+)').$

Denoting by D^\pm the relation $(R_0 \circ C^\mp)^{-1} \circ (R_0 \circ C^\pm)$ we have

(iii) $(\rho_0(R_1 - iJ_1 - \partial_t)E^+)^*(\rho_0H(R_2 - iJ_2 - \partial_t)E^-) \in I^{-N-7/2}(\mathcal{M} \times \mathcal{M}, (D^-)'),$
(iv) $(\rho_0(R_1 - iJ_1 - \partial_t)E^-)^*(\rho_0H(R_2 - iJ_2 - \partial_t)E^+) \in I^{-N-7/2}(\mathcal{M} \times \mathcal{M}, (D^+)').$

Proof: (i) According to [28, Thm. 25.2.2] and Lemma 5.7

$$(\rho_0(R_1 - iJ_1 - \partial_t)E^-)^* \in I^{-N-9/4}(\mathcal{M} \times \Sigma, ((R_0 \circ C^-)^{-1})).$$

We first note that the composition $(R_0 \circ C^-)^{-1} \circ (R_0 \circ C^-)$ equals C^- : In fact, $(R_0 \circ C^-)^{-1}$ is the set of all $(y, \eta; x_o, \xi_o)$, where $(x_o, \xi_o) \in T^*\Sigma$, y is joined to x_o by a null geodesic γ , $\eta \in N_-$ is cotangent to γ at y and the projection $P_\gamma(\eta)|_{T_{x_o}\Sigma}$ of the parallel transport of η along γ

coincides with ξ_o . The codimension of $(R_0 \circ C^-)^{-1} \times (R_0 \circ C^-)$ in $T^*\mathcal{M} \times T^*\Sigma \times T^*\Sigma \times T^*\mathcal{M}$ therefore equals $4 \dim \Sigma + 2$, and we have

$$\begin{aligned} & \text{codim}((R_0 \circ C^-)^{-1} \times (R_0 \circ C^-)) + \text{codim}(T^*\mathcal{M} \times \text{diag}(T^*\Sigma) \times T^*\mathcal{M}) \\ &= 6 \dim \Sigma + 2 \\ &= \text{codim}((R_0 \circ C^-)^{-1} \times (R_0 \circ C^-)) \cap (T^*\mathcal{M} \times \text{diag}(T^*\Sigma) \times T^*\mathcal{M}). \end{aligned}$$

In particular, the intersection of $(R_0 \circ C^-)^{-1} \times (R_0 \circ C^-)$ and $T^*\mathcal{M} \times \text{diag}(T^*\Sigma) \times T^*\mathcal{M}$ is transversal in $T^*\mathcal{M} \times T^*\Sigma \times T^*\Sigma \times T^*\mathcal{M}$, hence clean with excess 0.

Given $(y, \eta; x_o, \xi_o; x_o, \xi_o; \tilde{y}, \tilde{\eta})$ in the intersection, the element (x_o, ξ_o) is uniquely determined by (y, η) and $(\tilde{y}, \tilde{\eta})$. The mapping

$$(y, \eta; x_o, \xi_o; x_o, \xi_o; \tilde{y}, \tilde{\eta}) \mapsto (y, \eta; \tilde{y}, \tilde{\eta})$$

therefore is proper. The pre-image of each element is a single point, hence a connected set. We can apply the composition theorem [28, Thm. 25.2.3] and obtain the assertion. The proof of (ii), (iii) and (iv) is analogous. \blacksquare

We can now finish the proof of Theorem 5.3. According to (66) and the following remarks we have to find the wavefront set of

$$(\rho_0(R_1 - iJ_1 - \partial_t)(E^+ + E^-))^*(\rho_0 H(R_2 - iJ_2 - \partial_t)(E^+ + E^-)).$$

By Proposition B.10 we have, for an arbitrary canonical relation Λ ,

$$I^\mu(\mathcal{M} \times \mathcal{M}, \Lambda) \subset H^s(\mathcal{M} \times \mathcal{M})$$

if $\mu + \frac{1}{2} \dim \mathcal{M} + s < 0$; moreover, the wavefront set of elements of $I^\mu(\mathcal{M} \times \mathcal{M}, \Lambda)$ is a subset of Λ . Lemma 5.8 therefore immediately implies (65). \blacksquare

5.2 Construction on a compact Cauchy surface

Following the idea in [31] we shall now show that one can construct adiabatic vacuum states on any globally hyperbolic spacetime \mathcal{M} with compact Cauchy surface Σ .

In Gaussian normal coordinates w.r.t. Σ the metric reads

$$g_{\mu\nu} = \begin{pmatrix} 1 & \\ & -h_{ij}(t, \mathbf{x}) \end{pmatrix}$$

and the Klein-Gordon operator reduces to

$$\square_g + m^2 = \frac{1}{\sqrt{\mathfrak{h}}} \partial_t(\sqrt{\mathfrak{h}} \partial_t \cdot) - \Delta_\Sigma + m^2,$$

where h_{ij} is the induced Riemannian metric on Σ , \mathfrak{h} its determinant and Δ_Σ the Laplace-Beltrami operator w.r.t. h_{ij} acting on Σ . Following [31, Eq. (130)ff.] there exist operators $P_1^{(N)}, P_2^{(N)}$, $N = 0, 1, 2, \dots$, of the form

$$\begin{aligned} P_1^{(N)} &= -a^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) - \frac{1}{\sqrt{\mathfrak{h}}} \partial_t \sqrt{\mathfrak{h}} \\ P_2^{(N)} &= a^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) - \partial_t \end{aligned}$$

with $a^{(N)} = a^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) \in \mathcal{C}^\infty([-T, T], L^1(\Sigma))$ such that

$$P_1^{(N)} \circ P_2^{(N)} - (\square_g + m^2) = s_N(t, \mathbf{x}, D_{\mathbf{x}}) \quad (71)$$

with $s_N \in \mathcal{C}^\infty([-T, T], L^{-N}(\Sigma))$. In fact one gets

$$a^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) = -iA^{1/2} + \sum_{\nu=1}^{N+1} b^{(\nu)}(t, \mathbf{x}, D_{\mathbf{x}});$$

here A is the self-adjoint extension of $-\Delta_\Sigma + m^2$ on $L^2(\Sigma)$, so that $A^{1/2}$ is an elliptic pseudodifferential operator of order 1. The $b^{(\nu)}$ are elements of $\mathcal{C}^\infty([-T, T], L^{1-\nu}(\Sigma))$ defined recursively so that (71) holds. One then sets similarly as in [31, Eq. (134)]

$$j^{(N)}(t, \mathbf{x}, \xi) := -\frac{1}{2i} \sum_{\nu=1}^{N+1} \left[b^{(\nu)}(t, \mathbf{x}, \xi) - \overline{b^{(\nu)}(t, \mathbf{x}, -\xi)} \right] \in S^0 \quad (72)$$

$$r^{(N)}(t, \mathbf{x}, \xi) := \frac{1}{2} \sum_{\nu=1}^{N+1} \left[b^{(\nu)}(t, \mathbf{x}, \xi) + \overline{b^{(\nu)}(t, \mathbf{x}, -\xi)} \right] \in S^0 \quad (73)$$

$$J(t) := A^{1/2} + \frac{1}{2} \left[j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^* \right] \in L^1$$

$$R(t) := \frac{1}{2} \left[r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^* \right] \in L^0.$$

Lemma 5.9 *We can change the operator J defined above by a family of regularizing operators such that the assumptions of Theorem 5.1 are met.*

Proof: It is easily checked that a pseudodifferential operator on \mathbb{R}^n with symbol $\overline{a(x, \xi)}$ maps $\mathcal{C}_0^\infty(\mathbb{R}^n, \mathbb{R})$ to $L_{\mathbb{R}}^2(\mathbb{R}^n)$ (i.e. commutes with complex conjugation) iff $a(x, \xi) = \overline{a(x, -\xi)}$. The symbols $j^{(N)}$ and $r^{(N)}$ have this property by construction.

The operator family $R(t) = \frac{1}{2} (r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^*) \in L^0$ is bounded and symmetric, hence selfadjoint. Moreover, it commutes with complex conjugation: If $v \in L_{\mathbb{R}}^2(\Sigma, d^3\sigma)$, then $R(t)v$ is real-valued, since for every $u \in L_{\mathbb{R}}^2(\Sigma, d^3\sigma)$

$$2\langle u, R(t)v \rangle = \langle u, (r^{(N)} + r^{(N)*})v \rangle = \langle u, r^{(N)}v \rangle + \langle r^{(N)}u, v \rangle \in \mathbb{R}.$$

The operator $A^{1/2}$ maps $\mathcal{C}_0^\infty(\Sigma, \mathbb{R})$ to $L_{\mathbb{R}}^2(\Sigma, d^3\sigma)$ by (61); it is selfadjoint on $\mathcal{D}(A^{1/2}) = H^1(\Sigma)$. Hence J defines a selfadjoint family of pseudodifferential operators of order 1; it

is invariant under complex conjugation. Moreover, its principal symbol is $\sqrt{h^{ij}\xi_i\xi_j} > 0$. According to [44, Ch. II, Lemma 6.2] there exists a family of regularizing operators $J_\infty = J_\infty(t)$ such that $J + J_\infty$ is strictly positive. Replacing J_∞ by $\frac{1}{2}(J_\infty + CJ_\infty C)$, where C here denotes the operator of complex conjugation, we obtain an operator which is both strictly positive and invariant under complex conjugation. It differs from J by a regularizing family. \blacksquare

Theorem 5.10 *For $N = 0, 1, 2, \dots$ we let*

$$\Lambda_N(f_1, f_2) = \frac{1}{2} \langle [(R - iJ)\rho_0 - \rho_1] E f_1, J^{-1} [(R - iJ)\rho_0 - \rho_1] E f_2 \rangle$$

with J modified as in Lemma 5.9. Then Λ_N is the two-point function of a (pure) adiabatic vacuum state of order N .

Proof: By Theorem 5.1 and Lemma 5.9, Λ_N defines the two-point function of a (pure) quasifree state. We write

$$\begin{aligned} R(t) &= \frac{1}{2} r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + \frac{1}{2} r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^* \\ J(t) &= \frac{1}{2} (A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})) + \frac{1}{2} (A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^*) + j_\infty(t, \mathbf{x}, D_{\mathbf{x}}) \end{aligned}$$

with $r^{(N)}, j^{(N)}$ as in (72), (73) and j_∞ the regularizing modification of Lemma 5.9. We shall use Theorem 5.3 to analyze the wavefront set of Λ_N . We decompose

$$\begin{aligned} \Lambda_N(f_1, f_2) &= \\ &\frac{1}{8} \langle [(r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) - i(A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + 2j_\infty(t, \mathbf{x}, D_{\mathbf{x}}))) \rho_0 - \rho_1] E f_1 \\ &+ [(r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^* - i(A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^*)) \rho_0 - \rho_1] E f_1, \\ &J(t)^{-1} [(r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) - i(A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + 2j_\infty(t, \mathbf{x}, D_{\mathbf{x}}))) \rho_0 - \rho_1] E f_2 \\ &+ J(t)^{-1} [(r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^* - i(A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^*)) \rho_0 - \rho_1] E f_2 \rangle. \end{aligned} \quad (74)$$

Now we let

$$\begin{aligned} \tilde{Q}_1(t) &:= A^{1/2} + i(r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) - ij^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})) + \frac{i}{\sqrt{\hbar}} \partial_t \sqrt{\hbar} \\ &= i \left(a^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) + \frac{1}{\sqrt{\hbar}} \partial_t \sqrt{\hbar} \right) = -iP_1^{(N)} \end{aligned} \quad (75)$$

and

$$\tilde{Q}_2(t) := A^{1/2} + i(r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^* - ij^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})^*) + \frac{i}{\sqrt{\hbar}} \partial_t \sqrt{\hbar}. \quad (76)$$

Equation (71) implies that

$$\begin{aligned} &i\tilde{Q}_1(t) (r^{(N)}(t, \mathbf{x}, D_{\mathbf{x}}) - i(A^{1/2} + j^{(N)}(t, \mathbf{x}, D_{\mathbf{x}})) - 2ij_\infty(t, \mathbf{x}, D_{\mathbf{x}}) - \partial_t) \\ &= P_1^{(N)} \left(P_2^{(N)} - 2ij_\infty(t, \mathbf{x}, D_{\mathbf{x}}) \right) \\ &= \square_g + m^2 + \tilde{s}_N(t, \mathbf{x}, D_{\mathbf{x}}) \end{aligned} \quad (77)$$

where \tilde{s}_N differs from s_N in (71) by an element in $\mathcal{C}^\infty([-T, T], L^{-\infty}(\Sigma))$. Next we note that (71) is equivalent to the identity

$$\left(-r^{(N)} + i(A^{1/2} + j^{(N)}) - \frac{1}{\sqrt{\mathfrak{h}}} \partial_t \sqrt{\mathfrak{h}} \right) (r^{(N)} - i(A^{1/2} + j^{(N)}) - \partial_t) = \square_g + m^2 + s_N$$

which in turn is equivalent to

$$\begin{aligned} & (-r^{(N)} + i(A^{1/2} + j^{(N)})) (r^{(N)} - i(A^{1/2} + j^{(N)})) - \frac{1}{\sqrt{\mathfrak{h}}} \partial_t \left(\sqrt{\mathfrak{h}} (r^{(N)} - i(A^{1/2} + j^{(N)})) \right) \\ &= -\Delta_\Sigma + m^2 + s_N \end{aligned}$$

or - taking adjoints and conjugating with the operator C of complex conjugation -

$$\begin{aligned} & -C (r^{(N)*} + i(A^{1/2} + j^{(N)*})) C C (r^{(N)*} + i(A^{1/2} + j^{(N)*})) C \\ & \quad - \frac{1}{\sqrt{\mathfrak{h}}} \partial_t \left(\sqrt{\mathfrak{h}} C (r^{(N)*} + i(A^{1/2} + j^{(N)*})) C \right) \\ &= C(-\Delta_\Sigma + m^2 + s_N^*) C = -\Delta_\Sigma + m^2 + C s_N^* C. \end{aligned} \tag{78}$$

Here we have used the fact that

$$\left[\partial_t \left(\sqrt{\mathfrak{h}} (r^{(N)} - i(A^{1/2} + j^{(N)})) \right) \right]^* = \partial_t \left[\sqrt{\mathfrak{h}} (r^{(N)} - i(A^{1/2} + j^{(N)})) \right]^*.$$

Using that $r^{(N)*}$, $j^{(N)*}$ and $A^{1/2}$ commute with C , (78) reads

$$\begin{aligned} & - (r^{(N)*} - i(A^{1/2} + j^{(N)*})) (r^{(N)*} - i(A^{1/2} + j^{(N)*})) - \frac{1}{\sqrt{\mathfrak{h}}} \partial_t \left(\sqrt{\mathfrak{h}} (r^{(N)*} - i(A^{1/2} + j^{(N)*})) \right) \\ &= -\Delta_\Sigma + m^2 + C s_N^* C. \end{aligned}$$

Adding the time derivatives, it follows that

$$\begin{aligned} & i\tilde{Q}_2(t) (r^{(N)*} - i(A^{1/2} + j^{(N)*}) - \partial_t) \\ &= \left(-r^{(N)*} + i(A^{1/2} + j^{(N)*}) - \frac{1}{\sqrt{\mathfrak{h}}} \partial_t \sqrt{\mathfrak{h}} \right) (r^{(N)*} - i(A^{1/2} + j^{(N)*}) - \partial_t) \\ &= \square_g + m^2 + C s_N^* C. \end{aligned} \tag{79}$$

Note that the operators \tilde{Q}_1 and \tilde{Q}_2 , defined by Eq.s (75) and (76), are not yet pseudodifferential operators since their symbols will not decay in the covariable of t , say τ , if we take derivatives w.r.t. the covariables of \mathbf{x} , say ξ . To make them pseudodifferential operators we choose a finite number of coordinate neighborhoods $\{U_j\}$ for Σ , which yields finitely many coordinate neighborhoods for $(-T, T) \times \Sigma$. As (t, \mathbf{x}) varies over $(-T, T) \times U_j$, the negative light cone will not intersect a fixed conic neighborhood \mathcal{N} of $\{\xi = 0\}$ in $T^*((-T, T) \times U_j)$. We choose a real-valued function χ which is smooth on $T^*((-T, T) \times U_j)$, zero for $|(\tau, \xi)| \leq 1/2$, homogeneous of degree zero for $|(\tau, \xi)| \geq 1$ such that

$$\begin{aligned} \chi(t, \mathbf{x}, \tau, \xi) &= 0 \quad \text{on a conic neighborhood of } \{\xi = 0\} \\ \chi(t, \mathbf{x}, \tau, \xi) &= 1 \quad \text{outside } \mathcal{N}. \end{aligned} \tag{80}$$

We now let $X := \text{op } \chi$. Then

$$Q_1 := X\tilde{Q}_1 \quad \text{and} \quad Q_2 := X\tilde{Q}_2$$

are pseudodifferential operators due to (80). Their principal symbols are $((h^{ij}\xi_i\xi_j)^{1/2} - \tau)\chi(t, \mathbf{x}, \tau, \xi)$, so that their characteristic set does not intersect N_- . Eq.s (77), (79) and the fact that $(\square_g + m^2)E^- = 0$ show that the assumption of Theorem 5.3 is satisfied for each of the four terms arising from the decomposition of Λ_N in (74). This yields the assertion. ■

Lemma 5.8 explicitly shows that the non-Hadamard like singularities of the two-point function Λ_N in Theorem 5.10 (i.e. those not contained in the canonical relation C^+) are either pairs of purely negative frequency singularities lying on a common bicharacteristic (C^-) or pairs of mixed positive/negative frequency singularities (D^\pm) which lie on bicharacteristics that are “reflected” by the Cauchy surface. They may have spacelike separation.

For the states constructed in Theorem 5.10 one can explicitly find the Bogoljubov B -operator, which was introduced in the proof of Theorem 4.7(ii), in terms of the operators R and J . Applying the criterion of Lemma 4.11(iii) one can check the unitary equivalence of the GNS-representations generated by these states. A straightforward (but tedious) calculation shows that unitary equivalence already holds for $N \geq 0$, thus improving the statement of Theorem 4.7(ii) for these particular examples.

6 Adiabatic vacua on Robertson-Walker spaces

By introducing adiabatic vacua on Robertson-Walker spaces Parker [38] was among the first to construct a quantum field theory in a non-trivial background spacetime. A mathematically precise version of his construction and an analysis of the corresponding Hilbert space representations along the same lines as in our Section 4 were given by Lüders & Roberts [35]. Relying on their work we want to show in this section that these adiabatic vacua on Robertson-Walker spaces are indeed adiabatic vacua in the sense of our Definition 3.2. This justifies our naming and gives a mathematically intrinsic meaning to the “order” of an adiabatic vacuum. In [31] one of us had claimed to have shown that all adiabatic vacua on Robertson-Walker spaces are Hadamard states. This turned out to be wrong in general, when the same question was investigated for Dirac fields [24]². So the present section also serves to correct this mistake. Our presentation follows [31].

In order to be able to apply our Theorem 5.3 without technical complications we restrict our attention to Robertson-Walker spaces with compact spatial sections. These are the 4-dim. Lorentz manifolds $\mathcal{M} = \mathbb{R} \times \Sigma$ where Σ is regarded as being embedded in \mathbb{R}^4 as

$$\Sigma = \{x \in \mathbb{R}^4; (x^0)^2 + \sum_{i=1}^3 (x^i)^2 = 1\} \cong S^3,$$

²We want to thank S. Hollands for discussions about this point.

and \mathcal{M} is endowed with the homogeneous and isotropic metric

$$ds^2 = dt^2 - a(t)^2 \left[\frac{dr^2}{1-r^2} + r^2(d\theta^2 + \sin^2 \theta d\varphi^2) \right]; \quad (81)$$

here $\varphi \in [0, 2\pi], \theta \in [0, \pi], r \in [0, 1)$ are polar coordinates for the unit ball in \mathbb{R}^3 , and a is a strictly positive smooth function. In [31] it was shown that an adiabatic vacuum state of order n (as defined in [35]) is a pure quasifree state on the Weyl algebra of the Klein-Gordon field on the spacetime (81) given by a one-particle Hilbert space structure w.r.t. a fixed Cauchy surface $\Sigma_t = \{t = \text{const.}\} = \Sigma \times \{t\}$ (equipped with the induced metric from (81))

$$\begin{aligned} k_n : \Gamma &\rightarrow \mathcal{H}_n := \overline{k_n(\Gamma)} \subset L^2(\Sigma_t) \\ (q, p) &\mapsto (2J_n)^{-1/2} [(R_n - iJ_n)q - p] \end{aligned}$$

of the form (60) of Theorem 5.1, where the operator families $R_n(t), J_n(t)$ acting on $L^2(\Sigma, d^3\sigma)$ are defined in the following way:

$$\begin{aligned} (R_n f)(t, \mathbf{x}) &:= -\frac{1}{2} \int d\mu(\vec{k}) \left(3 \frac{\dot{a}(t)}{a(t)} + \frac{\dot{\Omega}_k^{(n)}(t)}{\Omega_k^{(n)}(t)} \right) \tilde{f}(t, \vec{k}) \phi_{\vec{k}}(\mathbf{x}) \\ (J_n f)(t, \mathbf{x}) &:= \int d\mu(\vec{k}) \Omega_k^{(n)}(t) \tilde{f}(t, \vec{k}) \phi_{\vec{k}}(\mathbf{x}), \end{aligned} \quad (82)$$

with t in some fixed finite interval $I \subset \mathbb{R}$, say. Here, $\{\phi_{\vec{k}}, \vec{k} := (k, l, m), k = 0, 1, 2, \dots; l = 0, 1, \dots, k; m = -l, \dots, l\}$ are the t -independent eigenfunctions of the Laplace-Beltrami operator Δ_Σ w.r.t. the Riemannian metric

$$s_{ij} = \begin{pmatrix} \frac{1}{1-r^2} & & \\ & r^2 & \\ & & r^2 \sin^2 \theta \end{pmatrix} \quad (83)$$

on the hypersurface Σ :

$$\Delta_\Sigma \phi_{\vec{k}} \equiv \left\{ (1-r^2) \frac{\partial^2}{\partial r^2} + \frac{2-3r^2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta(\theta, \varphi) \right\} \phi_{\vec{k}} = -k(k+2) \phi_{\vec{k}},$$

where $\Delta(\theta, \varphi) := \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}$ is the Laplace operator on S^2 . They form an orthonormal basis of $L^2(\Sigma, d^3\sigma)$ with $d^3\sigma := r^2(1-r^2)^{-1/2} dr \sin \theta d\theta d\varphi$. $\tilde{\cdot}$ denotes the generalized Fourier transform

$$\begin{aligned} \tilde{\cdot} : L^2(\Sigma, d^3\sigma) &\rightarrow L^2(\tilde{\Sigma}, d\mu(\vec{k})) \\ f &\mapsto \tilde{f}(\vec{k}) := \int_\Sigma d^3\sigma \overline{\phi_{\vec{k}}(\mathbf{x})} f(\mathbf{x}), \end{aligned} \quad (84)$$

which is a unitary map from $L^2(\Sigma, d^3\sigma)$ to $L^2(\tilde{\Sigma}, d\mu(\vec{k}))$ where $\tilde{\Sigma}$ is the space of values of $\vec{k} = (k, l, m)$ equipped with the measure $\int d\mu(\vec{k}) := \sum_{k=0}^\infty \sum_{l=0}^k \sum_{m=-l}^l$ [35]. (Note that (84)

is defined w.r.t. Σ with the metric s_{ij} , Eq. (83), and not w.r.t. Σ_t with the metric $a^2(t)s_{ij}$.) The inverse is given by

$$f(\mathbf{x}) = \int d\mu(\vec{k}) \tilde{f}(\vec{k}) \phi_{\vec{k}}(\mathbf{x}).$$

Using duality and interpolation of the Sobolev spaces one deduces

Lemma 6.1

$$H^s(\Sigma) = \left\{ f = \int d\mu(\vec{k}) \tilde{f}(\vec{k}) \phi_{\vec{k}}; \int d\mu(\vec{k}) (1 + k^2)^s |\tilde{f}(\vec{k})|^2 < \infty \right\}.$$

The Klein-Gordon operator associated to the metric (81) is given by

$$\square_g + m^2 = \frac{\partial^2}{\partial t^2} + 3 \frac{\dot{a}}{a} \frac{\partial}{\partial t} - \frac{1}{a^2} \Delta_\Sigma + m^2. \quad (85)$$

The functions $\Omega_k^{(n)}(t)$, $n \in \mathbb{N}_0$, in (82) were introduced by Lüders & Roberts. $\Omega_k^{(n)}(t)$ is strictly positive and plays the role of a generalized frequency which is determined by a WKB approximation to Eq. (85). It is iteratively defined by the following recursion relations

$$\begin{aligned} (\Omega_k^{(0)})^2 &:= \omega_k^2 \equiv \frac{k(k+2)}{a^2} + m^2 \\ (\Omega_k^{(n+1)})^2 &= \omega_k^2 - \frac{3}{4} \left(\frac{\dot{a}}{a} \right)^2 - \frac{3}{2} \frac{\ddot{a}}{a} + \frac{3}{4} \left(\frac{\dot{\Omega}_k^{(n)}}{\Omega_k^{(n)}} \right)^2 - \frac{1}{2} \frac{\ddot{\Omega}_k^{(n)}}{\Omega_k^{(n)}}. \end{aligned} \quad (86)$$

In the following we shall study the analytic properties of these functions. We shall see that, using (86), we may express $\Omega_k^{(n)}$ as a function of t and ω_k . As a function of these two variables, it turns out to behave like a classical pseudodifferential symbol. In Lemma 6.2 below we shall derive the corresponding estimates and expansions for $(t, \omega_k) \in I \times \mathbb{R}_+$. It is a little unusual to consider a ‘covariable’ in \mathbb{R}_+ ; in later applications, however, we will have $\omega_k = \sqrt{k(k+2)/a^2 + m^2}$ bounded away from zero, so that the behaviour of ω_k near zero is irrelevant.

We first observe that $(\Omega_k^{(n+1)})^2$ can be determined by an iteration involving only $(\Omega_k^{(n)})^2$ and its time derivatives: Since, for an arbitrary F , we have $\partial_t(F^2)/F^2 = 2\dot{F}/F$, we obtain

$$(\Omega_k^{(n+1)})^2 = \omega_k^2 - \frac{3}{4} \left(\frac{\dot{a}}{a} \right)^2 - \frac{3}{2} \frac{\ddot{a}}{a} + \frac{1}{16} \left(\frac{\frac{d}{dt} \left((\Omega_k^{(n)})^2 \right)}{\Omega_k^{(n)2}} \right)^2 - \frac{1}{4} \frac{d}{dt} \left(\frac{\frac{d}{dt} \left((\Omega_k^{(n)})^2 \right)}{(\Omega_k^{(n)})^2} \right). \quad (87)$$

An induction argument shows that $(\Omega_k^{(n)})^2 - \omega_k^2$ is a rational function in ω_k of degree ≤ 0 with coefficients in $\mathcal{C}^\infty(I)$. Indeed this is trivially true for $n = 0$. Suppose it is proven for some fixed n . We write

$$(\Omega_k^{(n)})^2 - \omega_k^2 = r(t, \omega_k) = \frac{p(t, \omega_k)}{q(t, \omega_k)} \quad (88)$$

with polynomials p and q in ω_k such that $\deg(p) \leq \deg(q)$ and the leading coefficient of q is 1. Then

$$\frac{\frac{d}{dt} \left((\Omega_k^{(n)})^2 \right)}{(\Omega_k^{(n)})^2} = \frac{2\omega_k \dot{\omega}_k + \dot{r}}{\omega_k^2 + r}. \quad (89)$$

In view of the fact that

$$\dot{\omega}_k = -\frac{\dot{a}}{a} \left(\omega_k - \frac{m^2}{\omega_k} \right) \quad \text{and} \quad \dot{r} = \frac{q \partial_{\omega_k} p - p \partial_{\omega_k} q}{q^2} \dot{\omega}_k + \frac{q \partial_t p - p \partial_t q}{q^2},$$

(89) is again rational of degree 0 and the leading coefficient of the polynomial in the denominator again equals 1. The same is true for the time derivatives of (89). The recursion formula (87) then shows the assertion for $n + 1$.

Next we observe that also $\frac{d^l}{dt^l} \left((\Omega_k^{(n)})^2 - \omega_k^2 \right)$ is a rational function of ω_k with coefficients in $\mathcal{C}^\infty(I)$ of degree ≤ 0 . Moreover, this shows that, for sufficiently large ω_k (equivalently for sufficiently large k), $(\Omega_k^{(n)})^2$ is a strictly positive function (uniformly in $t \in I$). We may redefine $(\Omega_k^{(n)})^2$ for small values of ω_k so that it is strictly positive and bounded away from zero on $I \times \mathbb{R}_+$. It makes sense to take its square root, and in the following we shall denote this function by $\Omega_k^{(n)}$. We note:

Lemma 6.2 $\Omega_k^{(n)}$, considered as a function of $(t, \omega) \in I \times \mathbb{R}_+$, is an element of $S_{cl}^1(I \times \mathbb{R}_+)$, i.e.

$$\partial_t^l \partial_\omega^m \Omega_k^{(n)}(t, \omega) = \mathcal{O}(\langle \omega \rangle^{1-m}) \quad (90)$$

and, in addition, $\Omega_k^{(n)}$ has an asymptotic expansion $\Omega_k^{(n)} \sim \sum_{j=0}^{\infty} (\Omega_k^{(n)})_j$ into symbols $(\Omega_k^{(n)})_j \in S^{1-j}$ which are positively homogeneous for large ω . Its principal symbol is ω . With the same understanding

$$\frac{\dot{\Omega}_k^{(n)}}{\Omega_k^{(n)}} \in S_{cl}^0(I \times \mathbb{R}_+), \quad (91)$$

$$(\Omega_k^{(n+1)})^2 - (\Omega_k^{(n)})^2 \in S_{cl}^{-2n}(I \times \mathbb{R}_+). \quad (92)$$

Proof: By induction, (90) is immediate from (88) together with the formulae

$$\partial_t \sqrt{\omega^2 + r(t, \omega)} = \frac{1}{2} \frac{\partial_t r(t, \omega)}{\sqrt{\omega^2 + r(t, \omega)}} \quad \text{and} \quad \partial_\omega \sqrt{\omega^2 + r(t, \omega)} = \frac{1}{2} \frac{2\omega + \partial_\omega r(t, \omega)}{\sqrt{\omega^2 + r(t, \omega)}}.$$

Relation (91) is immediate from (89), noting that $2\dot{\Omega}_k^{(n)}/\Omega_k^{(n)} = \frac{d}{dt} \left((\Omega_k^{(n)})^2 \right) / (\Omega_k^{(n)})^2$. In both cases the existence of the asymptotic expansion follows from [44, Ch. II, Thm. 3.2] and the expansion

$$\sqrt{\omega^2 + r(t, \omega)} = \omega \sqrt{1 + \frac{r(t, \omega)}{\omega^2}} = \omega \sum_{j=0}^{\infty} \binom{1/2}{j} \left(\frac{r(t, \omega)}{\omega^2} \right)^j$$

valid for large ω . The principal symbol of $\Omega_k^{(n)}$ is ω since $(\Omega_k^{(n)})^2 = \omega^2$ modulo rational functions of degree ≤ 0 , as shown above (cf. Eq. (88)). In order to show (92) we write, following Lüders & Roberts,

$$(\Omega_k^{(n+1)})^2 = (\Omega_k^{(n)})^2(1 + \epsilon_{n+1});$$

this yields [35, Eq. (3.9)]

$$\begin{aligned} \epsilon_{n+1} = & \frac{1}{\omega^2} \frac{1}{(1 + \epsilon_1) \cdots (1 + \epsilon_n)} \left(\frac{1}{4} \frac{\dot{\omega}}{\omega} \frac{\dot{\epsilon}_n}{1 + \epsilon_n} + \frac{1}{8} \frac{\dot{\epsilon}_1}{1 + \epsilon_1} \frac{\dot{\epsilon}_n}{1 + \epsilon_n} + \cdots \right. \\ & \left. + \frac{1}{8} \frac{\dot{\epsilon}_{n-1}}{1 + \epsilon_{n-1}} \frac{\dot{\epsilon}_n}{1 + \epsilon_n} + \frac{5}{16} \frac{\ddot{\epsilon}_n^2}{1 + \epsilon_n} - \frac{1}{4} \frac{\ddot{\epsilon}_n}{1 + \epsilon_n} \right). \end{aligned}$$

We know already that $(\Omega_k^{(1)})^2 - (\Omega_k^{(0)})^2 = (\Omega_k^{(1)})^2 - \omega^2$ is rational in ω of degree ≤ 0 , hence ϵ_1 is rational of degree -2 . Noting that $\dot{\epsilon}_n = (\partial_\omega \epsilon_n) \dot{\omega} + \partial_t \epsilon_n$, we deduce from the above recursion that ϵ_n is rational of degree $-2n$. This completes the argument. \blacksquare

The operators R_n and J_n , Eq. (82), are unitarily equivalent to multiplication operators on $L^2(\tilde{\Sigma}, d\mu(\vec{k}))$. From the fact that $\dot{\Omega}_k^{(n)}/\Omega_k^{(n)}$ is bounded and $\Omega_k^{(n)}$ is strictly positive with principal symbol ω_k (Lemma 6.2) we can immediately deduce that the assumptions of Theorem 5.1 are satisfied if we let $\text{dom } J(t) = H^1(\Sigma)$ for $t \in I$.

We are now ready to state the theorem that connects the adiabatic vacua of Lüders & Roberts [35] to our more general Definition 3.2:

Theorem 6.3 *For fixed t let*

$$\Lambda_n(f, g) := \langle (R_n - iJ_n - \partial_t)Ef, J_n^{-1}(R_n - iJ_n - \partial_t)Eg \rangle_{L^2(\Sigma_t)}$$

be the two-point function of a pure quasifree state of the Klein-Gordon field on the Robertson-Walker spacetime (81) with R_n, J_n given by Eq.s (82) and (86). Then

$$WF^{ts}(\Lambda_n) \subset \begin{cases} \emptyset, & s < -\frac{1}{2} \\ C^+, & -\frac{1}{2} \leq s < 2n + \frac{3}{2} \end{cases},$$

i.e. Λ_n describes an adiabatic vacuum state of order $2n$ in the sense of our Definition 3.2.

To prove the theorem we shall need the following observations:

Lemma 6.4 *Let $m \in \mathbb{R}$. Let M be a compact manifold and $A : \mathcal{D}(M) \rightarrow \mathcal{D}'(M)$ a linear operator. Suppose that, for each $k \in \mathbb{N}$, we can write*

$$A = P_k + R_k \tag{93}$$

where P_k is a pseudodifferential operator of order m and R_k is an integral operator with a kernel function in $C^k(M \times M)$. Then A is a pseudodifferential operator of order m .

Proof: Generalizing a result by R. Beals [4], Coifman & Meyer showed the following: A linear operator $T : \mathcal{D}(M) \rightarrow \mathcal{D}'(M)$ is a pseudodifferential operator of order 0 if and only if T as well as its iterated commutators with smooth vector fields are bounded on $L^2(M)$ [10, Thm. III.15]. As a corollary, T is a pseudodifferential operator of order m if and only if T and its iterated commutators induce bounded maps $L^2(M) \rightarrow H^{-m}(M)$. Given the iterated commutator of A with, say, l vector fields V_1, \dots, V_l , we write $A = P_k + R_k$ with $k \geq l + |m|$. The iterated commutator $[V_1, [\dots [V_l, P_k] \dots]]$ is a pseudodifferential operator of order m and hence induces a bounded map $L^2(M) \rightarrow H^{-m}(M)$. The analogous commutator with R_k has an integral kernel in $\mathcal{C}^{k-l}(M \times M)$. As $k - l \geq |m|$, it furnishes even a bounded operator $L^2(M) \rightarrow H^{|m|}(M)$. \blacksquare

Lemma 6.5 *Let $\mu \in \mathbb{Z}$ and $b = b(t, \tau) \in S_{cl}^\mu(I \times \mathbb{R})$ with principal symbol $b_{-\mu}(t)\tau^\mu$. Replacing τ by $\omega_k(t) = \left(\frac{k(k+2)}{a^2(t)} + m^2\right)^{1/2}$, b defines a family $\{B(t); t \in I\}$ of operators $B(t) : \mathcal{D}(\Sigma) \rightarrow \mathcal{D}'(\Sigma)$ by*

$$\widetilde{(B(t)f)}(t, \vec{k}) := b(t, \omega_k(t))\tilde{f}(\vec{k}).$$

We claim that this is a smooth family of pseudodifferential operators of order μ with principal symbol

$$\sigma^{(\mu)}(B(t)) = b_{-\mu}(t)(|\xi|_\Sigma/a(t))^\mu, \quad (94)$$

where the length $|\xi|_\Sigma$ of a covector ξ is taken w.r.t. the (inverse of the) metric (83).

Note that for the definition of $B(t)$ we only need to know $b(t, \tau)$ for $\tau \geq m$. We may therefore also apply this result to the symbols that appear in Lemma 6.2.

Proof: The fact that b is a classical symbol allows us to write, for each N ,

$$b(t, \tau) = \sum_{j=-\mu}^N b_j(t)\tau^{-j} + b^{(N)}(t, \tau), \quad (95)$$

where $b_j \in \mathcal{C}^\infty(I)$ and $|\partial_t^j \partial_\tau^l b^{(N)}(t, \tau)| \leq C_{jl}(1 + |\tau|)^{-N}$ for all $t \in I$ and $\tau \geq \epsilon$, $\epsilon > 0$ fixed. (Note that we will not obtain the estimates for all τ , since we have a fully homogeneous expansion in (95), but as we shall substitute τ by ω_k and ω_k is bounded away from 0, this will not be important.) Equation (95) induces an analogous decomposition of B :

$$B(t) = \sum_{j=-\mu}^N B_j(t) + B^{(N)}(t),$$

where $B_j(t)$ is given by

$$\widetilde{(B_j(t)f)}(t, \vec{k}) = b_j(t)\omega_k(t)^{-j}\tilde{f}(\vec{k})$$

and $B^{(N)}(t)$ by

$$\widetilde{(B^{(N)}(t)f)}(t, \vec{k}) = b^{(N)}(t, \omega_k(t))\tilde{f}(\vec{k}).$$

In view of the fact that $\Delta_\Sigma \phi_{\vec{k}} = -k(k+2)\phi_{\vec{k}}$, we have

$$B_j(t) = b_j(t) (m^2 - \Delta_\Sigma/a^2(t))^{-j/2}.$$

According to Seeley [43], B_j is a smooth family of pseudodifferential operators of order $-j$. Next, we observe that, by (90), $\partial_t^l \omega_k = \mathcal{O}(\omega_k)$ and hence, for each $l \in \mathbb{N}$,

$$|\partial_t^l (b^{(N)}(t, \omega_k(t)))| \leq C(1 + \omega_k(t))^{-N} \leq C'(1 + k)^{-N}$$

for all $t \in I$. Lemma 6.1 therefore shows that, for each $s \in \mathbb{R}$

$$\partial_t^l B^{(N)}(t) : H^s(\Sigma) \rightarrow H^{s+N}(\Sigma) \quad (96)$$

is bounded, uniformly in $t \in I$. On the other hand, it is well known that a linear operator T which maps $H^{-s-k}(\Sigma)$ to $H^{s+k}(\Sigma)$ for some $s > 3/2$ ($\dim \Sigma = 3$) has an integral kernel of class \mathcal{C}^k on $\Sigma \times \Sigma$. It is given by $K(x, y) = \langle T \delta_y, \delta_x \rangle$. Choosing $N > 3 + 2k$, the family $B^{(N)}$ will therefore have integral kernels of class \mathcal{C}^k . Now we apply Lemma 6.4 to conclude that B is a smooth family of pseudodifferential operators of order μ . Since B_j is of order $-j$ the principal symbol is that of $B_{-\mu} = b_{-\mu}(t) (m^2 - \Delta_\Sigma/a^2(t))^{-\mu/2}$. This yields (94). ■

Now let us define the family of operators $A_n(t)$ acting on $L^2(\Sigma, d^3\sigma)$ by

$$(A_n f)(t, \mathbf{x}) := \int d\mu(\vec{k}) a^{(n)}(t, k) \tilde{f}(t, \vec{k}) \phi_{\vec{k}}(\mathbf{x}),$$

with $a^{(n)}$ given by the function

$$a^{(n)}(t, k) := \frac{3}{2} \frac{\dot{a}}{a} - \frac{1}{2} \frac{\dot{\Omega}_k^{(n)}}{\Omega_k^{(n)}} - i\Omega_k^{(n)}.$$

Moreover let

$$Q_n := iX(\partial_t + A_n(t)),$$

where $X := \text{op } \chi$ and $\chi = \chi(t, \mathbf{x}, \tau, \xi)$ is as in (80).

Lemma 6.6 $A_n \in \mathcal{C}^\infty(I, L_{cl}^1(\Sigma))$ with principal symbol $\sigma^{(1)}(A_n(t)) = i|\xi|_\Sigma/a(t)$. Q_n is a pseudodifferential operator of order 1 on $I \times \Sigma$ with real-valued principal symbol whose characteristic does not intersect N_- .

Proof: We apply Lemma 6.5 in connection with Lemma 6.2 to see that $A_n \in \mathcal{C}^\infty(I, L_{cl}^1(\Sigma))$. The operator Q_n clearly is an element of $L_{cl}^1(I \times \Sigma)$. Outside a small neighborhood of $\{\xi = 0\}$ its characteristic set is

$$\{(t, \mathbf{x}, \tau, \xi) \in T^*(I \times \Sigma); -\tau + |\xi|_\Sigma/a(t) = 0\}.$$

Since $N_- = \{\tau = -|\xi|_\Sigma/a(t)\}$, the intersection is empty. ■

Proof of Theorem 6.3: In view of Theorem 5.3 we only have to check that

$$Q_n(R_n - iJ_n - \partial_t)E^- = S^{(2n)}E^- \quad (97)$$

for a pseudodifferential operator $S^{(2n)}$ of order $-2n$. A straightforward computation shows that $(\partial_t + A_n)(R_n - iJ_n - \partial_t)$ is the operator defined by

$$- \left(\partial_t^2 + 3\frac{\dot{a}}{a}\partial_t + \omega_k^2 + (\Omega_k^{(n)})^2 - (\Omega_k^{(n+1)})^2 \right).$$

Now $\partial_t^2 + 3\frac{\dot{a}}{a}\partial_t + \omega_k^2$ induces $\square_g + m^2$, Eq. (85), while, by Lemma 6.2 combined with Lemma 6.5, $(\Omega_k^{(n)})^2 - (\Omega_k^{(n+1)})^2$ induces an element of $\mathcal{C}^\infty(I, L^{-2n}(\Sigma))$. Composing with the operator X from the left and noting that $(\square_g + m^2)E^- = 0$, we obtain (97). ■

7 Physical interpretation

Using the notion of the Sobolev wavefront set (Definition B.1) we have generalized in this paper the previously known positive frequency conditions to define a large new class of quantum states for the Klein-Gordon field on arbitrary globally hyperbolic spacetime manifolds (Definition 3.2). Employing the techniques of pseudodifferential and Fourier integral operators we have explicitly constructed examples of them on spacetimes with a compact Cauchy surface (Theorem 5.10). We call these states adiabatic vacua because on Robertson-Walker spacetimes they include a class of quantum states which is already well-known under this name (Theorem 6.3). We order the adiabatic vacua by a real number N which describes the Sobolev order beyond which the positive frequency condition may be perturbed by singularities of a weaker nature. Our examples show that these additional singularities may be of negative frequency or even non-local type (Lemma 5.8). Hadamard states are naturally included in our definition as the adiabatic states of infinite order.

To decide which orders of adiabatic vacua are physically admissible we have investigated their corresponding GNS-representations: Adiabatic vacua of order $N > 5/2$ generate a quasiequivalence class of local factor representations (in other words, a unique local primary folium). For pure states on a spacetime with compact Cauchy surface - a case which often occurs in applications - this holds true already for $N > 3/2$ (Theorems 4.5 and 4.7). Physically, locally quasiequivalent states can be thought of as having a finite energy density relative to each other. Primarity means that there are no classical observables contained in the local algebras. Hence there are no local superselection rules, i.e. the local states can be coherently superimposed without restriction. For $N > 3/2$ the local von Neumann algebras generated by these representations contain no observables which are localized at a single point (Theorem 4.12). Together with quasiequivalence this implies that all the states become indistinguishable upon measurements in smaller and smaller spacetime regions (Corollary 4.13). This complies well with the fact that the correlation functions have the same leading short-distance singularities, whence the states should have the same high

energy behaviour. Finally, the algebras are maximal in the sense of Haag duality (Theorem 4.15) and additive (Lemma 2.5). For a more thorough discussion of all these properties in the framework of algebraic quantum field theory we refer to [21]. Taken together, all these results suggest that adiabatic vacua of order $N > 5/2$ are physically meaningful states.

Furthermore we expect that the energy momentum tensor of the Klein-Gordon field can be defined in these states by an appropriate regularisation generalizing the corresponding results for Hadamard states [8, 50] and adiabatic vacua on Robertson-Walker spaces [39].

However, all the mentioned physical properties of the GNS-representations are of a rather universal nature and therefore cannot serve to distinguish between different types of states. How can we physically discern an adiabatic state of order N from one of order N' , say, or from an Hadamard state? To answer this question we investigate the response of a quantum mechanical model detector (a so-called Unruh detector [5, 46]) to the coupling with the Klein-Gordon field in an N -th order adiabatic vacuum state. So let us assume we are given an adiabatic state ω_N of order N of the Klein-Gordon quantum field $\hat{\Phi}$ on the spacetime \mathcal{M} and its associated GNS-triple $(\mathcal{H}_{\omega_N}, \pi_{\omega_N}, \Omega_{\omega_N})$ as in Proposition 2.4(b). We consider a detector that moves on a worldline $\gamma : \mathbb{R} \rightarrow \mathcal{M}, \tau \mapsto x(\tau)$, in \mathcal{M} and is described as a quantum mechanical system by a Hilbert space \mathcal{H}_D and a free time evolution w.r.t. proper time τ . It shall be determined by a free Hamiltonian H_0 with a discrete energy spectrum $E_0 < E_1 < E_2 < \dots$, E_0 being the groundstate energy of H_0 (e.g. a harmonic oscillator). We assume that the detector has negligible extension and is coupled to the quantum field $\hat{\Phi}$ via the interaction Hamiltonian

$$H_I := \lambda M(\tau) \hat{\Phi}(x(\tau)) \chi(\tau) \quad (98)$$

acting on $\mathcal{H}_D \otimes \mathcal{H}_{\omega_N}$, where $\lambda \in \mathbb{R}$ is a small coupling constant, $M(\tau) = e^{iH_0\tau} M(0) e^{-iH_0\tau}$ the monopole moment operator characterizing the detector and $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ a cutoff function that describes the adiabatic switching on and off of the interaction. To calculate transition amplitudes between states of $\mathcal{H}_D \otimes \mathcal{H}_{\omega_N}$ under the interaction (98) one uses most conveniently the interaction picture, in which the field $\hat{\Phi}$ and the operator M evolve with the free time evolution (but the full coupling to the gravitational background) whereas the time evolution of the states is determined by the interaction H_I . In this formulation the perturbative S -matrix is given by [5, 7]

$$\begin{aligned} S &= \mathbf{1} + \sum_{j=1}^{\infty} \frac{(-i)^j}{j!} \int d\tau_1 \dots \int d\tau_j T[H_I(\tau_1) \dots H_I(\tau_j)] \\ &= \mathbf{1} + \sum_{j=1}^{\infty} \frac{(-i\lambda)^j}{j!} \int d\tau_1 \chi(\tau_1) \dots \int d\tau_j \chi(\tau_j) T[M(\tau_1) \dots M(\tau_j)] T[\hat{\Phi}(x(\tau_1)) \dots \hat{\Phi}(x(\tau_j))], \end{aligned} \quad (99)$$

where T denotes the operation of time ordering. Let us assume that the detector is prepared in its ground state $|E_0\rangle$ prior to switching on the interaction, and calculate in first order

perturbation theory ($j = 1$ in (99)) the transition amplitude between the incoming state $\psi_{in} := |E_0\rangle \otimes \Omega_{\omega_N} \in \mathcal{H}_D \otimes \mathcal{H}_{\omega_N}$ and some outgoing state $\psi_{out} := |E_n\rangle \otimes \psi$, $n \neq 0$, where $|E_n\rangle \in \mathcal{H}_D$ is the eigenstate of H_0 corresponding to the energy E_n and ψ some one-particle state in the Fock space \mathcal{H}_{ω_N} (the scalar products of $\hat{\Phi}(x)\Omega_{\omega_N}$ with other states vanish in a quasifree representation):

$$\langle \psi_{out}, S\psi_{in} \rangle = -i\lambda \langle E_n | M(0) | E_0 \rangle \int d\tau \chi(\tau) e^{i(E_n - E_0)\tau} \langle \psi | \hat{\Phi}(x(\tau)) \Omega_{\omega_N} \rangle.$$

From this we obtain the probability $P(E_n)$ that a transition to the state $|E_n\rangle$ occurs in the detector by summing over a complete set of (unobserved) one-particle states in \mathcal{H}_{ω_N} :

$$\begin{aligned} P(E_n) &= \lambda^2 |\langle E_n | M(0) | E_0 \rangle|^2 \int d\tau_1 \int d\tau_2 e^{-i(E_n - E_0)(\tau_1 - \tau_2)} \chi(\tau_1) \chi(\tau_2) \Lambda_N(x(\tau_1), x(\tau_2)) \\ &= \lambda^2 |\langle E_n | M(0) | E_0 \rangle|^2 \mathcal{F}(E_n - E_0). \end{aligned}$$

Here, $|\langle E_n | M(0) | E_0 \rangle|^2$ describes the model dependent sensitivity of the detector, whereas

$$\mathcal{F}(E) := \int_{-\infty}^{\infty} d\tau_1 \int_{-\infty}^{\infty} d\tau_2 e^{-iE(\tau_1 - \tau_2)} \chi(\tau_1) \chi(\tau_2) \Lambda_N(x(\tau_1), x(\tau_2))$$

is the well-known expression for the detector response function depending on the two-point function Λ_N of the adiabatic state ω_N . Inspection of the formula shows that it is in fact obtained from $\Lambda_N \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ by restricting Λ_N to $\gamma \times \gamma \subset \mathcal{M} \times \mathcal{M}$, multiplying this restricted distribution pointwise by $\chi \otimes \chi$ and taking the Fourier transform at $(-E, E)$:

$$\mathcal{F}(E) = 2\pi ((\Lambda_N|_{\gamma \times \gamma}) \cdot (\chi \otimes \chi))^\wedge(-E, E).$$

It follows from the very definition of Λ_N (Definition 3.2) and Proposition B.7 that $\Lambda_N|_{\gamma \times \gamma}$ is a well-defined distribution on $\mathbb{R} \times \mathbb{R}$ if $N > 3/2$, since $N^*(\gamma)$ consists only of space-like covectors. It holds

$$WF^s(\Lambda_N|_{\gamma \times \gamma}) \subset \varphi_*(C^+) \quad \text{for } s < N - 3/2,$$

where φ_* is the pullback of the embedding $\varphi : \gamma \times \gamma \rightarrow \mathcal{M} \times \mathcal{M}$. We now observe that

$$\{(\tau_1, -E; \tau_2, E) \in \mathbb{R}^4; E \geq 0\} \cap \varphi_*(C^+) = \emptyset \quad (100)$$

(this observation was already made by Fewster [17] in the investigation of energy mean values of Hadamard states). Hence there is an open cone Γ in $\mathbb{R}^2 \setminus \{0\}$ containing $(-E, E)$, $E > 0$, such that $WF^s(\Lambda_N|_{\gamma \times \gamma}) \cap \Gamma = \emptyset$. By (102) we can write $(\Lambda_N|_{\gamma \times \gamma}) \cdot (\chi \otimes \chi) = u_1 + u_2$ with $u_1 \in H_{loc}^s(\mathbb{R}^2)$ for $s < N - 3/2$ and $WF(u_2) \cap \Gamma = \emptyset$. Since $(\Lambda_N|_{\gamma \times \gamma}) \cdot (\chi \otimes \chi)$ has compact support we can assume without loss of generality that also u_1 and u_2 have compact supports. From $WF(u_2) \cap \Gamma = \emptyset$ it follows then that

$$\hat{u}_2(\xi) = \mathcal{O}(\langle \xi \rangle^{-k}) \quad \forall k \in \mathbb{N} \quad \forall \xi \in \Gamma,$$

whereas $u_1 \in H_{comp}^s(\mathbb{R}^2)$ implies that

$$\begin{aligned} & D^\alpha u_1 \in L_{comp}^2(\mathbb{R}^2) \quad \text{for } |\alpha| \leq s < N - 3/2, \text{ cf. Prop. B.3} \\ \Rightarrow & (D^\alpha u_1)^\wedge(\xi) = \xi^\alpha \hat{u}_1(\xi) \text{ is bounded} \\ \Rightarrow & \hat{u}_1(\xi) = \mathcal{O}(\langle \xi \rangle^{-|\alpha|}). \end{aligned}$$

Taken together, we find that $((\Lambda_N|_{\gamma \times \gamma}) \cdot (\chi \otimes \chi))^\wedge(\xi) = \mathcal{O}(\langle \xi \rangle^{-[N-3/2]})$ for $\xi \in \Gamma$, where $[N - 3/2] := \max\{n \in \mathbb{N}_0; n < N - 3/2\}$. Since $(-E, E) \in \Gamma, E > 0$, we can now conclude that

$$\mathcal{F}(E) = \mathcal{O}(\langle E \rangle^{-[N-3/2]})$$

for an adiabatic vacuum state of order $N > 3/2$. (Note that this estimate could be improved for the states constructed in Section 5 by taking into account that for them the singularities of lower order are explicitly known, cf. Lemma 5.8, and the sub-leading singularities also satisfy relation (100).) This means that the probability of a detector, moving in an adiabatic vacuum of order N , to get excited to the energy E decreases like $E^{-[N-3/2]}$ for large E , in an Hadamard state it decreases faster than any inverse power of E . We can therefore interpret adiabatic states of lower order as higher excited states of the quantum field. One should however keep in mind that all the states usually considered in elementary particle physics (on a static spacetime, say) are of the Hadamard type: ground states and thermodynamic equilibrium states are Hadamard states [31], particle states satisfy the microlocal spectrum condition (the generalization of the Hadamard condition to higher n -point functions) [8]. We do not know by which physical operation an adiabatic state of finite order could be prepared.

Although all results in this paper are concerned with the free Klein-Gordon field, it is clear that our Definition 3.2 is capable of a generalization to higher n -point functions of an interacting quantum field theory in analogy to the microlocal spectrum condition of Brunetti et al. [8]. In order to treat the pointwise product $(\Lambda_N)^2$ we write

$$(\Lambda_N)^2 = (\Lambda_H)^2 + (\Lambda_N - \Lambda_H)^2 + 2(\Lambda_N - \Lambda_H)\Lambda_H,$$

where Λ_H is the two-point function of any Hadamard state. It follows from Proposition B.6, Lemma 3.3, and Lemma 5.2 that these pointwise products are well-defined if $N > -1$. It is well-known that

$$WF'((\Lambda_H)^2) \subset C^+ \oplus C^+,$$

where $C^+ \oplus C^+ := \{(x_1, \xi_1 + \eta_1; x_2, \xi_2 + \eta_2) \in T^*(\mathcal{M} \times \mathcal{M}) \setminus 0; (x_1, \xi_1; x_2, \xi_2), (x_1, \eta_1; x_2, \eta_2) \in C^+\}$ [29, Thm. 8.2.10]. The regularity of the other two terms can be estimated by Theorems 8.3.1 and 10.2.10 in [30] such that finally

$$WF'^s((\Lambda_N)^2) \subset C^+ \oplus C^+ \quad \text{if } s < N - 3.$$

Higher powers of Λ_N can be treated similarly. Thus, for sufficiently large adiabatic order N , finite Wick powers (with finitely many derivatives) can be defined. This should be sufficient

for the perturbative construction of a quantum field theory with an interaction Lagrangian involving a fixed number of derivatives and powers of the fields. Obviously one has to require more and more regularity of the states if one wants to define higher and higher Wick powers. This complies with a recent result of Hollands & Ruan [25].

It is also clear that the notion of adiabatic vacua can be extended to other field theory models than merely the scalar field. A first step in this direction has been taken by Hollands [24] for Dirac fields.

Finally we want to point out that, although the whole analysis in this paper has been based on a given \mathcal{C}^∞ -manifold \mathcal{M} with smooth Lorentz metric g , the notion of adiabatic vacua should be particularly relevant for manifolds with \mathcal{C}^k -metric. Typical examples that occur in general relativity are star models: here the metric outside the star satisfies Einstein's vacuum field equations and is matched on the boundary \mathcal{C}^1 to the metric inside the star where it satisfies Einstein's equations with an energy momentum tensor of a suitable matter model as a source term. In such a situation Hadamard states cannot even be defined on a part of the spacetime that contains the boundary of the star, whereas adiabatic states up to a certain order should still be meaningful. This remark could e.g. be relevant for the derivation of the Hawking radiation from a realistic stellar collapse to a black hole.

A Sobolev spaces

$H^s(\mathbb{R}^n)$, $s \in \mathbb{R}$, is the set of all tempered distributions u on \mathbb{R}^n whose Fourier transforms \hat{u} are regular distributions satisfying

$$\|u\|_{H^s(\mathbb{R}^n)}^2 := \int \langle \xi \rangle^{2s} |\hat{u}(\xi)|^2 d^n \xi < \infty.$$

For a domain $\mathcal{U} \subset \mathbb{R}^n$ we let

$$H^s(\mathcal{U}) := \{r_{\mathcal{U}}u; u \in H^s(\mathbb{R}^n)\}$$

be the space of all restrictions to \mathcal{U} of H^s -distributions on \mathbb{R}^n , equipped with the quotient topology

$$\|u\|_{H^s(\mathcal{U})} := \inf\{\|U\|_{H^s(\mathbb{R}^n)}; U \in H^s(\mathbb{R}^n), r_{\mathcal{U}}U = u\}.$$

Moreover, we denote by $H_0^s(\overline{\mathcal{U}})$ the space of all elements in $H^s(\mathbb{R}^n)$ whose support is contained in $\overline{\mathcal{U}}$. If \mathcal{U} is bounded with smooth boundary, then it follows from [28, Thm. B.2.1] that $\mathcal{C}_0^\infty(\mathcal{U})$ is dense in $H_0^s(\overline{\mathcal{U}})$ for every s and that $H_0^s(\overline{\mathcal{U}})$ is the dual space of $H^s(\mathcal{U})$ with respect to the extension of the sesquilinear form

$$\int \bar{u}v d^n x, \quad u \in \mathcal{C}_0^\infty(\mathcal{U}), v \in \mathcal{C}^\infty(\overline{\mathcal{U}}).$$

If Σ is a compact manifold without boundary we choose a covering by coordinate neighborhoods with associated coordinate maps, say $\{U_j, \kappa_j\}_{j=1, \dots, J}$ with a subordinate partition of

unity $\{\varphi_j\}_{j=1,\dots,J}$. Given a distribution u on Σ , we shall say that $u \in H^s(\Sigma)$ if, for each j , the push-forward of $\varphi_j u$ under κ_j is an element of $H^s(\mathbb{R}^n)$. It is easy to see that this definition is independent of the choices made for U_j, κ_j and φ_j . The space $H^s(\Sigma)$ is a Hilbert space with the norm

$$\|u\|_{H^s(\Sigma)} := \left(\sum_{j=1}^J \|(\kappa_j)_*(\varphi_j u)\|_{H^s(\mathbb{R}^n)}^2 \right)^{1/2}.$$

We denote by Δ the Laplace-Beltrami operator with respect to an arbitrary metric on Σ . Then we have

$$H^{2k}(\Sigma) = \{u \in L^2(\Sigma); (1 - \Delta)^k u \in L^2(\Sigma)\}$$

for $k = 0, 1, 2, \dots$: Clearly, the left hand side is a subset of the right hand side. Conversely, we may assume that u has support in a single coordinate neighborhood, so that we can look at the push-forward u_* under the coordinate map. The fact that both u_* and $((1 - \Delta)^k u)_*$ belong to $L^2(\mathbb{R}^n)$ implies that $u_* \in H^{2k}(\mathbb{R}^n)$, hence $u \in H^{2k}(\Sigma)$. Moreover, this consideration shows that the two topologies are equivalent (and in particular independent of the choice of metric on Σ).

We may identify $H^{-s}(\Sigma)$ with the dual of $H^s(\Sigma)$ with respect to the L^2 -inner product in Σ .

Now let Σ be a (possibly) non-compact Riemannian manifold which is geodesically complete. The Laplace-Beltrami operator $\Delta : \mathcal{C}_0^\infty(\Sigma) \rightarrow \mathcal{C}_0^\infty(\Sigma)$ is essentially selfadjoint by Chernoff's theorem [9]. We can therefore define the powers $(1 - \Delta)^{s/2}$ for all $s \in \mathbb{R}$. By $H^s(\Sigma)$ we denote the completion of $\mathcal{C}_0^\infty(\Sigma)$ with respect to the norm

$$\|u\|_{H^s(\Sigma)} := \|(1 - \Delta)^{s/2} u\|_{L^2(\Sigma)}.$$

For $s \in 2\mathbb{N}_0$, this shows that $H^{2k}(\Sigma)$ is the set of all $u \in L^2(\Sigma)$ for which $(1 - \Delta)^k u \in L^2(\Sigma)$. We deduce that this definition coincides with the previous one if Σ is compact and $s = 2k$; using complex interpolation, cf. [44, Ch. I, Thm. 4.2], equality holds for all $s \geq 0$. Moreover, we can define a sesquilinear form

$$\langle \cdot, \cdot \rangle : H^{-s}(\Sigma) \times H^s(\Sigma) \rightarrow \mathbb{C}$$

by letting

$$\langle u, v \rangle := \left((1 - \Delta)^{-s/2} u, (1 - \Delta)^{s/2} v \right)_{L^2(\Sigma)}.$$

This allows us to identify $H^{-s}(\Sigma)$ with the dual of $H^s(\Sigma)$, as in the compact case. In particular, the definition of the Sobolev spaces on compact manifolds coincides also for negative s .

Now suppose that \mathcal{O} is a relatively compact subset of Σ . We let $H^s(\mathcal{O}) := r_{\mathcal{O}} H^s(\Sigma)$, the restriction to \mathcal{O} of H^s -distributions on Σ , endowed with the quotient topology

$$\|u\|_{H^s(\mathcal{O})} := \inf \{ \|U\|_{H^s(\Sigma)}; U \in H^s(\Sigma), r_{\mathcal{O}} U = u \}.$$

This definition is local: If \mathcal{O}' is another relatively compact subset with smooth boundary containing $\overline{\mathcal{O}}$, then we can find a function $f \in \mathcal{C}_0^\infty(\mathcal{O}')$ with $f \equiv 1$ on \mathcal{O} . Hence, whenever there exists a $U \in H^s(\Sigma)$ with $r_{\mathcal{O}}U = u$, then there is a $U_1 \in H^s(\Sigma)$ with $\text{supp } U_1 \subset \mathcal{O}'$ and $r_{\mathcal{O}}U_1 = u$, namely $U_1 = fU$. We therefore obtain the same space and the same topology, if we replace the right hand side by

$$\inf\{\|U\|_{H^s(\Sigma)}; U \in H^s(\Sigma), \text{supp } U \subset \mathcal{O}', r_{\mathcal{O}}U = u\}.$$

Indeed, both definitions yield the same space, which also is a Banach space with respect to both norms. As the first norm can be estimated by the second, the open mapping theorem shows that both are equivalent. Note that $H^s(\mathcal{O})$ is independent of the particular choice of \mathcal{O}' .

On $\mathcal{C}_0^\infty(\mathcal{O})$ the topology of $H^s(\Sigma)$ is independent of the choice of the Riemannian metric; moreover it coincides with that induced from $H^s(\mathbb{R}^n)$ via the coordinate maps: This follows from the fact that, for $s = 0, 2, 4, \dots$, the spaces $H^s(\Sigma)$ are the domains of powers of the Laplacian, together with interpolation and duality. As a consequence, $H^s(\mathcal{O})$ does not depend on the choice of the metric, and its topology is that induced by the Euclidean H^s -topology.

Finally we define the local Sobolev spaces

$$\begin{aligned} H_{loc}^s(\Sigma) &:= \{u \in \mathcal{D}'(\Sigma); \int \langle \xi \rangle^{2s} |\widehat{\kappa_*(\varphi u)}(\xi)|^2 d^n \xi < \infty \text{ for all coordinate maps} \\ &\quad \kappa : \mathcal{U} \rightarrow \mathbb{R}^n, \mathcal{U} \subset \Sigma, \text{ and all } \varphi \in \mathcal{C}_0^\infty(\mathcal{U})\} \\ H_{comp}^s(\Sigma) &:= \{u \in H_{loc}^s(\Sigma); \text{supp } u \text{ compact}\}. \end{aligned}$$

We have the following inclusions of sets

$$H_{comp}^s(\mathcal{O}) \subset H_{comp}^s(\Sigma) \subset H_{loc}^s(\Sigma) \subset H^s(\mathcal{O}) \subset H_{loc}^s(\mathcal{O})$$

for any relatively compact subset \mathcal{O} of Σ .

B Microlocal analysis with finite Sobolev regularity

The \mathcal{C}^∞ -wavefront set WF of a distribution u characterizes the directions in Fourier space which cause the appearance of singularities of u . It does however not specify the strength with which the different directions contribute to the singularities. To give a precise quantitative measure of the strength of singular directions of u the notion of the H^s -wavefront set WF^s was introduced by Duistermaat & Hörmander [16]. It is the mathematical tool which we use in the main part of the paper to characterize the adiabatic vacua of a quantum field on a curved spacetime manifold. To make the paper reasonably self-contained we present the definition of WF^s and collect some results of the calculus related to it which are otherwise spread over the literature. They are mainly taken from [16, 20, 27, 30, 44]. All other notions

from microlocal analysis which we use can also be found there or, in a short synopsis, in [31]. In the following let X denote an open subset of \mathbb{R}^n .

Definition B.1 *Let $u \in \mathcal{D}'(X)$, $x_0 \in X$, $\xi_0 \in \mathbb{R}^n \setminus \{0\}$, $s \in \mathbb{R}$. We say that u is H^s (microlocally) in (x_0, ξ_0) or that (x_0, ξ_0) is not in the H^s -wavefront set of u ($(x_0, \xi_0) \notin WF^s(u)$) if there is a test function $\varphi \in \mathcal{C}_0^\infty(X)$ with $\varphi(x_0) \neq 0$ and an open conic neighborhood Γ of ξ_0 in $\mathbb{R}^n \setminus \{0\}$ such that*

$$\int_{\Gamma} \langle \xi \rangle^{2s} |\widehat{\varphi u}(\xi)|^2 d^n \xi < \infty, \quad (101)$$

where $\langle \xi \rangle := (1 + |\xi|^2)^{1/2}$.

Note that, since $\varphi u \in \mathcal{E}'(X)$, there is for all $(x, \xi) \in X \times \mathbb{R}^n \setminus 0$ a sufficiently small $s \in \mathbb{R}$ such that $(x, \xi) \notin WF^s(u)$. From the definition the following **properties of WF^s** are immediate:

- (i) $WF^s(u)$ is a local property of u , depending only on an infinitesimal neighborhood of a point x_0 , in the following sense:

If $u \in \mathcal{D}'(X)$, $\varphi \in \mathcal{C}_0^\infty(X)$ with $\varphi(x_0) \neq 0$ then

$$(x_0, \xi_0) \in WF^s(u) \Leftrightarrow (x_0, \xi_0) \in WF^s(\varphi u)$$

- (ii) $WF^s(u)$ is a closed cone in $X \times (\mathbb{R}^n \setminus \{0\})$, i.e. in particular

$$(x, \xi) \in WF^s(u) \Rightarrow (x, \lambda \xi) \in WF^s(u) \quad \forall \lambda > 0.$$

- (iii)

$$WF^s(u) = \emptyset \Leftrightarrow u \in H_{loc}^s(X)$$

- (iv)

$$(x, \xi) \in WF^s(u) \Leftrightarrow \forall v \in H_{loc}^s(X) : (x, \xi) \in WF(u - v) \quad (102)$$

- (v)

$$WF^{s_1}(u) \subset WF^{s_2}(u) \subset WF(u) \quad \forall s_1 \leq s_2$$

- (vi)

$$WF^s(u_1 + u_2) \subset WF^s(u_1) \cup WF^s(u_2)$$

- (vii)

$$WF(u) = \overline{\bigcup_{s \in \mathbb{R}} WF^s(u)}$$

As an example consider the δ -distribution in $\mathcal{D}'(\mathbb{R}^n)$. One easily calculates from the criterion of the definition

$$WF^s(\delta) = \begin{cases} \emptyset, & s < -n/2 \\ \{(0, \xi); \xi \in \mathbb{R}^n \setminus \{0\}\}, & s \geq -n/2. \end{cases} \quad (103)$$

The following proposition gives an important characterization of the H^s -wavefront set in terms of pseudodifferential operators. Remember that $S_{\rho,\delta}^m(X \times \mathbb{R}^n)$ is the space of symbols of order m and type ρ, δ ($m \in \mathbb{R}$, $0 \leq \delta, \rho \leq 1$), and $L_{\rho,\delta}^m(X)$ the corresponding space of pseudodifferential operators on X .

Proposition B.2 *Let $u \in \mathcal{D}'(X)$. Then*

$$WF^s(u) = \bigcap_{\substack{A \in L_{1,0}^0 \\ Au \in H_{loc}^s(X)}} char A = \bigcap_{\substack{A \in L_{1,0}^s \\ Au \in L_{loc}^2(X)}} char A, \quad (104)$$

where the intersection is taken over all properly supported classical pseudodifferential operators A (having principal symbol $a(x, \xi)$) and $char A := a^{-1}(0) \setminus 0$ is the characteristic set of A .

Also the **pseudolocal property** of pseudodifferential operators can be stated in a refined way taking into account the finite Sobolev regularity:

Proposition B.3 *If $A \in L_{\rho,\delta}^m(X)$ is properly supported, with $0 \leq \delta < \rho \leq 1$, and $u \in \mathcal{D}'(X)$, then*

$$WF^{s-m}(Au) \subset WF^s(u)$$

for all $s \in \mathbb{R}$, in particular

$$A : H_{loc}^s(X) \rightarrow H_{loc}^{s-m}(X).$$

From Propositions B.2 and B.3 we can draw the following important **conclusions**:

- (i) Since the principal symbol of a pseudodifferential operator is an invariant function on the cotangent bundle T^*X we see from (104) that $WF^s(u)$ is well-defined as a subset of $T^*X \setminus 0$, i.e. does not depend on a particular choice of coordinates. By a partition of unity one can therefore define $WF^s(u)$ for any paracompact smooth manifold \mathcal{M} and $u \in \mathcal{D}'(\mathcal{M})$ as a subset of $T^*\mathcal{M} \setminus 0$ and all results in this appendix remain valid when replacing X by \mathcal{M} .
- (ii) If $Au \in H_{loc}^s(X)$ for some properly supported $A \in L_{1,0}^m(X)$ then

$$WF^{s+m}(u) \subset char A. \quad (105)$$

This follows from Proposition B.2 because, choosing some elliptic $B \in L_{1,0}^{-m}(X)$, we have $BA \in L_{1,0}^0(X)$ and, by Proposition B.3, $BAu \in H_{loc}^{s+m}(X)$, and therefore, by (104), $WF^{s+m}(u) \subset char(BA) = char(A)$.

(iii) If $A \in L^{-\infty}(X)$, then $WF(Au) = \emptyset$ and hence $WF^s(Au) = \emptyset$ for all $s \in \mathbb{R}$.

(iv) If $A \in L_{\rho,\delta}^m(X)$, $0 \leq \delta < \rho \leq 1$, is a properly supported elliptic pseudodifferential operator, $u \in \mathcal{D}'(X)$, then

$$WF^{s-m}(Au) = WF^s(u)$$

for all $s \in \mathbb{R}$.

This is a consequence of the fact that an elliptic pseudodifferential operator has a parametrix, i.e. there is a properly supported $Q \in L_{\rho,\delta}^{-m}(X)$ with $QAu = u + Ru$ and $AQu = u + R'u$ for some $R, R' \in L^{-\infty}(X)$. Therefore, by Proposition B.3,

$$WF^s(u) = WF^s(QAu) \subset WF^{s-m}(Au) \subset WF^s(u).$$

The behaviour of $WF^s(u)$ for hyperbolic operators (like the Klein-Gordon operator, which plays an important role in this work) is determined by the theorem of **propagation of singularities** due to Duistermaat & Hörmander [16, Thm. 6.1.1']. It states in particular that, if u satisfies $Au \in H_{loc}^s(X)$ for $A \in L_{1,0}^m(X)$ with real principal symbol $a(x, \xi)$ which is homogeneous of degree m , then $WF^{s+m-1}(u)$ consists of complete bicharacteristics of A , i.e. complete integral curves in $a^{-1}(0) \subset T^*X$ of the Hamiltonian vectorfield

$$H_a(x, \xi) := \sum_{i=1}^n \left[\frac{\partial a(x, \xi)}{\partial x^i} \frac{\partial}{\partial \xi_i} - \frac{\partial a(x, \xi)}{\partial \xi_i} \frac{\partial}{\partial x^i} \right].$$

The precise statement is as follows:

Proposition B.4 *Let $A \in L_{1,0}^m(X)$ be a properly supported pseudodifferential operator with real principal symbol $a(x, \xi)$ which is homogeneous of degree m . If $u \in \mathcal{D}'(X)$ and $Au = f$ it follows for any $s \in \mathbb{R}$ that*

$$WF^{s+m-1}(u) \setminus WF^s(f) \subset a^{-1}(0) \setminus 0$$

and $WF^{s+m-1}(u) \setminus WF^s(f)$ is invariant under the Hamiltonian vectorfield H_a .

It is well-known that the wavefront set gives sufficient criteria when two distributions can be pointwise multiplied, composed or restricted to submanifolds. We reconsider these operations from the point of view of finite Sobolev regularity and obtain weaker conditions in terms of WF^s . We start with the regularity of the tensor product of two distributions:

Proposition B.5 *Let $X \subset \mathbb{R}^n, Y \subset \mathbb{R}^m$ be open sets and $u \in \mathcal{D}'(X), v \in \mathcal{D}'(Y)$.*

Then the tensor product $w := u \otimes v \in \mathcal{D}'(X \times Y)$ satisfies

$$WF^r(w) \subset WF^s(u) \times WF^t(v) \cup WF^s(u) \times WF^t(v) \cup \begin{cases} (\text{supp } u \times \{0\}) \times WF^t(v) \cup WF^s(u) \times (\text{supp } v \times \{0\}), & r = s + t \\ (\text{supp } u \times \{0\}) \times WF^s(u) \cup WF^t(v) \times (\text{supp } v \times \{0\}), & r = \min\{s, t, s + t\}. \end{cases}$$

The proof of this proposition can be adapted from the proof of Lemma 11.6.3 in [30].

The pointwise product of two distributions $u_1, u_2 \in \mathcal{D}'(X)$ – if it exists – is defined by convolution of Fourier transforms as the distribution $v \in \mathcal{D}'(X)$ such that $\forall x \in X \exists f \in \mathcal{D}(X)$ with $f = 1$ near x such that for all $\xi \in \mathbb{R}^n$

$$\widehat{f^2 v}(\xi) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \widehat{f u_1}(\eta) \widehat{f u_2}(\xi - \eta) d^n \eta$$

with absolutely convergent integral. It is clear that for the integral to be absolutely convergent it is sufficient that $\widehat{f u_1}(\eta)$ and $\widehat{f u_2}(\xi - \eta)$ decay sufficiently fast in the opposite directions η resp. $-\eta$, i.e. that u_1 and u_2 are in Sobolev spaces of sufficiently high order at (x, η) resp. $(x, -\eta)$. The precise condition is the following:

Proposition B.6 *Let $u_1, u_2 \in \mathcal{D}'(X)$. Suppose that $\forall (x, \xi) \in T^*X \setminus 0 \exists s_1, s_2 \in \mathbb{R}$ with $s_1 + s_2 \geq 0$ such that $(x, \xi) \notin WF^{s_1}(u_1)$ and $(x, -\xi) \notin WF^{s_2}(u_2)$.*

Then the pointwise product $u_1 u_2$ exists.

For a proof see [37].

Next we consider the restriction of distributions to submanifolds. Let Σ be an $(n - 1)$ -dimensional hypersurface of X (i.e. there exists a \mathcal{C}^∞ -embedding $\varphi : \Sigma \rightarrow X$) with conormal bundle

$$N^*\Sigma := \{(\varphi(y), \xi) \in T^*X; y \in \Sigma, \varphi_*(\xi) = 0\}.$$

We can define the restriction $u_\Sigma \in \mathcal{D}'(\Sigma)$ of $u \in \mathcal{D}'(X)$ to Σ – if it exists – as the mapping $f \mapsto \langle u \cdot (f \delta_\Sigma), 1 \rangle$, where $f \delta_\Sigma : \mathcal{C}^\infty(X) \rightarrow \mathbb{C}$ is the distribution given by $(f \delta_\Sigma)(g) := \int_\Sigma f g$, $f \in \mathcal{D}(\Sigma)$. If Σ is locally given by $x^0 = 0$ then $f \delta_\Sigma$ is locally given by $f(\mathbf{x}) \delta(x^0)$, where $\delta(x^0)$ is the delta-function in the x^0 -variable. By a consideration analogous to (103) we see that

$$WF^s(f \delta_\Sigma) \subset \begin{cases} \emptyset, & s < -1/2 \\ N^*\Sigma, & s \geq -1/2 \end{cases}. \quad (106)$$

We obtain

Proposition B.7 *Let $u \in \mathcal{D}'(X)$ with $WF^s(u) \cap N^*\Sigma = \emptyset$ for some $s > 1/2$.*

Then the restriction u_Σ of u is a well-defined distribution in $\mathcal{D}'(\Sigma)$, and

$$WF^{r-1/2}(u_\Sigma) \subset \varphi_* WF^r(u) := \{(y, \varphi_*(\xi)) \in T^*\Sigma; (\varphi(y), \xi) \in WF^r(u)\}$$

for all $r > 1/2$.

Proof: Let $s > 1/2$ and $WF^s(u) \cap N^*\Sigma = \emptyset$. It follows from (106) and Proposition B.6 that the product $u \cdot f \delta_\Sigma$ is defined. Suppose that $(y, \eta) \in WF^{r-1/2}(u_\Sigma)$ for some $r > 1/2$. By (102) we have $(y, \eta) \in WF(u_\Sigma - w)$ for each $w \in H_{loc}^{r-1/2}(\Sigma)$. Since the restriction operator $H_{loc}^r(X) \rightarrow H_{loc}^{r-1/2}(\Sigma)$ is onto [44, Ch. I, Thm. 3.5], there exists a $v \in H_{loc}^r(X)$ for each w such that $w = v_\Sigma$. Hence we have for every $v \in H_{loc}^r(X)$

$$(y, \eta) \in WF(u_\Sigma - v_\Sigma) = WF((u - v)_\Sigma) \subset \varphi_* WF(u - v)$$

where we have used the standard result on the wavefront set of a restricted distribution [26, Thm. 2.5.11']. Applying (102) again we obtain the assertion. \blacksquare

The proposition can easily be generalized to submanifolds of higher codimension by repeated projection. From Proposition B.5 and B.7 one can get an estimate for the H^s -wavefront set of the pointwise product in Proposition B.6 when noticing that $u_1 u_2$ is the pull-back of $u_1 \otimes u_2$ under the map $\varphi : X \rightarrow X \times X$, $x \mapsto (x, x)$ and that $\varphi_*(\xi_1, \xi_2) = \xi_1 + \xi_2$. This estimate, however, is rather poor and we will not present it here, better information on the regularity of products can be gained e.g. from [30, Thm. 8.3.1 and Thm. 10.2.10].

Proposition B.8 *Let $X \subset \mathbb{R}^n, Y \subset \mathbb{R}^m$ be open sets, $u \in \mathcal{C}_0^\infty(Y)$ and let $\mathcal{K} \in \mathcal{D}'(X \times Y)$ be the kernel of the continuous map $K : \mathcal{C}_0^\infty(Y) \rightarrow \mathcal{D}'(X)$.*

Then we have for all $s \in \mathbb{R}$

$$WF^s(Ku) \subset WF_X^s(\mathcal{K}) := \{(x, \xi) \in T^*X \setminus 0; (x, \xi; y, 0) \in WF^s(\mathcal{K}) \text{ for some } y \in Y\}.$$

Proof: Assume that $(x, \xi; y, 0) \notin WF^s(\mathcal{K})$ for some $(x, \xi) \in T^*X \setminus 0, y \in Y$. By (102) we can write $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ with $\mathcal{K}_1 \in H_{loc}^s(X \times Y)$ and $(x, \xi; y, 0) \notin WF(\mathcal{K}_2)$. Since $Ku = K_1 u + K_2 u$ and $WF(K_2 u) \subset WF_X(\mathcal{K}_2)$ it follows that $(x, \xi) \notin WF(K_2 u)$. It remains to be shown that $K_1 u \in H_{loc}^s(X)$, because then it follows from (102) that $(x, \xi) \notin WF^s(Ku)$, i.e. $WF^s(Ku) \subset WF_X^s(\mathcal{K})$.

To this end we localize \mathcal{K}_1 with test functions $\varphi \in \mathcal{C}_0^\infty(X)$ and $\psi \in \mathcal{C}_0^\infty(Y)$ such that $\psi = 1$ on $\text{supp } u$ and estimate for $\varphi(K_1 u) = \varphi(K_1 \psi u) = \int \mathcal{K}'_1(x, y) u(y) d^m y \in \mathcal{E}'(X)$, where $\mathcal{K}'_1(x, y) := \varphi(x) \mathcal{K}_1(x, y) \psi(y)$:

$$\begin{aligned} \int d^n \xi (1 + |\xi|^2)^s |\widehat{\varphi(K_1 u)}(\xi)|^2 &= \int d^n \xi (1 + |\xi|^2)^s \left| \int d^m \eta \hat{\mathcal{K}}'_1(\xi, -\eta) \hat{u}(\eta) \right|^2 \\ &\leq \int d^n \xi (1 + |\xi|^2)^s \int d^m \eta (1 + |\eta|^2)^t |\hat{\mathcal{K}}'_1(\xi, -\eta)|^2 \\ &\quad \int d^m \theta (1 + |\theta|^2)^{-t} |\hat{u}(\theta)|^2 \\ &= C \int d^n \xi \int d^m \eta (1 + |\xi|^2)^s (1 + |\eta|^2)^t |\hat{\mathcal{K}}'_1(\xi, -\eta)|^2 \\ &\leq C \int d^n \xi \int d^m \eta (1 + |\xi|^2 + |\eta|^2)^s |\hat{\mathcal{K}}'_1(\xi, -\eta)|^2 \end{aligned}$$

which is finite since $\mathcal{K}'_1 \in H_{comp}^s(X \times Y)$. The last estimate was obtained by putting $t := 0$ if $s \geq 0$, and $t := s$ if $s < 0$. \blacksquare

In the next proposition we generalize this result to the case where u is a distribution in $\mathcal{E}'(Y)$. Then Ku – if it exists – is defined as the distribution in $\mathcal{D}'(X)$ such that, for $\varphi \in \mathcal{C}_0^\infty(X)$,

$$\langle Ku, \varphi \rangle = \langle \mathcal{K}(1 \otimes u), \varphi \otimes 1 \rangle.$$

Proposition B.9 *Let $X \subset \mathbb{R}^n, Y \subset \mathbb{R}^m$ be open sets, $\mathcal{K} \in \mathcal{D}'(X \times Y)$ be the kernel of the continuous map $K : \mathcal{C}_0^\infty(Y) \rightarrow \mathcal{D}'(X), u \in \mathcal{E}'(Y)$ and denote*

$$WF_Y^{s'}(\mathcal{K}) := \{(y, \eta) \in T^*Y \setminus 0; (x, 0; y, -\eta) \in WF^s(\mathcal{K}) \text{ for some } x \in X\}.$$

*If $\forall (y, \eta) \in T^*Y \setminus 0 \exists s_1, s_2 \in \mathbb{R}$ with $s_1 + s_2 \geq 0$ such that*

$$(y, \eta) \notin WF_Y^{s_1}(\mathcal{K}) \cap WF^{s_2}(u), \quad (107)$$

then Ku exists. If, in addition, $WF_Y(\mathcal{K}) = \emptyset$ and $K(H_{\text{comp}}^s(Y)) \subset H_{\text{loc}}^{s-\mu}(X)$, then

$$WF^{s-\mu}(Ku) \subset WF'(\mathcal{K}) \circ WF^s(u) \cup WF_X(\mathcal{K}),$$

*where $WF'(\mathcal{K}) := \{(x, \xi; y, -\eta) \in T^*X \times T^*Y; (x, \xi; y, \eta) \in WF(\mathcal{K})\}$ is to be regarded as a relation mapping elements of T^*Y to elements in T^*X .*

Proof: For the first part of the statement we only have to check that the product $\mathcal{K}(1 \otimes u)$ exists. Indeed, by Proposition B.5 we have $WF^{s_2}(1 \otimes u) \subset (X \times \{0\}) \times WF^{s_2}(u)$ and, because of (107), for no point $(y, \eta) \in T^*Y \setminus 0$ is $(x, 0; y, -\eta)$ in $WF^{s_1}(\mathcal{K})$ and at the same time $(x, 0; y, \eta)$ in $WF^{s_2}(1 \otimes u)$. Therefore, according to Proposition B.6, the pointwise product $\mathcal{K}(1 \otimes u)$ exists.

Given an open conic neighborhood Γ of $WF^s(u)$ in T^*Y , we can write $u = u_1 + u_2$ with $u_1 \in H_{\text{loc}}^s(Y)$ and $WF(u_2) \subset \Gamma$. This is immediate from (102) with the help of a microlocal partition of unity. By assumption we have $Ku_1 \in H_{\text{loc}}^{s-\mu}(Y)$, and hence, by [29, Thm. 8.2.13],

$$\begin{aligned} WF^{s-\mu}(Ku) &\subset WF(Ku_2) \subset WF'(\mathcal{K}) \circ WF(u_2) \cup WF_X(\mathcal{K}) \\ &\subset WF'(\mathcal{K}) \circ \Gamma \cup WF_X(\mathcal{K}). \end{aligned}$$

Since Γ was arbitrary, we obtain

$$WF^{s-\mu}(Ku) \subset WF'(\mathcal{K}) \circ WF^s(u) \cup WF_X(\mathcal{K}).$$

■

The assumptions in the last proposition are tailored for application to the case that \mathcal{K} is the kernel of a Fourier integral operator. Indeed, if $K \in I_\rho^\mu(X \times Y, C')$, $1/2 < \rho \leq 1$, where C' is locally the graph of a canonical transformation from $T^*Y \setminus 0$ to $T^*X \setminus 0$, then $WF(\mathcal{K}) \subset C'$ [26, Thm. 3.2.6] and $K(H_{\text{comp}}^s(Y)) \subset H_{\text{loc}}^{s-\mu}(X)$ [28, Cor. 25.3.2] and the proposition applies. For pseudodifferential operators we have $C' = id$ and hence we get back the result of Proposition B.3. In the next proposition we give information about the smoothness of the kernel \mathcal{K} itself:

Proposition B.10 *Let $K \in I_\rho^\mu(X \times Y, \Lambda)$, $1/2 < \rho \leq 1$, where Λ is a closed Lagrangean submanifold of $T^*(X \times Y) \setminus 0$, and $\mathcal{K} \in \mathcal{D}'(X \times Y)$ its kernel. Then $WF^s(\mathcal{K}) \subset WF(\mathcal{K}) \subset \Lambda$, more precisely*

$$\begin{aligned} WF^s(\mathcal{K}) = \emptyset &\quad \text{if } s < -\mu - \frac{n+m}{4}, \\ \lambda \in WF^s(\mathcal{K}) &\quad \text{if } s \geq -\mu - \frac{n+m}{4} \text{ and } \lambda \in \Lambda \text{ is a non-characteristic point of } K. \end{aligned}$$

$K \in I_\rho^\mu(X \times Y, \Lambda)$ is said to be non-characteristic at a point $\lambda \in \Lambda$ if the principal symbol has an inverse (as a symbol) in a conic neighborhood of λ . A proof of the proposition can be found in [16, Thm. 5.4.1].

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