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The Generally Covariant Locality Principle – A New Paradigm for Local Quantum Field Theory

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Dedicated to Rudolf Haag on the occasion of his eightieth birthday

Abstract: A new approach to the model-independent description of quantum field theories will be introduced in the present work. The main feature of this new approach is to incorporate in a local sense the principle of general covariance of general relativity, thus giving rise to the concept of a *locally covariant quantum field theory*. Such locally covariant quantum field theories will be described mathematically in terms of covariant functors between the categories, on one side, of globally hyperbolic spacetimes with isometric embeddings as morphisms and, on the other side, of *-algebras with unital injective *-monomorphisms as morphisms. Moreover, locally covariant quantum fields can be described in this framework as natural transformations between certain functors. The usual Haag-Kastler framework of nets of operator-algebras over a fixed spacetime background-manifold, together with covariant automorphic actions of the isometry-group of the background spacetime, can be re-gained from this new approach as a special case. Examples of this new approach are also outlined. In case that a locally covariant quantum field theory obeys the time-slice axiom, one can naturally associate to it certain automorphic actions, called "relative Cauchy-evolutions", which describe the dynamical reaction of the quantum field theory to a local change of spacetime background metrics. The functional derivative of a relative Cauchy-evolution with respect to the spacetime metric is found to be a divergence-free quantity which has, as will be demonstrated in an example, the significance of an energy-momentum tensor (up to addition of scalar functions) for the locally covariant quantum field theory. Furthermore, we discuss the functorial properties of state spaces of locally covariant quantum field theories that entail the validity of the principle of local definiteness.

1. Introduction

Quantum field theory incorporates two main principles into quantum physics, locality and covariance. Locality expresses the idea that quantum processes can be localized in space and time [and, at the level of observable quantities, that causally separated processes are exempt from any uncertainty relations restricting their commensurability]. The principle of Poincaré-covariance within special relativity states that there are no preferred Lorentzian coordinates for the description of physical processes, and thereby the concept of an absolute space as an arena for physical phenomena is abandoned. Yet it is still meaningful to speak of events in terms of spacetime points as entities of a given, fixed spacetime background in the setting of special relativistic physics.

In general relativity, however, spacetime points lose this a priori meaning (cf. the discussion of the "hole argument" in general relativity in [34]). The principle of general covariance forces one to regard spacetime points simultaneously as members of several, locally diffeomorphic spacetimes. It is rather the relations between distinguished events that have a physical interpretation.

This principle should also be observed when quantum field theory in the presence of gravitational fields is discussed. A first approximation to such situations is to consider quantum fields on a given, curved Lorentzian background spacetime where the sources of the gravitational curvature are described classically and independently of the dynamics of the quantum fields in that background. Due to the weakness of gravitational interactions compared to elementary particle interactions, this is expected to be a reasonable approximation which nevertheless has a range of applicability where nontrivial phenomena occur, like particle creation in strong, or rapidly varying, gravitational fields. The most prominent effects of that sort are the Hawking effect [24] and the Fulling-Unruh effect [19, 48].

For quantum field theory on Minkowski spacetime, one demands that quantum fields behave covariantly under Poincaré-transformations, and there are distinct states, like the vacuum state, or (multi-) particle states tied to the Wigner-type particle concept. Such states are natural reference states which allow to fix physical quantities in comparison with experiments. In contradistinction to this familiar case, a generic spacetime manifold need not possess any (non-trivial) spacetime symmetries (isometries), and thus there is in general no restrictive concept of covariance for quantum fields propagating on an arbitrary, but fixed curved background spacetime. (A similar problem arises already for quantum fields in flat spacetime coupled to outer classical fields, and most of what follows applies, mutatis mutandis, also to this case.)

This lack of covariance is a source of serious ambiguities in quantum field theory on curved spacetime, such as the lack of a natural candidate of a vacuum state or a Wigner-type particle concept. In turn, this leads to ambiguities in the concrete determination of physical quantities. This problem was observed some time ago by Wald [52] in his discussion of a renormalization prescription for defining the energy-momentum tensor of a quantized field on a curved spacetime M with metric tensor $\boldsymbol{g} = g_{\mu\nu}$.

One can define a renormalization procedure for the energy-momentum tensor of a free quantum field on a curved spacetime by picking a quasifree Hadamard state ω as "reference state" and normal ordering of creation and annihilation operators in the GNS-representation of ω. In this way, one arrives at an expression for the quantized energy-momentum tensor as an operator valued distribution, but the problem is the dependence on the reference state ω: On a generic spacetime without symmetries, there is in general no preferred quasifree Hadamard state, like the vacuum on Minkowski spacetime which is selected by invariance with respect to spacetime symmetries. In order to restrict this ambiguity, Wald imposed as a further requirement a principle of locality and covariance that states that the energy-momentum tensor should only locally depend on the spacetime metric; we will outline this condition further below.

A similar problem occurred in the definition of Wick-polynomials and of renormalized perturbation theory on Lorentzian manifolds. We will discuss here the case of the Wick square, as an illustration of other cases, like the energy-momentum tensor. The definition of a normal ordered product, or Wick-square, of a field operator $\varphi(x)$ in the GNS-representation of the reference state ω may be given in form of the coincidence limit

$$:\varphi^2:_\omega(x) = \lim_{y \to x} (\varphi(x)\varphi(y) - \omega(\varphi(x)\varphi(y))) .$$

(The limit procedure has to be properly defined, see, e.g. [7].) Due to the non-unique choice of a reference state, it turns out that choosing instead of ω a different reference state ω' results in changing $:\varphi^2:_\omega(x)$ to

$$:\varphi^2:_{\omega'}(x) =:\varphi^2:_\omega(x) + f(x)$$

with some smooth function f. This ambiguity would actually not be very serious at the level of a description of a quantum field theory in terms of operator algebras, but it enters into the definition of time-ordered products of Wick-polynomials from which, in turn, local S-matrix functionals are derived in the sense of perturbation theory whose matrix elements may be compared with physical processes modelled by interacting fields on curved spacetime [6]. Furthermore, a more serious ambiguity enters in the course of the process of infinite renormalization of ultraviolet divergencies in defining the time-ordered product of Wick-polynomials. There remains a freedom that corresponds to adding certain products of differential operators contracted with Wick-polynomials to the Lagrangian. While one can show [6] that the perturbative classification of interacting scalar field theories on curved spacetimes is independent of that freedom, the predictive power of the local S-matrix thus obtained is somewhat limited because the "renormalization constants" now are, in fact, functions depending on the spacetime points. Therefore, it seems most desirable to invoke a suitable locality and covariance principle so as to reduce that ambiguity affecting the S-matrix in a similar way as was done by Wald for the case of the energy-momentum tensor. And, in fact, in recent work by Hollands and Wald [26], this task has been attacked successfully. We should like to point out that related ideas concerning the renormalization of physical quantities for quantum fields in flat spacetime coupled to outer electromagnetic fields have been proposed earlier by Dosch and Müller [14].

Let us now briefly look at the locality and covariance condition imposed by Wald [52] in order to reduce the ambiguity of the renormalized energy-momentum tensor of the free, massless scalar field. The condition may be formulated as follows. Suppose that one has a prescription for obtaining $T^{\text{ren}}_{\mu\nu}(x)$ on *any* curved spacetime. Then such a prescription is local and covariant if the following holds: Whenever one has two spacetimes M and M' equipped with metrics $\boldsymbol{g}$ and $\boldsymbol{g}'$, respectively, and for some (arbitrary) open subset U of M an isometric diffeomorphism $\kappa : U \to U'$ onto an open subset U' of M' (so that $\kappa_*\boldsymbol{g} = \boldsymbol{g}'$), then it is required that

$$\alpha'_\kappa(T'^{\text{ren}}_{\mu\nu}(x')) = \kappa_* T^{\text{ren}}_{\mu\nu}(x') , \quad x' \in U' ,$$

where $\alpha'_\kappa : \mathcal{A}_{M'}(U') \to \mathcal{A}_M(U)$ is the canonical isomorphism between the local CCR-algebras $\mathcal{A}_{M'}(U')$ of the Klein-Gordon field on M' and $\mathcal{A}_M(U)$ of the Klein-Gordon field on M (cf. [11, 52]), and $T^{\text{ren}}_{\mu\nu}$ is the renormalized energy-momentum tensor.

The crucial content of this condition is that it allows an intrinsic definition of the energy-momentum tensor for an arbitrary globally hyperbolic spacetime, independent of the question whether it is part of a larger spacetime. Its basic requisite is the unique construction of the free scalar field on any globally hyperbolic spacetime.

The further formalization of this property is the main purpose of the present article. The most general and most efficient mathematical framework for such a discussion is provided by the operator-algebraic approach to quantum field theory which was initiated by Haag and Kastler [23] for quantum field theory on Minkowski spacetime, see also the monographs [21, 1]. In Sect. 2, we will define a local, generally covariant quantum field theory as a covariant functor between the category of globally hyperbolic (four-dimensional) spacetime manifolds with isometric embeddings as morphisms and the category of C^*-algebras with monomorphisms as morphisms. This generalizes similar approaches, such as the notion of a local, covariant quantum field recently used in [26], and is very similar to the concept of a covariant field theory over the class of globally hyperbolic manifolds defined in [47]. The latter is a generalization of ideas in [12] where also the setting of categories and functors was used. Our approach seems to have the advantage of generalizing in a natural manner at the same time all these mentioned concepts as well as related ideas on generally covariant quantum field theories which appear e.g. in the famous "Missed opportunities" collection by Dyson [16], or in the works [3, 18, 21, 35]. We will indicate that the theory of a free, scalar Klein-Gordon field on globally hyperbolic spacetimes is an example for our functorial description of a quantum field theory. Moreover, it will turn out that the more common concept of a quantum field theory on a fixed spacetime background described in terms of an isotonous map from bounded open subregions to C^*-algebras which is covariant when the spacetime possesses isometries (as in the original Haag-Kastler approach on Minkowski-spacetime, as will be indicated below) is actually a consequence of our functorial description. We will also see that there is a natural notion of equivalence of locally covariant quantum field theories induced by the concept of equivalent functors. It will then turn out that the Klein-Gordon fields with different mass terms provide examples for inequivalent theories.

Section 3 is devoted to a study of the functorial properties of state spaces for locally covariant quantum field theories. A state space will be introduced as a contravariant functor between the category of globally hyperbolic spacetimes and the category of dual spaces of C^*-algebras, with duals of C^*-algebraic embeddings as morphisms. State spaces will be characterized which have the property that their "local folia" are invariant under the functorial action of isometric embeddings of spacetime manifolds. These will be seen to obey the principle of local definiteness proposed by Haag, Narnhofer and Stein [22]. We will indicate that the quasifree states of the Klein-Gordon field which fulfill the microlocal spectrum condition [7] or equivalently, the Hadamard condition [36, 31], induce such a state space.

In Sect. 4 we will demonstrate that to locally covariant quantum field theories obeying the time-slice axiom one can associate a dynamics in the form of automorphic actions, referred to as "relative Cauchy-evolution", which describe the reaction of the quantum field theory on local perturbations of the spacetime metric. We will show that the functional derivative of such relative Cauchy-evolutions with respect to the spacetime-metric is divergence-free. This functional derivative has, in analogy to the case of classical field theory, the significance of an energy-momentum tensor up to additon of scalar functions, and in fact we will also show that for the free Klein-Gordon field the functional derivative of the relative Cauchy-evolution agrees with the commutator action of the energy momentum tensor in representations of quasifree Hadamard states.

Finally, in Sect. 5, we will show that the construction of locally covariant Wick-polynomials by Hollands and Wald [26] may be understood as a solution of a cohomological problem.

Some technical details appear in an Appendix.

2. The Generally Covariant Locality Principle

2.1. Some geometrical preliminaries. In what follows, we will be concerned with four-dimensional, globally hyperbolic spacetimes, so it is appropriate to summarize some of their basic properties. For further discussion, see e.g. [25, 51]. We note that the condition of global hyperbolicity doesn't appear to be very restrictive on physical grounds. Its main purpose is to rule out certain causal pathologies.

We denote a spacetime by $(M, \boldsymbol{g})$ where M is a smooth, four-dimensional manifold (smooth meaning here C^∞, and Hausdorff, paracompact, and connected) and $\boldsymbol{g}$ is a Lorentzian metric on M (taken to be of signature $(+1, -1, -1, -1)$). Also, we always assume that the spacetimes we consider are orientable and time-orientable. The latter means that there exists a C^∞-vectorfield u on M which is everywhere timelike, i.e. $\boldsymbol{g}(u, u) > 0$. A smooth curve $\gamma : I \to M$, I being a connected subset of $\mathbb{R}$, is called causal if $\boldsymbol{g}(\dot\gamma, \dot\gamma) \geq 0$, where $\dot\gamma$ denotes the tangent vector of γ. Given the global timelike vector field u on M, one calls a causal curve γ future-directed if $\boldsymbol{g}(u, \dot\gamma) > 0$ all along γ, and analogously one calls γ past-directed if $\boldsymbol{g}(u, \dot\gamma) < 0$. This induces a globally consistent notion of time-direction in the spacetime $(M, \boldsymbol{g})$. For any point $x \in M$, $J^\pm(x)$ denotes the set of all points in M which can be connected to x by a future(+)/past(−)-directed causal curve $\gamma : I \to M$ so that $x = \gamma(\inf I)$. Two subsets O_1 and O_2 in M are called causally separated if they cannot be connected by a causal curve, i.e. if for all $x \in \overline{O_1}$, $J^\pm(x)$ has empty intersection with $\overline{O_2}$. By $O^\perp$ we denote the causal complement of O, i.e. the largest open set in M which is causally separated from O.

An orientable and time-orientable spacetime $(M, \boldsymbol{g})$ is called globally hyperbolic if for each pair of points $x, y \in M$ the set $J^-(y) \cap J^+(x)$ is compact whenever it is non-empty. This property can be shown to be equivalent to the existence of a smooth foliation of M in Cauchy-surfaces, where a smooth hypersurface of M is called a Cauchy-surface if it is intersected exactly once by each inextendible causal curve in $(M, \boldsymbol{g})$ (for precise definition of inextendible causal curve, see the indicated references). A particular feature of globally hyperbolic spacetimes is the fact that the Cauchy-problem (inital value problem) for linear hyperbolic wave-equations is well-posed and that such wave-equations possess unique retarded and advanced fundamental solutions on those spacetimes. It should also be observed that global hyperbolicity makes no reference to spacetime isometries.

Of some importance later on will be the concept of isometric embedding. Let $(M_1, \boldsymbol{g}_1)$ and $(M_2, \boldsymbol{g}_2)$ be two globally hyperbolic spacetimes. A map $\psi : M_1 \to M_2$ is called an isometric embedding (of $(M_1, \boldsymbol{g}_1)$ into $(M_2, \boldsymbol{g}_2)$) if ψ is a diffeomorphism onto its range $\psi(M_1)$ (i.e. the map $\bar\psi : M_1 \to \psi(M_1) \subset M_2$ is a diffeomorphism) and if ψ is an isometry, that is, $\psi_* \boldsymbol{g}_1 = \boldsymbol{g}_2 \restriction \psi(M_1)$.

2.2. Quantum field theories as covariant functors. It is a famous saying attributed to E. Nelson that quantum field theory is a functor (see [37], Sect. X.7 for a full quotation). This refers to the map of second quantization, mapping the category of Hilbert-spaces with unitaries as morphisms to that of C*-algebras with unit-preserving $*$-homomorphisms as morphisms. In a similar light, topological quantum field theories have already at an early stage been couched in the framework of categories and functors [2]. Here, we wish to put forward that quantum field theory is indeed a covariant functor, but in the more fundamental and physical sense of implementing the principles of locality and general covariance, as discussed in the Introduction. As already pointed out, our approach provides a natural generalization both of the usual abstract formulation of quantum field theory in terms of isotonous families of operator algebras indexed by bounded open subregions of a fixed background spacetime, and of other approaches to diffeomorphism-covariant quantum field theory; we will discuss this further below. We first have to define the categories involved in our formulation of locally covariant quantum field theory. (See [32] as a general reference on categories and functors.) The two categories we shall use are the following:

$\mathfrak{Man}$: This category consists of a class of objects $\mathrm{Obj}(\mathfrak{Man})$ formed by all four-dimensional, globally hyperbolic spacetimes $(M, \boldsymbol{g})$ that are oriented and time-oriented. Given any two such objects $(M_1, \boldsymbol{g}_1)$ and $(M_2, \boldsymbol{g}_2)$, the morphisms $\psi \in \mathrm{hom}_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$ are taken to be the isometric embeddings $\psi : (M_1, \boldsymbol{g}_1) \to (M_2, \boldsymbol{g}_2)$ of $(M_1, \boldsymbol{g}_1)$ into $(M_2, \boldsymbol{g}_2)$ as defined above, but with the additional constraints that

- (i) if $\gamma : [a, b] \to M_2$ is any causal curve and $\gamma(a), \gamma(b) \in \psi(M_1)$ then the whole curve must be in the image $\psi(M_1)$, i.e., $\gamma(t) \in \psi(M_1)$ for all $t \in]a, b[$;
- (ii) the isometric embedding preserves orientation and time-orientation of the embedded spacetime.

The composition rule for any $\psi \in \mathrm{hom}_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$ and $\psi' \in \mathrm{hom}_{\mathfrak{Man}}((M_2, \boldsymbol{g}_2), (M_3, \boldsymbol{g}_3))$ is to define its composition $\psi' \circ \psi$ as the composition of maps. Hence $\psi' \circ \psi : (M_1, \boldsymbol{g}_1) \to (M_3, \boldsymbol{g}_3)$ is a well-defined map which is obviously a diffeomorphism onto its range $\psi'(\psi(M_1))$ and clearly isometric; also the properties (i) and and (ii) are obviously fulfilled, and hence $\psi' \circ \psi \in \mathrm{hom}_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_3, \boldsymbol{g}_3))$. The associativity of the composition rule follows from the associativity of the composition of maps. Clearly, each $\mathrm{hom}_{\mathfrak{Man}}((M, \boldsymbol{g}), (M, \boldsymbol{g}))$ possesses a unit element, given by the identity map $\mathrm{id}_M : x \mapsto x, x \in M$.

$\mathfrak{Alg}$: This is the category whose class of objects $\mathrm{Obj}(\mathfrak{Alg})$ is formed by all C^*-algebras possessing unit elements, and the morphisms are faithful (injective) unit-preserving $*$-homomorphisms. Given $\alpha \in \mathrm{hom}_{\mathfrak{Alg}}(\mathcal{A}_1, \mathcal{A}_2)$ and $\alpha' \in \mathrm{hom}_{\mathfrak{Alg}}(\mathcal{A}_2, \mathcal{A}_3)$, the composition $\alpha' \circ \alpha$ is again defined as the composition of maps and easily seen to be an element in $\mathrm{hom}_{\mathfrak{Alg}}(\mathcal{A}_1, \mathcal{A}_3)$. The unit element in $\mathrm{hom}_{\mathfrak{Alg}}(\mathcal{A}, \mathcal{A})$ is for any $A \in \mathrm{Obj}(\mathfrak{Alg})$ given by the identical map $\mathrm{id}_{\mathcal{A}} : A \mapsto A, A \in \mathcal{A}$.

Remarks. (A) Requirement (i) on the morphisms of $\mathfrak{Man}$ is introduced in order that the induced and intrinsic causal structures coincide for the embedded spacetime $\psi(M_1) \subset M_2$. Aspects of this condition are discussed in [29]. Condition (ii) might, in fact, be relaxed; the resulting structure, allowing also isometric embeddings which reverse spatial and time orientation, could accomodate a discussion of PCT-theorems. We hope to report elsewhere on this topic.

(B) Clearly, one may envisage variations on the categories introduced here. Our present choices might have to be changed or supplemented by other structures, depending on the situations considered. For example, instead of choosing for $\mathrm{Obj}(\mathfrak{Alg})$ the class of C^*-algebras with unit elements, one could consider $*$-algebras, Borchers-algebras, or von Neumann algebras; we have chosen C^*-algebras for definiteness. Moreover, one could also allow more general objects than globally hyperbolic spacetimes in $\mathrm{Obj}(\mathfrak{Man})$, or endow these objects with additional structures, e.g. spin-structures, as in [12, 47]. For discussing the locality and covariance structures of observables, however, the present approach appears sufficient.

Now we are in position to define the concept of locally covariant quantum field theory.

Definition 2.1. (*i*) *A* **locally covariant quantum field theory** *is a covariant functor* $\mathscr{A}$ *between the two categories* $\mathfrak{Man}$ *and* $\mathfrak{Alg}$*, i.e., writing* α_ψ *for* $\mathscr{A}(\psi)$*, in typical diagramatic form:*

$$\begin{array}{ccc} (M, \boldsymbol{g}) & \xrightarrow{\psi} & (M', \boldsymbol{g}') \\ \mathscr{A}\downarrow & & \downarrow\mathscr{A} \\ \mathscr{A}(M, \boldsymbol{g}) & \xrightarrow{\alpha_\psi} & \mathscr{A}(M', \boldsymbol{g}') \end{array}$$

together with the covariance properties

$$\alpha_{\psi'} \circ \alpha_\psi = \alpha_{\psi' \circ \psi}\,, \quad \alpha_{\mathrm{id}_M} = \mathrm{id}_{\mathscr{A}(M,\boldsymbol{g})}\,,$$

for all morphisms $\psi \in \hom_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$*, all morphisms* $\psi' \in \hom_{\mathfrak{Man}}((M_2, \boldsymbol{g}_2), (M_3, \boldsymbol{g}_3))$ *and all* $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$.

(*ii*) *A locally covariant quantum field theory described by a covariant functor* $\mathscr{A}$ *is called* **causal** *if the following holds: Whenever there are morphisms* $\psi_j \in \hom_{\mathfrak{Man}}((M_j, \boldsymbol{g}_j), (M, \boldsymbol{g}))$*,* $j = 1, 2$*, so that the sets* $\psi_1(M_1)$ *and* $\psi_2(M_2)$ *are causally separated in* $(M, \boldsymbol{g})$*, then one has*

$$\left[\alpha_{\psi_1}(\mathscr{A}(M_1, \boldsymbol{g}_1)), \alpha_{\psi_2}(\mathscr{A}(M_2, \boldsymbol{g}_2))\right] = \{0\}\,,$$

where $[\mathcal{A}, \mathcal{B}] = \{AB - BA : A \in \mathcal{A}, B \in \mathcal{B}\}$ *for subsets* $\mathcal{A}$ *and* $\mathcal{B}$ *of an algebra.*

(*iii*) *We say that a locally covariant quantum field theory given by the functor* $\mathscr{A}$ *obeys the* **time-slice axiom** *if*

$$\alpha_\psi(\mathscr{A}(M, \boldsymbol{g})) = \mathscr{A}(M', \boldsymbol{g}')$$

holds for all $\psi \in \hom_{\mathfrak{Man}}((M, \boldsymbol{g}), (M', \boldsymbol{g}'))$ *such that* $\psi(M)$ *contains a Cauchy-surface for* $(M', \boldsymbol{g}')$.

Thus, a locally covariant quantum field theory is an assignment of C^*-algebras to (all) globally hyperbolic spacetimes so that the algebras are identifiable when the spacetimes are isometric, in the indicated way. Note that we use the term "local" in the sense of "geometrically local" in the definition which shouldn't be confused with the meaning of locality in the sense of Einstein causality. Causality properties are further specified in (*ii*) and (*iii*) of Def. 2.1. Causality means that the algebras $\alpha_{\psi_1}(\mathscr{A}(M_1, \boldsymbol{g}_1))$ and $\alpha_{\psi_2}(\mathscr{A}(M_2, \boldsymbol{g}_2))$ commute elementwise in the larger algebra $\mathscr{A}(M, \boldsymbol{g})$ when the subregions $\psi_1(M_1)$ and $\psi_2(M_2)$ of M are causally separated (with respect to $\boldsymbol{g}$). This property is expected to hold generally for observable quantities which can be localized in certain subregions of spacetimes. The time slice axiom (*iii*) (also called strong Einstein causality, or existence of a causal dynamical law, cf. [21]) says that an algebra of observables on a globally hyperbolic spacetime is already determined by the algebra of observables localized in any neighbourhood of a Cauchy-surface.

Before continuing, some remarks on related approaches are in order now. In [16], Dyson suggested that one should attempt to generalize the usual Haag-Kastler framework of a general description of quantum field theories on Minkowski spacetime, as we have sketched it in the Introduction, to general spacetime manifolds in such a way that the covariance group $\mathcal{P}_+^\uparrow$ is replaced by the diffeomorphism group. An approach which is very close in spirit to Dyson's suggestion is due to Bannier [3] who constructed, on $\mathbb{R}^4$ as fixed background manifold, a generalized CCR-algebra of the Klein-Gordon field of fixed mass on which the diffeomorphism group acts covariantly by C^*-automorphisms. Bannier's approach may therefore be regarded as a realization of a functor $\mathscr{A}$ with the above properties but where the domain-category $\mathfrak{Man}$ is replaced by the subcategory $\mathfrak{Man}_{\mathbb{R}^4}$ whose objects are the globally hyperbolic spacetimes $(M, \boldsymbol{g})$ having $M = \mathbb{R}^4$ as spacetime manifolds, and globally hyperbolic sub-spacetimes of those. However, it appears that the restriction to a fixed background manifold like $\mathbb{R}^4$ is artificial, and at variance with the principles of general relativity. This is supported by the results in [47] where an approach similar to the one presented here was taken, and which "localizes" Dimock's formulation in [11, 12] where a functorial approach to generally covariant quantum field theory seems to have been proposed for the first time. Like Bannier's work, however, Dimock's proposal lacks the "locality" aspect of general covariance and therefore doesn't completely reveal its strength. It was shown in [47] that the combination of general covariance and (geometrical) locality leads, together with a few other, natural requirements, to a spin-statistics theorem for quantum fields on curved spacetimes.

A nice feature of the just given definition of a locally covariant quantum field theory lies in the fact that there is a natural concept of equivalence of such theories in terms of equivalence of the corresponding functors. Let $\mathscr{A}$ and and $\mathscr{A}'$ denote two locally covariant quantum field theories, i.e. functors between $\mathfrak{Man}$ and $\mathfrak{Alg}$ as in Def. 2.1. Then, a *natural transformation* between $\mathscr{A}$ and $\mathscr{A}'$ is a family $\{\beta_{(M,\boldsymbol{g})}\}_{(M,\boldsymbol{g})\in\mathfrak{Man}}$ of $*$-monomorphisms $\beta_{(M,\boldsymbol{g})} : \mathscr{A}(M, \boldsymbol{g}) \to \mathscr{A}'(M, \boldsymbol{g})$ such that the following commutative diagram is valid whenever ψ is a morphism in $\hom_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$:

$$\begin{array}{ccc} \mathscr{A}(M_1, \boldsymbol{g}_1) & \xrightarrow{\beta_{(M_1,\boldsymbol{g}_1)}} & \mathscr{A}'(M_1, \boldsymbol{g}_1) \\ \alpha_\psi \downarrow & & \downarrow \alpha'_\psi \\ \mathscr{A}(M_2, \boldsymbol{g}_2) & \xrightarrow{\beta_{(M_2,\boldsymbol{g}_2)}} & \mathscr{A}'(M_2, \boldsymbol{g}_2) \end{array}$$

Thus, in particular, one has

$$\beta_{(M_2,\boldsymbol{g}_2)} \circ \alpha_\psi = \alpha'_\psi \circ \beta_{(M_1,\boldsymbol{g}_1)} \,.$$

If all the $\beta_{(M,\boldsymbol{g})}$ are bijective, one says that the natural transformation $\{\beta_{(M,\boldsymbol{g})}\}_{(M,\boldsymbol{g})\in\mathfrak{Man}}$ is an *equivalence* (or isomorphism) between $\mathscr{A}$ and $\mathscr{A}'$ and that, hence, $\mathscr{A}$ and $\mathscr{A}'$ are *equivalent*. Such an equivalence means that the quantum field theories described by $\mathscr{A}$ and $\mathscr{A}'$ are physically indistinguishable. Conversely, if $\mathscr{A}$ and $\mathscr{A}'$ cannot be related by such an equivalence, they are to be regarded as physically different.

An example for a pair of theories which are not equivalent is given by the Klein-Gordon fields corresponding to different masses. We will discuss this at the end of Sect. 2.4.

2.3. The Klein-Gordon field. The simplest and best studied example of a quantum field theory in curved spacetime is the scalar Klein-Gordon field. As was shown by Dimock [11], its local C^*-algebras can be constructed easily on each globally hyperbolic spacetime, giving rise to a functor $\mathscr{A}$. To summarize this construction, let $(M, \boldsymbol{g})$ be an object in $\mathrm{Obj}(\mathfrak{Man})$. Global hyperbolicity entails the well-posedness of the Cauchy-problem for the scalar Klein-Gordon equation on $(M, \boldsymbol{g})$,

$$(\nabla^\mu \nabla_\mu + m^2 + \xi R)\varphi = 0 \tag{1}$$

(for smooth, real-valued φ) where ∇ is the covariant derivative of $\boldsymbol{g}$, $m \geq 0$ and $\xi \geq 0$ are constants, and R is the scalar curvature of $\boldsymbol{g}$. Moreover, it implies that there exist uniquely determined advanced and retarded fundamental solutions of the Klein-Gordon equation, $E^{\text{adv/ret}} : C_0^\infty(M, \mathbb{R}) \to C^\infty(M, \mathbb{R})$. Here, $C^\infty(M, \mathbb{R})$ denotes the space of smooth, real-valued test functions on M, and $C_0^\infty(M, \mathbb{R})$ the subset of those test functions having compact support. The difference $E = E^{\text{adv}} - E^{\text{ret}}$ is called the causal propagator of the Klein-Gordon equation. Let us denote the range $E(C_0^\infty(M, \mathbb{R}))$ by $\mathcal{R}$ (or, sometimes, by $\mathcal{R}(M, \boldsymbol{g})$ for clarity). It can be shown (cf. [11]) that defining

$$\sigma(Ef, Eh) = \int_M f(Eh)\, d\mu_{\boldsymbol{g}}\,, \quad f, h \in C_0^\infty(M, \mathbb{R})\,,$$

where $d\mu_{\boldsymbol{g}}$ is the metric-induced volume form on M, endowes $\mathcal{R}$ with a symplectic form, and thus $(\mathcal{R}, \sigma)$ is a symplectic space. To this symplectic space one can associate its Weyl-algebra $\mathfrak{W}(\mathcal{R}, \sigma)$, which is generated by a family of unitary elements $W(\varphi)$, $\varphi \in \mathcal{R}$, satisfying the CCR in exponentiated form ("Weyl-relations"),

$$W(\varphi)W(\tilde{\varphi}) = \mathrm{e}^{-i\sigma(\varphi,\tilde{\varphi})/2}W(\varphi + \tilde{\varphi})\,.$$

Now, when the constants m and ξ are kept fixed independently of $(M, \boldsymbol{g})$, the symplectic space $(\mathcal{R}, \sigma)$ is entirely determined by $(M, \boldsymbol{g})$, and so is $\mathfrak{W}(\mathcal{R}, \sigma)$. Setting therefore $\mathscr{A}(M, \boldsymbol{g}) = \mathfrak{W}(\mathcal{R}(M, \boldsymbol{g}), \sigma_{(M,\boldsymbol{g})})$, one obtains a candidate for a covariant functor $\mathscr{A}$ with the properties of Def. 2.1. What remains to be checked is the covariance property. Thus, let $\psi \in \hom_{\mathfrak{Man}}((M, \boldsymbol{g}), (M', \boldsymbol{g}'))$ and let us denote by $E, \mathcal{R}, \sigma$ the propagator, range-space, and symplectic form corresponding to the Klein-Gordon equation (1) on $(M, \boldsymbol{g})$, and by $E', \mathcal{R}', \sigma'$ their counterparts with respect to $(M', \boldsymbol{g}')$. Moreover, we denote by $E^\psi, \mathcal{R}^\psi, \sigma^\psi$ the analogous objects for the spacetime $(\psi(M), \psi_*\boldsymbol{g})$. It was shown in [11] that, writing $\psi_*\varphi = \varphi \circ \psi^{-1}$, there holds $E^\psi = \psi_* \circ E \circ \psi_*{}^{-1}$, $\mathcal{R}^\psi = \psi_*\mathcal{R}$, and

$$\sigma(Ef, Eh) = \sigma^\psi(E^\psi \psi_* f, E^\psi \psi_* h) = \sigma^\psi(\psi_* Ef, \psi_* Eh).$$

Thus ψ_* furnishes a symplectomorphism between $(\mathcal{R}, \sigma)$ and $(\mathcal{R}^\psi, \sigma^\psi)$, and hence, by a standard theorem [5], there is a C^*-algebraic isomorphism $\tilde{\alpha}_\psi : \mathfrak{W}(\mathcal{R}, \sigma) \to \mathfrak{W}(\mathcal{R}^\psi, \sigma^\psi)$ so that

$$\tilde{\alpha}_\psi(W(\varphi)) = W^\psi(\psi_*(\varphi))\,, \quad \varphi \in \mathcal{R}, \tag{2}$$

where $W^\psi(\,.\,)$ denote the CCR-generators of $\mathfrak{W}(\mathcal{R}^\psi, \sigma^\psi)$.

While these observations are already contained in Dimock's work [11], we add another one which is important in the present context: Since $\psi : M \to \psi(M) \subset M'$ is a metric isometry, it holds that $\psi_*\boldsymbol{g} = \boldsymbol{g}' \restriction \psi(M)$. And hence the fact that the advanced and retarded fundamental solutions of the Klein-Gordon operator are uniquely determined on a globally hyperbolic spacetime implies that $E^\psi = \chi_{\psi(M)}E' \restriction C_0^\infty(\psi(M), \mathbb{R})$, where $\chi_{\psi(M)}$ is the characteristic function of $\psi(M)$ and that, moreover, $\mathcal{R}^\psi$ can be identified with $E'(C_0^\infty(\psi(M), \mathbb{R}))$ and σ^ψ with $\sigma' \restriction \mathcal{R}^\psi$. Therefore, denoting by $\iota_\psi : \psi(M) \to M'$ the canonical injection $\iota_\psi(x') = x'$, the map T^ψ which assigns to each element Ef, $f \in C_0^\infty(M, \mathbb{R})$, the element $E'\iota_{\psi *}f$ in $(\mathcal{R}', \sigma')$ is a symplectic map from $(\mathcal{R}^\psi, \sigma^\psi)$ into $(\mathcal{R}', \sigma')$, and thus one obtains a C^*-algebraic monomorphism $\tilde{\alpha}_{\iota_\psi} : \mathfrak{W}(\mathcal{R}^\psi, \sigma^\psi) \to \mathfrak{W}(\mathcal{R}', \sigma')$ by

$$\tilde{\alpha}_{\iota_\psi}(W^\psi(\phi)) = W'(T^\psi\phi)\,, \quad \phi \in \mathcal{R}^\psi\,, \tag{3}$$

where $W'(\,.\,)$ denote the Weyl-generators of $\mathfrak{W}(\mathcal{R}', \sigma')$. Hence, setting $\alpha_\psi = \tilde{\alpha}_{\iota_\psi} \circ \tilde{\alpha}_\psi$, we have a C^*-algebraic monomorphism $\alpha_\psi : \mathscr{A}(M, \boldsymbol{g}) \to \mathscr{A}(M', \boldsymbol{g}')$. The covariance property $\alpha_{\psi' \circ \psi} = \alpha_{\psi'} \circ \alpha_\psi$ for $\psi \in \hom_{\mathfrak{Man}}((M, \boldsymbol{g}), (M', \boldsymbol{g}'))$ and $\psi' \in \hom_{\mathfrak{Man}}((M', \boldsymbol{g}'), (M'', \boldsymbol{g}''))$ is an easy consequence of the construction of α_ψ, i.e. of the relations (2) and (3). It was also shown in [11] that causality and the time-slice axiom are fulfilled in each $\mathfrak{W}(\mathcal{R}, \sigma)$ in the following sense: (i) If $f, h \in C_0^\infty(M, \mathbb{R})$ with $\operatorname{supp} f \subset (\operatorname{supp} h)^\perp$, then $W(Ef)$ and $W(Eh)$ commute, (ii) if N is an open neighbourhood of a Cauchy-surface Σ in M, then there is for each $f \in C_0^\infty(M, \mathbb{R})$ some $h \in C_0^\infty(N, \mathbb{R})$ with $W(Ef) = W(Eh)$. We collect these findings in the following:

Theorem 2.2. *If one defines for each* $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$ *the* C^**-algebra* $\mathscr{A}(M, \boldsymbol{g})$ *as the CCR-algebra* $\mathfrak{W}(\mathcal{R}(M, \boldsymbol{g}), \sigma_{(M,\boldsymbol{g})})$ *of the Klein-Gordon equation* (1) *(with* m, ξ *fixed for all* $(M, \boldsymbol{g})$*), and for each* $\psi \in \hom_{\mathfrak{Man}}((M, \boldsymbol{g}), (M', \boldsymbol{g}'))$ *the* C^**-algebraic monomorphism* $\alpha_\psi = \tilde{\alpha}_{\iota_\psi} \circ \tilde{\alpha}_\psi : \mathscr{A}(M, \boldsymbol{g}) \to \mathscr{A}(M', \boldsymbol{g}')$ *according to* (2) *and* (3)*, then one obtains a functor* $\mathscr{A}$ *with the properties of Def. 2.1. Moreover, this functor is causal and fulfills the time-slice axiom.*

In this sense, the free Klein-Gordon field theory is a locally covariant quantum field theory.

2.4. Recovering algebraic quantum field theory. Now we address the issue of regaining the usual setting of algebraic quantum field theory on a fixed globally hyperbolic spacetime from a locally covariant quantum field theory, i.e. from a covariant functor $\mathscr{A}$ with the properties listed above. It may be helpful for readers not too familiar with the algebraic approach to quantum field theory on Minkowski spacetime that we briefly summarize the Haag-Kastler framework [23] so that it becomes apparent in which way the usual description of algebraic quantum field theory is regained via Prop. 2.3 from our functorial approach. In the Haag-Kastler framework, the basic structure of the formal description of a quantum system is given by a map $O \mapsto \mathcal{A}(O)$ assigning to each open, bounded region O a C^*-algebra $\mathcal{A}(O)$. This "local C^*-algebra" is supposed to contain all the (bounded) observables of the quantum system at hand that can be measured "at times and locations" within the spacetime region O; e.g., if the system is described by a hermitian scalar quantum field $\varphi(x)$, then $\mathcal{A}(O)$ may be taken as the operator-algebra generated by all exponentiated field operators $e^{i\varphi(f)}$, where the test-functions f are supported in O, and the smeared field-operators are $\varphi(f) = \int d^4x\, f(x)\varphi(x)$. Hence, one has the condition of isotony, demanding that $\mathcal{A}(O_1) \subset \mathcal{A}(O)$ whenever $O_1 \subset O$. It is also assumed that the local algebras all contain a common unit element, denoted by $\mathbf{1}$. Moreover, as the local algebras contain observables, it is usually demanded that they commute elementwise when their respective localization regions are spacelike separated.

The locality concept being thus formulated, the notion of special relativistic covariance is given the following form: Collecting all local observables in the minimal C^*-algebra $\mathcal{A}$ containing all local algebras $\mathcal{A}(O)$,[1] there ought to be for each element $L \in \mathcal{P}_+^\uparrow$ (i.e., the proper, orthochronous Poincaré group) a C^*-algebra automorphism

[1] This minimal C^*-algebra is, as a consequence of the isotony condition, well-defined and called the inductive limit of the family $\{\mathcal{A}(O)\}$, where O ranges over all bounded open subsets of Minkowski spacetime.

$\alpha_L : \mathcal{A} \to \mathcal{A}$ so that

$$\alpha_{L_1} \circ \alpha_{L_2} = \alpha_{L_1 \circ L_2}\,, \quad L_1, L_2 \in \mathcal{P}_+^{\uparrow}\,,$$

where $L_1 \circ L_2$ denotes the composition of elements in $\mathcal{P}_+^{\uparrow}$.

Let $(M, \boldsymbol{g})$ be an object in Obj($\mathfrak{Man}$). We denote by $\mathcal{K}(M, \boldsymbol{g})$ the set of all open subsets in M which are relatively compact and contain with each pair of points x and y also all $\boldsymbol{g}$-causal curves in M connecting x and y (cf. condition (ii) in the definition of $\mathfrak{Man}$). Given $O \in \mathcal{K}(M, \boldsymbol{g})$, we denote by $\boldsymbol{g}_O$ the Lorentzian metric restricted to O, so that $(O, \boldsymbol{g}_O)$ (with the induced orientation and time-orientation) is a member of Obj($\mathfrak{Man}$). Then the injection map $\iota_{M,O} : (O, \boldsymbol{g}_O) \to (M, \boldsymbol{g})$, i.e. the identical map restricted to O, is an element in $\hom_{\mathfrak{Man}}((O, \boldsymbol{g}_O), (M, \boldsymbol{g}))$. With this notation, we obtain the following assertion.

Proposition 2.3. *Let $\mathscr{A}$ be a functor with the properties stated in Def. 2.1, and define a map $\mathcal{K}(M, \boldsymbol{g}) \ni O \mapsto \mathcal{A}(O) \subset \mathscr{A}(M, \boldsymbol{g})$ by setting*

$$\mathcal{A}(O) := \alpha_{M,O}(\mathscr{A}(O, \boldsymbol{g}_O))\,,$$

having abbreviated $\alpha_{M,O} \equiv \alpha_{\iota_{M,O}}$. Then the following statements hold:

(a) *The map fulfills isotony, i.e.*

$$O_1 \subset O_2 \Rightarrow \mathcal{A}(O_1) \subset \mathcal{A}(O_2) \quad \text{for all } O_1, O_2 \in \mathcal{K}(M, \boldsymbol{g})\,.$$

(b) *If there exists a group G of isometric diffeomorphisms $\kappa : M \to M$ (so that $\kappa_* \boldsymbol{g} = \boldsymbol{g}$) preserving orientation and time-orientation, then there is a representation $G \ni \kappa \mapsto \tilde{\alpha}_\kappa$ of G by C^*-algebra automorphisms $\tilde{\alpha}_\kappa : \mathcal{A} \to \mathcal{A}$ (where $\mathcal{A}$ denotes the minimal C^*-algebra generated by $\{\mathcal{A}(O) : O \in \mathcal{K}(M, \boldsymbol{g})\}$) such that*

$$\tilde{\alpha}_\kappa(\mathcal{A}(O)) = \mathcal{A}(\kappa(O))\,, \quad O \in \mathcal{K}(M, \boldsymbol{g})\,. \tag{4}$$

(c) *If, in addition, the theory given by $\mathscr{A}$ is causal, then it follows that*

$$[\mathcal{A}(O_1), \mathcal{A}(O_2)] = \{0\}$$

for all $O_1, O_2 \in \mathcal{K}(M, \boldsymbol{g})$ with O_1 causally separated from O_2.

(d) *Suppose that the theory $\mathscr{A}$ fulfills the time-slice axiom, and let Σ be a Cauchy-surface in $(M, \boldsymbol{g})$ and let $S \subset \Sigma$ be open and connected. Then for each $O \in \mathcal{K}(M, \boldsymbol{g})$ with $O \supset S$ it holds that*

$$\mathcal{A}(O) \supset \mathcal{A}(S^{\perp\perp}),$$

where $S^{\perp\perp}$ is the double causal complement of S, and $\mathcal{A}(S^{\perp\perp})$ is defined as the smallest C^*-algebra formed by all $\mathcal{A}(O_1)$, $O_1 \subset S^{\perp\perp}$, $O_1 \in \mathcal{K}(M, \boldsymbol{g})$.

Proof. (a) The proof of this statement is based on the covariance properties of the functor $\mathscr{A}$. To demonstrate that isotony holds, let O_1 and O_2 be in $\mathcal{K}(M, \boldsymbol{g})$ with $O_1 \subset O_2$. We denote by $\iota_{2,1} : (O_1, \boldsymbol{g}_{O_1}) \to (O_2, \boldsymbol{g}_{O_2})$ the canonical embedding obtained by restricting the identity map on O_2 to O_1, hence $\iota_{2,1} \in \hom_{\mathfrak{Man}}((O_1, \boldsymbol{g}_{O_1}), (O_2, \boldsymbol{g}_{O_2}))$. With the notation $\alpha_{\iota_{M,O_1}} \equiv \alpha_{M,1}$, etc., covariance of the functor $\mathscr{A}$ implies $\alpha_{M,1} = \alpha_{M,2} \circ \alpha_{2,1}$ and therefore,

$$\begin{aligned}\mathcal{A}(O_1) = \alpha_{M,1}(\mathscr{A}(O_1, \boldsymbol{g}_{O_1})) &= \alpha_{M,2}(\alpha_{2,1}(\mathscr{A}(O_1, \boldsymbol{g}_{O_1}))\\ &\subset \alpha_{M,2}(\mathscr{A}(O_2, \boldsymbol{g}_{O_2})) = \mathcal{A}(O_2),\end{aligned}$$

since $\alpha_{2,1}(\mathscr{A}(O_1, \boldsymbol{g}_{O_1})) \subset \mathscr{A}(O_2, \boldsymbol{g}_{O_2})$ by the very properties of the functor $\mathscr{A}$.

(b) To prove the second part of the statement, let $\kappa : (M, \boldsymbol{g}) \to (M, \boldsymbol{g})$ be a diffeomorphism preserving the metric as well as time-orientation and orientation. The functor assigns to it an automorphism $\alpha_\kappa : \mathscr{A}(M, \boldsymbol{g}) \to \mathscr{A}(M, \boldsymbol{g})$. Denoting by $\tilde{\kappa}$ the map $O \to \kappa(O), x \mapsto \kappa(x)$, there is an associated morphism $\alpha_{\tilde{\kappa}} : \mathscr{A}(O, \boldsymbol{g}_O) \to \mathscr{A}(\kappa(O), \boldsymbol{g}_{\kappa(O)})$. Hence we obtain the following sequence of equations:

$$
\begin{aligned}
\alpha_\kappa(\mathcal{A}(O)) &= \alpha_\kappa \circ \alpha_{M,O}(\mathscr{A}(O, \boldsymbol{g}_O)) = \alpha_{\kappa \circ \iota_{M,O}}(\mathscr{A}(O, \boldsymbol{g}_O)) \\
&= \alpha_{\iota_{M,\kappa(O)} \circ \tilde{\kappa}}(\mathscr{A}(O, \boldsymbol{g}_O)) = \alpha_{M,\kappa(O)} \circ \alpha_{\tilde{\kappa}}(\mathscr{A}(O, \boldsymbol{g}_O)) \\
&= \alpha_{M,\kappa(O)}(\mathscr{A}(\kappa(O), \boldsymbol{g}_{\kappa(O)})) = \mathcal{A}(\kappa(O)) .
\end{aligned}
$$

Since $\mathcal{A} \subset \mathscr{A}(M, \boldsymbol{g})$, it follows that defining $\tilde{\alpha}_\kappa$ as the restriction of α_κ to $\mathcal{A}$ yields an automorphism with the required properties. The group representation property is simply a consequence of the covariance properties of the functor yielding $\alpha_{\kappa_1} \circ \alpha_{\kappa_2} = \alpha_{\kappa_1 \circ \kappa_2}$ for any pair of members $\kappa_1, \kappa_2 \in G$ together with (4) which allows us to conclude that $\tilde{\alpha}_{\kappa_1} \circ \tilde{\alpha}_{\kappa_2} = \tilde{\alpha}_{\kappa_1 \circ \kappa_2}$.

(c) If O_1 and O_2 are causally separated members in $\mathcal{K}(M, \boldsymbol{g})$, then one can find a Cauchy-surface Σ in $(M, \boldsymbol{g})$ and a pair of disjoint subsets S_1 and S_2 of Σ, both of which are connected and relatively compact, so that $O_j \subset S_j^{\perp\perp}$, $j = 1, 2$. Now $S_j^{\perp\perp}$ are causally separated members of $\mathcal{K}(M, \boldsymbol{g})$, and equipped with the appropriate restrictions of $\boldsymbol{g}$ as metrics, they are globally hyperbolic spacetimes in their own right, and naturally embedded into $(M, \boldsymbol{g})$. According to the causal assumption on $\mathscr{A}$, it holds that $\mathcal{A}(S_j^{\perp\perp}) = \alpha_{M, S_j^{\perp\perp}}(\mathscr{A}(S_j^{\perp\perp}), \boldsymbol{g}_{S_j^{\perp\perp}})$ are pairwise commuting subalgebras of $\mathscr{A}(M, \boldsymbol{g})$, and due to isotony, $\mathcal{A}(O_j) \subset \mathcal{A}(S_j^{\perp\perp})$, so that $[\mathcal{A}(O_1), \mathcal{A}(O_2)] = \{0\}$.

(d) Consider $S^{\perp\perp}$, equipped with the appropriate restriction of $\boldsymbol{g}$, as a globally hyperbolic spacetime in its own right. Then S is a Cauchy-surface for that spacetime, and $O \cap S^{\perp\perp}$ is an open neighbourhood of the Cauchy-surface S. Hence there is an open neighbourhood N of S contained in $O \cap S^{\perp\perp}$ so that N, endowed with the restricted metric, is again a globally hyperbolic spacetime. By the time-slice axiom, it follows that $\alpha_{S^{\perp\perp},N}(\mathscr{A}(N)) = \mathscr{A}(S^{\perp\perp})$, where we have suppressed the metrics to ease notation. According to the functorial properties of $\mathscr{A}$ it follows that

$$
\mathcal{A}(O) \supset \mathcal{A}(N) = \mathcal{A}(S^{\perp\perp}) .
$$

This completes the proof. □

Thus, one can clearly see that, in the light of Prop. 2.3, the Haag-Kastler framework is a special consequence of our functorial approach.

As announced towards the end of Sect. 2.2, we now indicate that the theories of the Klein-Gordon field corresponding to different masses, $m_1 \neq m_2$, are inequivalent. To this end it suffices, in view of Prop. 2.3, to argue as follows. Let $O \mapsto \mathcal{A}_j(O)$, $j = 1, 2$, denote the C^*-algebraic nets on Minkowski spacetime derived from the locally covariant Klein-Gordon field theories $\mathscr{A}_1$ and $\mathscr{A}_2$ for the masses m_1 and m_2, and let $(\tilde{\alpha}_L^{(j)})_{L \in \mathcal{P}_+^\uparrow}$ be the associated covariant automorphic actions of the Poincaré group on $\mathcal{A}_j$. If an equivalence between $\mathscr{A}_1$ and $\mathscr{A}_2$ existed, then a simple variation of the proof of Prop. 2.3 shows that there must be an isomorphism $\beta : \mathcal{A}_1 \to \mathcal{A}_2$ such that

$$
\beta(\mathcal{A}_1(O)) = \mathcal{A}_2(O) \quad \text{and} \quad \beta \circ \tilde{\alpha}_L^{(1)} = \tilde{\alpha}_L^{(2)} \circ \beta
$$

hold for all $O \in \mathcal{K}(M_0, \boldsymbol{g}_0)$ (where $(M_0, \boldsymbol{g}_0)$ denotes Minkowski spacetime) and all $L \in \mathcal{P}_+^\uparrow$. Now, on each $\mathcal{A}_j$ there is a unique state ω_j that is invariant under the respective automorphic action of the Poincaré group and a ground state with respect to the corresponding action of timelike translations. Hence, one would have to conclude that $\omega_2 \circ \beta = \omega_1$ which, however, cannot hold, as it would imply that the spectra of the generators of the time-translations in the vacuum representations of the Klein-Gordon field for different masses coincide.

2.5. Quantum fields as natural transformations. We have just seen how a quantum field *theory* is defined in terms of a covariant functor. Thereby, an algebra is mapped via the monomorphism α_ψ into another algebra, but a priori there are no distinguished elements of the algebras which are mapped onto each other by that transformation.

As discussed in the Introduction, the energy-momentum tensor should possess a corresponding covariance property, and the same holds for other quantum fields. The definition of locally covariant fields given below may be considered as a generalization of the Gårding-Wightman approach to fields as operator-valued distributions. As there, the C*-algebraic formulation of quantum field theory turns out to be too rigid, in general, and we therefore replace the category $\mathfrak{Alg}$ of C*-algebras by the category $\mathfrak{TAlg}$ of topological *-algebras.

The definition may be given as follows: Consider a family $\Phi \equiv \{\Phi_{(M,\boldsymbol{g})}\}$, indexed by all spacetimes $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$, of quantum fields defined as "generalized algebra-valued distributions". That means there is a family $\{\mathcal{A}(M, \boldsymbol{g})\}$ of topological *-algebras indexed by all spacetimes in $\mathrm{Obj}(\mathfrak{Man})$, and for each spacetime $(M, \boldsymbol{g})$, $\Phi_{(M,\boldsymbol{g})} : C_0^\infty(M) \to \mathcal{A}(M, \boldsymbol{g})$ is a continuous map (not necessarily linear, this is why we refer to it as a "generalized" distribution). Consider in addition any morphism $\psi \in \hom_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$. Then we demand that there exists a continuous monomorphism $\alpha_\psi : \mathcal{A}(M_1, \boldsymbol{g}_1) \to \mathcal{A}(M_2, \boldsymbol{g}_2)$ so that,

$$\alpha_\psi(\Phi_{(M_1,\boldsymbol{g}_1)}(f)) = \Phi_{(M_2,\boldsymbol{g}_2)}(\psi_*(f)),$$

where $f \in C_0^\infty(M_1)$ is any test function and $\psi_*(f) = f \circ \psi^{-1}$ as before. (The push-forward ψ_* is well-defined here since $\psi^{-1} : \psi(M) \to M$ exists by injectivity of ψ.) The family $\{\Phi_{(M,\boldsymbol{g})}\}$ with these covariance conditions is called a *locally covariant* quantum field, and indeed, this definition was already used by Hollands and Wald [26, 27] in their construction of Wick polynomials and time ordered products. The concept of locally covariant fields has a beautiful functorial translation, as we shall next outline.

Let $\mathfrak{Test}$ denote the category of test function spaces on manifolds, i.e. the objects are spaces $C_0^\infty(M)$ of smooth, compactly supported test-functions on M and the morphisms are the push-forwards ψ_* of (injective) embeddings $\psi : M_1 \to M_2$ as described above.

Now let a locally covariant quantum field *theory* $\mathscr{A}$ be defined as a functor in the same manner as in Def. 2.1, but with the category $\mathfrak{TAlg}$ in place of the category $\mathfrak{Alg}$, and again following the convention to denote $\mathscr{A}(\psi)$ by α_ψ whenever ψ is any morphism in $\mathfrak{Man}$. Moreover, let $\mathscr{D}$ be the covariant functor between $\mathfrak{Man}$ and $\mathfrak{Test}$ assigning to each $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$ the test-function space $\mathscr{D}(M, \boldsymbol{g}) = C_0^\infty(M)$, and to each morphism ψ of $\mathfrak{Man}$ its push-forward: $\mathscr{D}(\psi) = \psi_*$. We regard the categories $\mathfrak{Test}$ and $\mathfrak{TAlg}$ as subcategories of the category of all topological spaces $\mathfrak{Top}$, and hence we are led to adopt the following:

Definition 2.4. *A* **locally covariant quantum field** Φ *is a natural transformation between the functors* $\mathscr{D}$ *and* $\mathscr{A}$*, i.e. for any object* $(M, \boldsymbol{g})$ *in* $\mathfrak{Man}$ *there exists a morphism* $\Phi_{(M,\boldsymbol{g})} : \mathscr{D}(M, \boldsymbol{g}) \to \mathscr{A}(M, \boldsymbol{g})$ *in* $\mathfrak{Top}$ *such that for each given morphism* $\psi \in \hom_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$ *the following diagram*

$$\begin{array}{ccc} \mathscr{D}(M_1, \boldsymbol{g}_1) & \xrightarrow{\Phi_{(M_1,\boldsymbol{g}_1)}} & \mathscr{A}(M_1, \boldsymbol{g}_1) \\ \psi_* \downarrow & & \downarrow \alpha_\psi \\ \mathscr{D}(M_2, \boldsymbol{g}_2) & \xrightarrow[\Phi_{(M_2,\boldsymbol{g}_2)}]{} & \mathscr{A}(M_2, \boldsymbol{g}_2) \end{array}$$

commutes.

The commutativity of the diagram means, explicitly, that

$$\alpha_\psi \circ \Phi_{(M_1,\boldsymbol{g}_1)} = \Phi_{(M_2,\boldsymbol{g}_2)} \circ \psi_*,$$

i.e., the requirement of covariance for fields.

Remarks. (A) This definition may of course be extended; instead of the test-function spaces $C_0^\infty(M)$ one may take smooth compactly supported sections of vector bundles, and monomorphisms of such more general test-sections spaces which are suitable pull-backs of vector-bundle monomorphisms. Also, one might include conditions on the wave-front set of the field-operators.

(B) The notion of causality may also be introduced in the obvious manner: One calls a locally covariant quantum field *causal* if for all $f, h \in \mathscr{D}(M, \boldsymbol{g})$ with causally separated supports it holds that $\Phi_{(M,\boldsymbol{g})}(f)$ and $\Phi_{(M,\boldsymbol{g})}(h)$ commute.

(C) One reason for allowing non-linear fields in the definitions of quantum fields as natural transformations is that it can be applied to more general objects. One would be the definition of a locally covariant S-matrix, patterned after the definition of the "local" S-matrix of Epstein and Glaser, see e.g. [6]. At the perturbative level (in the sense of formal power series) this amounts to showing that time-ordered products may be defined in such a way that they become locally covariant fields, as was done in [27]. At the non-perturbative level, it might be possible that the constraint of local covariance together with a dynamical generator property (in the spirit of Sect. 4) allows to fix the phase of the S-matrix. We hope to return elsewhere to this issue.

2.6. Free scalar Klein-Gordon field as a natural transformation. The present subsection serves the purpose of sketching two simple examples for locally covariant quantum fields. The first example is based on the Borchers-Uhlmann algebra which can be associated with each manifold M. It assigns to each differentiable manifold M a topological *-algebra $\mathfrak{B}(M)$ that is constructed as follows: Elements in $\mathfrak{B}(M)$ are sequences (f_n) $(n \in \mathbb{N}_0)$, where $f_0 \in \mathbb{C}$ and $f_n \in C_0^\infty(M^n)$ for $n > 0$, and only finitely many entries are non-zero. Addition and scalar multiplication are defined as usual for sequences with values in vector spaces, and the product $(f_n)(h_n)$ in $\mathfrak{B}(M)$ is defined as the sequence (j_n), where

$$j_n(x_1, \ldots, x_n) = \sum_{i+j=n} f_i(x_1, \ldots, x_i) h_j(x_{i+1}, \ldots, x_n), \quad (x_1, \ldots, x_n) \in M^n .$$

The $*$-operation is defined via $(f_n)^* = (\overset{=}{f}_n)$, where $\overset{=}{f}_n(x_1, \ldots, x_n) = \overline{f_n(x_n, \ldots, x_1)}$, the latter overlining meaning complex conjugation. The unit element is given by $\mathbf{1} = (1, 0, 0, \ldots)$. The algebra can be equipped with a fairly natural locally convex topology with respect to which it is complete. See [4, 43] (and also [18, 38] in the context of curved spacetime manifolds) for further discussion of the Borchers-Uhlmann algebra.

Given a morphism $\psi \in \hom_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$, one can lift it to an algebraic morphism $\alpha_\psi : \mathfrak{B}(M_1) \to \mathfrak{B}(M_2)$ by setting

$$\alpha_\psi((f_n)) = (\psi_*^{(n)} f_n),$$

where $\psi_*^{(n)}$ denotes the n-fold push-forward, given by $(\psi_*^{(n)} f_n)(y_1, \ldots, y_n) = f_n (\psi^{-1}(y_1), \ldots, \psi^{-1}(y_n))$. We thus obtain a covariant functor $\mathscr{A}$ between $\mathfrak{Man}$ and $\mathfrak{TAlg}$ by setting $\mathscr{A}(M, \boldsymbol{g}) = \mathfrak{B}(M)$ and $\mathscr{A}(\psi) = \alpha_\psi$ as just defined. A locally covariant quantum field Φ in the sense of Def. 2.4 may then be obtained by defining for $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$ and $f \in \mathscr{D}(M, \boldsymbol{g}) = C_0^\infty(M)$,

$$\Phi_{(M,\boldsymbol{g})}(f) = (f_n),$$

where $(f_n) \in \mathscr{A}(M, \boldsymbol{g}) = \mathfrak{B}(M)$ is the sequence with $f_1 = f$ and $f_n = 0$ for all $n \neq 1$. It is straightforward to check that this indeed satisfies all conditions for a natural transformation between the functors $\mathscr{D}$ and $\mathscr{A}$.

The Borchers-Uhlmann algebra, however, carries no dynamical information, which would have to be incorporated by passing to representations, or factorizing by ideals. In this spirit, we introduce as our second example the Klein-Gordon field as a locally covariant field. For $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$, let $J(M, \boldsymbol{g})$ be the (closed) two-sided ideal in $\mathfrak{B}(M)$ that is generated by all the terms

$$(f_n)(h_n) - (h_n)(f_n) - \sigma(Ef, Eh)\mathbf{1}$$

and

$$((\nabla^\mu \nabla_\mu + \xi R + m^2)(f_n)),$$

where the (f_n) and (h_n) in $\mathfrak{B}(M)$ are such that $f_1 = f$, $h_1 = h$, and all other entries in the sequences vanish; $E = E_{(M,\boldsymbol{g})}$ and $\sigma = \sigma_{(M,\boldsymbol{g})}$ are the propagator and symplectic form corresponding to the Klein-Gordon equation

$$(\nabla^\mu \nabla_\mu + \xi R + m^2)\varphi = 0 \tag{5}$$

on $(M, \boldsymbol{g})$ introduced in Subsect. 2.3. (Again it is assumed that the constants ξ and m are the same for all $(M, \boldsymbol{g})$).

Then we introduce a new functor $\mathscr{A}$ between $\mathfrak{Man}$ and $\mathfrak{TAlg}$, as follows: We define $\mathscr{A}(M, \boldsymbol{g}) = \mathfrak{B}(M)/J(M, \boldsymbol{g})$ and, denoting by $[\,.\,] : \mathfrak{B}(M) \to \mathfrak{B}(M)/J(M, \boldsymbol{g})$ the quotient map, we set for $\psi \in \hom_{\mathfrak{Man}}((M_1, \boldsymbol{g}_1), (M_2, \boldsymbol{g}_2))$,

$$\mathscr{A}(\psi)([(f_n)]) \equiv \alpha_\psi([(f_n)]) = [(\psi_*^{(n)} f_n)],$$

where $\psi_*^{(n)}$ is the n-fold push-forward of ψ defined above. The required properties of this definition of α_ψ to map $J(M_1, \boldsymbol{g}_1)$ into $J(M_2, \boldsymbol{g}_2)$, and $\alpha_{\psi \circ \psi'} = \alpha_\psi \circ \alpha_{\psi'}$, can be obtained by an argument similar to that in Subsect. 2.3 showing that the α_ψ defined there have the desired covariance properties.

With respect to this new functor $\mathscr{A}$, we may now define the generally covariant Klein-Gordon field Φ as a natural transformation according to Def. 2.4 through setting for $(M, \boldsymbol{g}) \in \mathrm{Obj}(M, \boldsymbol{g})$ and $f \in \mathscr{D}(M, \boldsymbol{g}) = C_0^\infty(M)$,

$$\Phi_{(M,\boldsymbol{g})}(f) = [(f_n)],$$

where, as above, (f_n) is the element in $\mathfrak{B}(M)$ with $f_1 = f$ and $f_n = 0$ for all $n \neq 1$. Again, the properties of a natural transformation are easily checked for this definition.

Moreover, locally covariant quantum fields Φ modelling the Klein-Gordon field (5) may be obtained from the functor $\mathscr{A}$ of Subsect. 2.3 describing the locally covariant quantum field theory of the Klein-Gordon field at C^*-algebraic level. We give only a rough sketch of the idea. Let $\mathscr{A}$ be the functor associated with the Klein-Gordon field in Subsect. 2.3. Let $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$, and let π be a Hilbert-space representation of the C^*-algebra $\mathscr{A}(M, \boldsymbol{g})$ on a representation Hilbert-space $\mathcal{H}$. We assume that there exists a dense subspace $\mathcal{V}$ of $\mathcal{H}$ so that, for each $f \in C_0^\infty(M, \mathbb{R})$, the field operator

$$\Phi_{(M,\boldsymbol{g})}(f) = \frac{1}{i} \left. \frac{d}{ds} \right|_{s=0} \pi(W(sEf))$$

exists as an (essentially) self-adjoint operator on $\mathcal{V}$, where E denotes the propagator and $W(\,.\,)$ the Weyl-algebra generators associated with the Klein-Gordon field on $(M, \boldsymbol{g})$. (The field operators can be extended to all complex-valued testfunctions by requiring complex linearity.) The notation used here already suggests how one may go about in order to try to obtain a locally covariant quantum field in this way. Supposing a quantum field $\Phi_{(M,\boldsymbol{g})}$ can be defined in this manner for all $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$ (from representations π for each spacetime), and that, for each $\psi \in \hom_{\mathfrak{Man}}((M, \boldsymbol{g}), (M', \boldsymbol{g}'))$, the assignment $\tilde{\alpha}_\psi(\Phi_{(M,\boldsymbol{g})}(f)) = \Phi_{(M',\boldsymbol{g}')}(\psi_* f)$ extends to a *-algebraic morphism $\tilde{\alpha}_\psi : \tilde{\mathscr{A}}(M, \boldsymbol{g}) \to \tilde{\mathscr{A}}(M', \boldsymbol{g}')$, where $\tilde{\mathscr{A}}(M, \boldsymbol{g})$ denotes the *-algebra formed by all the $\Phi_{(M,\boldsymbol{g})}(f)$, $f \in C_0^\infty(M)$, one obtains in this way a locally covariant quantum field Φ as a natural transformation.

3. States, Representations, and the Principle of Local Definiteness

3.1. Functorial description of a state space. The description of a physical system in terms of operator algebras requires also the concept of states so that expectation values of observables can be calculated. First, suppose that one is given a C^*-algebra $\mathcal{A}$ with unit element $\mathbf{1}$ modelling the algebra of observables of some physical system. A state is a linear functional $\omega : \mathcal{A} \to \mathbb{C}$ having the property of being positive, i.e. $\omega(A^*A) \geq 0$ $\forall A \in \mathcal{A}$, and normalized, i.e. $\omega(\mathbf{1}) = 1$. Thus, given any hermitian element $A \in \mathcal{A}$, the number $\omega(A)$ is interpreted as an expectation value of the observable A in the state ω.

There is an intimate relation between states on $\mathcal{A}$ and Hilbert-space representations of $\mathcal{A}$. If π is a linear $*$-representation of $\mathcal{A}$ by bounded linear operators on some Hilbert-space $\mathcal{H}$, then each positive density matrix ρ with unit trace on $\mathcal{H}$ induces a state $\omega(A) = \mathrm{tr}(\rho \cdot \pi(A))$, $A \in \mathcal{A}$, on $\mathcal{A}$. There is also a converse of that: For each state ω on $\mathcal{A}$ there exists a triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, consisting of a Hilbert-space $\mathcal{H}_\omega$, a linear $*$-representation π_ω of $\mathcal{A}$ by bounded linear operators on $\mathcal{H}_\omega$, and a unit vector $\Omega_\omega \in \mathcal{H}_\omega$ such that $\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle$ for all $A \in \mathcal{A}$. This triple is called the GNS-representation of ω (after Gelfand, Naimark and Segal); for its construction, see e.g. [5].

Now suppose that our set of observables arises in terms of a functor $\mathscr{A}$ describing a locally covariant quantum field theory. The question arises what the concept of a state might be in this case. The first, quite natural idea is to say that a state is a family $\{\omega_{(M,g)} : (M, g) \in \mathrm{Obj}(\mathfrak{Man})\}$ indexed by the members in the object-class $\mathfrak{Man}$, where each $\omega_{(M,g)}$ is a state on the C^*-algebra $\mathscr{A}(M, g)$. Usually, however, one is interested in states with particular properties, e.g., one would like to consider states $\omega_{(M,g)}$ fulfilling an appropriate variant of the "microlocal spectrum condition" [7] which can be seen as a replacement for the relativistic spectrum condition for quantum field theories on curved spacetime and which, for free fields, is equivalent to the Hadamard condition (cf. Sect. 2.3, and [36, 39]). One might wonder if, above that, there are families of states $\{\omega_{(M,g)} : (M, g) \in \mathrm{Obj}(\mathfrak{Man})\}$ that are distinguished by a property which in our framework would correspond to "local diffeomorphism invariance", namely,

$$\omega_{(M',g')} \circ \alpha_\psi = \omega_{(M,g)} \quad \text{on } \mathscr{A}(M, g)$$

for all $\psi \in \hom_{\mathfrak{Man}}((M, g), (M', g'))$. However, it has been shown in [26] that this invariance property cannot be realized for states of the free scalar field fulfilling the microlocal spectrum condition. Let us briefly sketch an argument showing that the above property will, in general, not be physically realistic. Let us consider two spacetimes (M_1, g_1) and (M_2, g_2), and assume that (M_1, g_1) is just Minkowski-spacetime. Moreover, it will be assumed that (M_2, g_2) consists of three regions which are themselves globally hyperbolic sub-spacetimes of (M_2, g_2): An "intermediate" region L_2 lying in the future of a region N_2^- and in the past of a region N_2^+. All these regions are assumed to contain Cauchy-surfaces, and it is also assumed that the regions $N_2^\pm$ are isometrically diffeomorphic to globally hyperbolic subregions $N_1^\pm$ of Minkowski spacetime (M_1, g_1) which likewise contain Cauchy-surfaces. By $\iota^\pm : N_1^\pm \to N_2^\pm$ we denote the corresponding isometric diffeomorphisms. We may, for the sake of concreteness, consider a free scalar field (cf. next section), and define the state ω_1 on $\mathscr{A}(M_1, g_1)$ to be its vacuum state (which fulfills the microlocal spectrum condition). Then the state $\omega_2^- = \omega_1 \circ \alpha_{\iota^-}^{-1}$ induces a state on $\mathscr{A}(N_2^-, g_{2,N_2^-})$ and thereby, since the free field obeys the time-slice axiom, it induces a state ω_2 on $\mathscr{A}(M_2, g_2)$ (which again fulfills the microlocal spectrum condition). Now the state ω_2 restricts to a state ω_2^+ on $\mathscr{A}(N_2^+, g_{2,N_2^+})$. However, if there is non-trivial curvature in the intermediate region L_2, then the state ω_2, which was a vacuum state on the "initial" region N_2^-, will no longer be a vacuum state on the "final" region N_2^+ [50]. The regions N_2^- and N_2^+ possess isometric subregions; it is no loss of generality to suppose that there is an isometric diffeomorphism $\psi : N_2^- \to N_2^+$. Then invariance in the above sense of the family of states $\omega_1, \omega_2, \omega_2^\pm$ demands that

$$\omega_2^+ \circ \alpha_\psi = \omega_2^- ,$$

but this is not the case (ω_2^- is (the restriction of) a vacuum state, ω_2^+ is (the restriction of) a non-vacuum state.) The counterexample is based on a form of "relative Cauchy-evolution", which is worth being studied in greater generality, and this will be the topic of Sect. 4.

In view of this negative result one finds oneself confronted with the question if there is a more general concept of "invariance" that can be attributed to families of states $\{\omega_{(M,g)} : (M, g) \in \mathrm{Obj}(\mathfrak{Man})\}$ for a locally covariant quantum field theory given by a functor $\mathscr{A}$. We will argue that there is a positive answer to that question: The local folia determined by states satisfying the microlocal spectrum condition are good candidates for minimal classes of states which are locally diffeomorphism covariant. To explain this, let us fix the relevant concepts some of which are, in fact, due to Haag [23].

Folium of a representation. Let $\mathcal{A}$ be a C^*-algebra and $\pi : \mathcal{A} \to B(\mathcal{H})$ a $*$-representation of $\mathcal{A}$ by bounded linear operators on a Hilbert space $\mathcal{H}$. The *folium* of π, denoted by $\boldsymbol{F}(\pi)$, is the set of all states ω' on $\mathcal{A}$ which can be written as

$$\omega'(A) = \mathrm{tr}(\rho \cdot \pi(A)) , \quad A \in \mathscr{A}(M, \boldsymbol{g}) .$$

In other words, the folium of a representation consists of all density matrix states in that representation.

Local quasi-equivalence and local normality. Let $\mathscr{A}$ be a locally covariant quantum field theory and let, for $(M, \boldsymbol{g})$ fixed, ω and $\tilde{\omega}$ be two states on $\mathscr{A}$. We will say that these states (or their GNS-representations, denoted by π and $\tilde{\pi}$, respectively) are *locally quasi-equivalent* if for all $O \in \mathcal{K}(M, \boldsymbol{g})$ the relation

$$\boldsymbol{F}(\pi \circ \alpha_{M,O}) = \boldsymbol{F}(\tilde{\pi} \circ \alpha_{M,O}) \tag{6}$$

is valid, where $\alpha_{M,O} = \alpha_{\iota_{M,O}}$ and $\iota_{M,O} : (O, \boldsymbol{g}_O) \to (M, \boldsymbol{g})$ is the natural embedding (cf. Prop. 2.3).

Moreover, we say that ω is *locally normal* to $\tilde{\omega}$ (or to the corresponding GNS-representation $\tilde{\pi}$) if

$$\omega \circ \alpha_{M,O} \in \boldsymbol{F}(\tilde{\pi} \circ \alpha_{M,O}) \tag{7}$$

holds for all $O \in \mathcal{K}(M, \boldsymbol{g})$.

Intermediate factoriality. Let ω be a state on $\mathscr{A}(M, \boldsymbol{g})$, then we define for each $O \in \mathcal{K}(M, \boldsymbol{g})$ the von Neumann algebra $\mathcal{M}_\omega(O) = \pi_\omega(\alpha_{M,O}(\mathscr{A}(M, \boldsymbol{g})))''$, the local von Neumann algebra of the region O with respect to the state ω. We say that the state ω fulfills the condition of *intermediate factoriality* if for each $O \in \mathcal{K}(M, \boldsymbol{g})$ there exist $O_1 \in \mathcal{K}(M, \boldsymbol{g})$ and a factorial von Neumann algebra $\mathcal{N}$ acting on the GNS-Hilbert-space $\mathcal{H}_\omega$ of ω so that

$$\mathcal{M}_\omega(O) \subset \mathcal{N} \subset \mathcal{M}_\omega(O_1) .$$

(We recall that a factorial von Neumann algebra $\mathcal{N}$ is a von Neumann algebra so that $\mathcal{N} \cap \mathcal{N}'$ contains only multiples of the unit operator.)

It is known that quasifree states of the free scalar field on globally hyperbolic spacetimes which fulfill the microlocal spectrum condition are locally quasi-equivalent (cf. Subsect. 3.2). Thus, local quasi-equivalence may be expected for states satisfying the microlocal spectrum condition. More generally, local normality can be interpreted as ruling out the possibility of local superselection rules. Also intermediate factoriality is known to hold for states of the free scalar field fulfilling the microlocal spectrum condition on globally hyperbolic spacetimes (cf. again Sect. 3). The condition of intermediate factoriality serves the purpose of eliminating the possible difference between the folium of a representation and the folium of any of its (non-trivial) subrepresentations (see Appendix **b**)). It can also be motivated as the consequence of a stricter formulation, known as "split property", which is expected to hold for all (also interacting) physically relevant quantum field theories on general grounds (cf. [41, 21, 9]) and is in fact known to hold for states of the free field fulfilling the microlocal spectrum condition in flat and curved spacetimes [8, 45], and for interacting theories in low dimensions [40]. We also note that the property of a state to fulfill the microlocal spectrum condition is a locally covariant property (owing to the covariant behaviour of wavefront sets of distributions under diffeomorphisms [28]) and thus, for a locally covariant quantum field theory it is natural to assume that, if $\omega_{(M',\boldsymbol{g}')}$ fulfills (any suitable variant of) the microlocal spectrum condition, then so does $\omega_{(M',\boldsymbol{g}')} \circ \alpha_\psi$ for any $\psi \in \hom_{\mathfrak{Man}}((M,\boldsymbol{g}),(M',\boldsymbol{g}'))$. In the case where also the folia of states (i.e., the folia of their GNS-representations) satisfying the microlocal spectrum condition coincide locally, one thus obtains the invariance of local folia under local diffeomorphisms for families of states satisfying the microlocal spectrum condition, more precisely, at the level of the GNS-representations of $\omega_{(M,\boldsymbol{g})}$ and $\omega_{(M',\boldsymbol{g}')}$,

$$\boldsymbol{F}(\pi_{(M',\boldsymbol{g}')} \circ \alpha_\psi \circ \alpha_{M,O}) = \boldsymbol{F}(\pi_{(M,\boldsymbol{g})} \circ \alpha_{M,O})$$

holds for all $\psi \in \hom_{\mathfrak{Man}}((M,\boldsymbol{g}),(M',\boldsymbol{g}'))$ and all $O \in \mathcal{K}(M,\boldsymbol{g})$. All these properties are known to hold for quasifree states of the free scalar field fulfilling the microlocal spectrum condition on global hyperbolic spacetimes, see Subsect. 3.2 for discussion.

Thus one can see that local diffeomorphism invariance really occurs at the level of local folia of states for $\mathscr{A}$. In this light, it appears natural to give a functorial description of the space of states that takes this form of local diffeomorphism invariance into account. To this end, it seems convenient to first introduce a new category, the category of state spaces.

$\mathfrak{Sts}$: An object $\boldsymbol{S} \in \mathrm{Obj}(\mathfrak{Sts})$ is a state space of a C^*-algebra $\mathcal{A}$. That is, $\boldsymbol{S}$ is a subset of the set of all states on $\mathcal{A}$ that is closed under taking finite convex combinations and operations $\omega(\,.\,) \mapsto \omega_A(\,.\,) = \omega(A^*\,.\,A)/\omega(A^*A)$, $A \in \mathcal{A}$. Morphisms between members $\boldsymbol{S}'$ and $\boldsymbol{S}$ of $\mathrm{Obj}(\mathfrak{Sts})$ are maps $\gamma^* : \boldsymbol{S}' \to \boldsymbol{S}$ that arise as the dual map of a C^*-algebraic monomorphism $\gamma : \mathcal{A} \to \mathcal{A}'$ via

$$\gamma^*\omega'(A) = \omega'(\gamma(A))\,, \quad \omega' \in \boldsymbol{S}', \quad A \in \mathcal{A}\,.$$

The category $\mathfrak{Sts}$ is therefore "dual" to the category $\mathfrak{Alg}$. The composition rules for morphisms should thus be obvious.

Now we can define a state space for a locally covariant quantum field theory in a functorial manner.

Definition 3.1. *Let $\mathscr{A}$ be a locally covariant quantum field theory.*

(i) *A* **state space** *for $\mathscr{A}$ is a contravariant functor $\boldsymbol{S}$ between $\mathfrak{Man}$ and $\mathfrak{Sts}$:*

$$\begin{array}{ccc} (M,\boldsymbol{g}) & \xrightarrow{\ \psi\ } & (M',\boldsymbol{g}') \\ {\scriptstyle S}\downarrow & & \downarrow{\scriptstyle S} \\ \boldsymbol{S}(M,\boldsymbol{g}) & \xleftarrow{\ \alpha_\psi^*\ } & \boldsymbol{S}(M',\boldsymbol{g}') \end{array}$$

where $\boldsymbol{S}(M,\boldsymbol{g})$ is a set of states on $\mathscr{A}(M,\boldsymbol{g})$ and α_ψ^* is the dual map of α_ψ; the contravariance property is

$$\alpha^*_{\tilde{\psi}\circ\psi} = \alpha^*_\psi \circ \alpha^*_{\tilde{\psi}}$$

together with the requirement that unit morphisms are mapped to unit morphisms.

(ii) *We say that a state space $\boldsymbol{S}$ is* **locally quasi-equivalent** *if Eq.* (6) *holds for any pair of states $\omega, \tilde{\omega} \in \boldsymbol{S}(M,\boldsymbol{g})$ (with GNS-representations $\pi, \tilde{\pi}$) whenever $(M,\boldsymbol{g}) \in$* $\mathrm{Obj}(\mathfrak{Man})$ *and $O \in \mathcal{K}(M,\boldsymbol{g})$.*

(iii) *A state space* $\boldsymbol{S}$ *is called* **locally normal** *if there exists a locally quasi-equivalent state space* $\tilde{\boldsymbol{S}}$ *so that for each* $\omega \in \boldsymbol{S}(M, \boldsymbol{g})$ *there is some* $\tilde{\omega} \in \tilde{\boldsymbol{S}}(M, \boldsymbol{g})$ *(with GNS-representation* $\tilde{\pi}$*) so that* (7) *holds for all* $O \in \mathcal{K}(M, \boldsymbol{g})$.

(iv) *We say that a state space* $\boldsymbol{S}$ *is* **intermediate factorial** *if each state* $\omega \in \boldsymbol{S}(M, \boldsymbol{g})$ *fulfills the condition of intermediate factoriality.*

We list a few direct consequences of the previous definitions.

Theorem 3.2. (a) *Let* $\boldsymbol{S}$ *be a state space which is intermediate factorial. Then for all spacetimes* $(M, \boldsymbol{g}), (M', \boldsymbol{g}') \in \mathrm{Obj}(\mathfrak{Man})$ *and all pairs of states* $\omega \in \boldsymbol{S}(M, \boldsymbol{g})$, $\omega' \in \boldsymbol{S}(M', \boldsymbol{g}')$ *with GNS-representations* π, π' *there holds*

$$\boldsymbol{F}(\pi' \circ \alpha_\psi \circ \alpha_{M,O}) = \boldsymbol{F}(\pi \circ \alpha_{M,O}), \quad O \in \mathcal{K}(M, \boldsymbol{g}), \tag{8}$$

if and only if the state space is locally quasi-equivalent.

(b) *If the state space* $\boldsymbol{S}$ *is locally normal, then there exists a family of states* $\{\omega_{(M,\boldsymbol{g})} : (M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})\}$ *on* $\mathscr{A}$ *with the property that each* $\omega \in \boldsymbol{S}(M, \boldsymbol{g})$ *is locally normal to* $\omega_{(M,\boldsymbol{g})}$.

(c) *If* $\tilde{\boldsymbol{S}}$ *is a locally quasi-equivalent and intermediate factorial state space, then one obtains a convex, locally normal state space* $\boldsymbol{S}$ *by defining* $\boldsymbol{S}(M, \boldsymbol{g})$ *as the set of all states which are locally normal to any state on* $\tilde{\boldsymbol{S}}(M, \boldsymbol{g})$.

Proof. In our proof, we will make use of the following statements:

(α) Let $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ be C^*-algebras with C^*-algebraic morphisms

$$\mathcal{A} \xrightarrow{\beta} \mathcal{B} \xrightarrow{\gamma} \mathcal{C},$$

and let ω be a state on $\mathcal{C}$. Then there holds

$$\boldsymbol{F}(\pi_\omega \circ \gamma \circ \beta) \supset \boldsymbol{F}(\pi_{\omega\circ\gamma} \circ \beta) \supset \boldsymbol{F}(\pi_{\omega\circ\gamma\circ\beta}),$$

where π_ν denotes the GNS-representation of the state ν; we will use this notation also below.

(β) Let $\mathcal{N}$ be a factorial von Neumann algebra on some Hilbert-space $\mathcal{H}$, and let $\mathcal{H}_\mathcal{N}$ be some $\mathcal{N}$-invariant closed, non-zero subspace. Then for every density matrix $\rho = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$, where the ϕ_i are unit vectors in $\mathcal{H}$, there exists a density matrix $\rho^\mathcal{N} = \sum_j \mu_j |\chi_j\rangle\langle\chi_j|$, where the χ_j are unit vectors in $\mathcal{H}_\mathcal{N}$, so that

$$\mathrm{tr}(\rho \cdot N) = \mathrm{tr}(\rho^\mathcal{N} \cdot N) \tag{9}$$

holds for all $N \in \mathcal{N}$.

These statements will be proved in the appendix.

(a) A first immediate observation is that $\alpha_\psi^* \boldsymbol{S}(M', \boldsymbol{g}') \subset \boldsymbol{S}(M, \boldsymbol{g})$ together with the condition of local quasi-equivalence imply

$$\boldsymbol{F}(\pi_{\omega'\circ\alpha_\psi} \circ \alpha_{M,O}) = \boldsymbol{F}(\pi \circ \alpha_{M,O}), \quad O \in \mathcal{K}(M, \boldsymbol{g}). \tag{10}$$

Now fix $O \in \mathcal{K}(M, \boldsymbol{g})$. According to the assumed condition of intermediate factoriality, there are a region $O_1 \in \mathcal{K}(M, \boldsymbol{g})$ and a factorial von Neumann algebra $\mathcal{N}$ so that

$$\mathcal{M}_{\omega'}(\psi(O)) \subset \mathcal{N} \subset \mathcal{M}_{\omega'}(\psi(O_1)).$$

Consequently, if we choose an arbitrary state $\omega_1 \in \boldsymbol{F}(\pi_{\omega'} \circ \alpha_\psi \circ \alpha_{M,O})$, then there exists, according to statement (β) above, a density matrix $\rho^{\mathcal{N}} = \sum_j \mu_j |\chi_j\rangle\langle\chi_j|$ with $\chi_j \in \mathcal{H}_{\mathcal{N}} = \overline{\mathcal{N}\Omega'}$ (where Ω' is the GNS-vector of ω') with the property

$$\omega_1(A) = \mathrm{tr}(\rho^{\mathcal{N}} \cdot \pi_{\omega'} \circ \alpha_\psi \circ \alpha_{M,O}(A)), \quad A \in \alpha_{M,O}(\mathscr{A}(O, \boldsymbol{g}_O)).$$

Therefore, the state is in particular given by a density matrix $\rho^{\mathcal{N}}$ in the GNS-representation of $\omega' \circ \alpha_{M',\psi(O_1)}$, so that ω_1 extends to a state

$$\overline{\omega}_1 \in \boldsymbol{F}(\pi_{\omega' \circ \alpha_{M',\psi(O_1)}}).$$

Owing to covariance, this in turn shows that

$$\overline{\omega}_1 \in \boldsymbol{F}(\pi_{\omega' \circ \alpha_\psi \circ \alpha_{M,O_1}}).$$

Restricting $\overline{\omega}_1$ again to $\omega_1 = \overline{\omega}_1 \circ \alpha_{M,O}$ on $\mathscr{A}(O, \boldsymbol{g}_O)$ yields

$$\omega_1 \in \boldsymbol{F}(\pi_{\omega' \circ \alpha_\psi} \circ \alpha_{M,O}).$$

In view of statement (α) above and because of (10), we have thus shown that (8) holds for all $O \in \mathcal{K}(M, \boldsymbol{g})$ if $\boldsymbol{S}$ is locally quasi-equivalent. The reverse implication, saying that (8) implies that $\boldsymbol{S}$ is locally quasi-equivalent, is evident.

(b) One may choose an arbitrary family of states $\omega_{(M,\boldsymbol{g})} \in \tilde{\boldsymbol{S}}(M, \boldsymbol{g})$; since each such choice of states is locally quasi-equivalent to any other, by definition each state in $\boldsymbol{S}(M, \boldsymbol{g})$ will be locally normal to $\omega_{(M,\boldsymbol{g})}$.

(c) If $\boldsymbol{S}$ is a state space, then it is clearly locally normal owing to the way it is defined. So it suffices to prove that $\boldsymbol{S}$ is a state space, and convex.

To show that $\boldsymbol{S}$ is a state space, it is enough to demontrate that

$$\alpha_\psi^*(\boldsymbol{S}(M', \boldsymbol{g}')) \subset \boldsymbol{S}(M, \boldsymbol{g}),$$

since the contravariance property of the α_ψ^*'s is inherited from the covariance property of the α_ψ's. Now if $\omega' \in \boldsymbol{S}(M', \boldsymbol{g}')$, then this means that

$$\omega' \circ \alpha_{M',O'} \in \boldsymbol{F}(\pi_{\hat{\omega}} \circ \alpha_{M',O'})$$

holds for all $O' \in \mathcal{K}(M', \boldsymbol{g}')$, where $\hat{\omega}$ is some element in $\tilde{\boldsymbol{S}}(M', \boldsymbol{g}')$. Using covariance one deduces from this relation

$$(\alpha_\psi^*\omega') \circ \alpha_{M,O} = \omega' \circ \alpha_\psi \circ \alpha_{M,O} \in \boldsymbol{F}(\pi_{\hat{\omega}} \circ \alpha_\psi \circ \alpha_{M,O}).$$

Then part (a) of the proposition entails

$$(\alpha_\psi^*\omega') \circ \alpha_{M,O} \in \boldsymbol{F}(\pi_{\tilde{\omega}} \circ \alpha_{M,O})$$

for all $O \in \mathcal{K}(M, \boldsymbol{g})$ with some $\tilde{\omega} \in \tilde{\boldsymbol{S}}(M, \boldsymbol{g})$, showing that $\alpha_\psi^*\omega' \in \boldsymbol{S}(M, \boldsymbol{g})$.

Finally, we show that $\boldsymbol{S}$ is convex. Let $\omega' = \lambda\omega_1 + (1-\lambda)\omega_2$ be a convex combination of two states ω_1 and ω_2 in $\boldsymbol{S}(M, \boldsymbol{g})$. Then $\omega_j \circ \alpha_{M,O} \in \boldsymbol{F}(\pi_{\tilde{\omega}} \circ \alpha_{M,O})$, $j = 1, 2$, for some state $\tilde{\omega} \in \tilde{\boldsymbol{S}}(M, \boldsymbol{g})$, and going back to the definition of the folium, this shows in fact that $\omega' \circ \alpha_{M,O} \in \boldsymbol{F}(\pi_{\tilde{\omega}} \circ \alpha_{M,O})$. Thus $\omega' \in \boldsymbol{S}(M, \boldsymbol{g})$, showing that $\boldsymbol{S}(M, \boldsymbol{g})$ is convex. □

Finally, we shall demonstrate that a locally normal and intermediate factorial state space induces a generally covariant realization of the principle of local definiteness proposed by Haag, Narnhofer and Stein [22]. This principle was introduced in the context of a net of observable algebras $\{\mathcal{A}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$ over a fixed, globally hyperbolic background spacetime $(M, \boldsymbol{g})$. The **principle of local definiteness** demands that there exists a Hilbert-space representation π of the C^*-algebra $\mathcal{A}$ generated by $\{\mathcal{A}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$ so that the set of states, $\mathcal{S}$, of the theory can be characterized as consisting of all states ω on $\mathcal{A}$ that can be extended to normal states on the local von Neumann algebras $\mathcal{M}(O) = \pi(\mathcal{A}(O))''$, $O \in \mathcal{K}(M, \boldsymbol{g})$. Furthermore, it was required in [22] that the local von Neumann algebras $\mathcal{M}(O)$ are factors, at least for a suitable collection of regions O. Here we take the point of view that one should replace this condition by the (weaker) condition of intermediate factoriality with respect to the family of local von Neumann algebras $\{\mathcal{M}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$ since this avoids having to specify precise geometric conditions on the regions O for which $\mathcal{M}(O)$ should be a factor.

Adopting this point of view, we may observe the following. Let $\mathscr{A}$ be a locally covariant quantum field theory with a locally normal and intermediate factorial state space $\boldsymbol{S}$, and for $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$, let $\{\mathcal{A}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$ be the net of C^*-algebras on $(M, \boldsymbol{g})$ induced by $\mathscr{A}$ according to Prop. 2.3. Let $\tilde{\omega}$ be any state in $\tilde{\boldsymbol{S}}(M, \boldsymbol{g})$, where $\tilde{\boldsymbol{S}}$ is a locally quasi-equivalent state space to which $\boldsymbol{S}$ is locally normal (cf. Def. 2.3(iii)), and denote by $\tilde{\pi}$ the corresponding GNS-representation. This representation induces a representation π of $\mathscr{A}$ via defining the representations $\pi \restriction \mathcal{A}(O)$ as $\tilde{\pi} \circ \alpha_{M,O}^{-1}$, and hence it induces the corresponding net of von Neumann algebras $\{\mathcal{M}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$. It is easy to see that each state $\omega \in \boldsymbol{S}(M, \boldsymbol{g})$ extends to a normal state on $\mathcal{M}(O)$ owing to local normality of $\boldsymbol{S}$; additionally $\{\mathcal{M}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$ satisfies the condition of intermediate factoriality because $\boldsymbol{S}$ is intermediate factorial. We formulate the result of this discussion subsequently as

Proposition 3.3. *If $\boldsymbol{S}$ is locally normal and intermediate factorial, then the set of states $\boldsymbol{S}(M, \boldsymbol{g})$ for $\{\mathcal{A}(O)\}_{O\in\mathcal{K}(M,\boldsymbol{g})}$ fulfills the principle of local definiteness, for each $(M, \boldsymbol{g})$ $\in \mathrm{Obj}(M, \boldsymbol{g})$.*

3.2. State space of the Klein-Gordon field distinguished by microlocal spectrum condition. For the locally covariant quantum field theory of the Klein-Gordon field, we will show in the present subsection that the microlocal spectrum condition selects a state space that is locally quasi-equivalent and intermediate factorial.

We have to provide some explanations first. Let $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$ and let E, $\mathfrak{W}(\mathcal{R}, \sigma)$ be defined with respect to the Klein-Gordon equation (1) on $(M, \boldsymbol{g})$. A state ω on $\mathfrak{W}(\mathcal{R}, \sigma)$ is called quasifree if its two-point function

$$w_2^{(\omega)}(f, h) = \partial_t \partial_\tau |_{t=\tau=0}\, \omega(W(tEf)W(\tau Eh))$$

exists for all $f, h \in C_0^\infty(M, \mathbb{R})$, and if ω is determined by $w_2^{(\omega)}$ according to

$$\omega(W(Ef)) = \mathrm{e}^{-w_2^{(\omega)}(f,f)} .$$

A quasifree state ω is a Hadamard state if its two-point function is of Hadamard form. This property is a constraint on the short-distance behaviour of the two-point function.

Qualitatively, it means that $w_2^{(\omega)}$ is a distribution on $C_0^\infty(M,\mathbb{R}) \times C_0^\infty(M,\mathbb{R})$ of the form

$$w_2^{(\omega)}(f,h) = \lim_{\epsilon\to 0} \int (G_\epsilon(x,y) + H_\omega(x,y)) f(x)h(y)\, d\mu_{\boldsymbol{g}}(x)\, d\mu_{\boldsymbol{g}}(y), \tag{11}$$

where H_ω is a smooth integral kernel depending on the state ω, while the singular part of $w_2^{(\omega)}$ is given as the limit of a family of integral kernels G_ϵ which are determined by the metric $\boldsymbol{g}$ and the Klein-Gordon equation via the so-called Hadamard recursion relations. The leading singularity is of the type 1/(squared geodesic distance from x to y). We refer to [31] for details. The Hadamard property can be equivalently expressed in terms of a condition on the wavefront set $\mathrm{WF}(w_2^{(\omega)})$ of the two-point function [36] (see also [39]): ω is a Hadamard state exactly if the pairs of covectors (x,η) and (x',η') which are in $\mathrm{WF}(w_2^{(\omega)})$ are such that their base-points x and x' lie on a lightlike geodesic, and the co-tangent vectors η and $-\eta'$ are co-tangent and co-parallel to that geodesic, with η future-pointing.

This characterization of the Hadamard condition in terms of a constraint on the wavefront set of the two-point function of a state is also referred to as the "microlocal spectrum condition" because it mimicks the usual, flat space spectrum condition in the sense of microlocal analysis; its advantage is that it may be formulated for general quantum field theories, in contrast to the Hadamard condition which requires that the 2-point function satisfies a hyperbolic wave-equation [7, 46]. We refer to the indicated references for further discussion. In the context of the present subsection, we will use "Hadamard condition" and "microlocal spectrum condition" synonymously.

Now let $\mathscr{A}$ be the locally covariant quantum field theory associated with the Klein-Gordon field as in Subsect. 2.3. It is important to note that, owing to the functorial transformation properties of wavefront sets under diffeomorphisms [28], a quasifree Hadamard state ω' on $\mathscr{A}(M',\boldsymbol{g}')$ induces a quasifree Hadamard state $\omega' \circ \alpha_\psi$ on $\mathscr{A}(M,g)$ whenever $\psi \in \mathrm{hom}_{\mathfrak{Man}}((M,\boldsymbol{g}),(M',\boldsymbol{g}'))$. Furthermore, it was shown in [20] that there exists a large set of quasifree Hadamard states for the Klein-Gordon field on every globally hyperbolic spacetime $(M,\boldsymbol{g})$. Moreover, the results in [44] show that the GNS-representations of quasifree Hadamard states are locally quasi-equivalent, and in [45] it was proved that the condition of intermediate factoriality is fulfilled for quasifree Hadamard states. We may thus summarize these results in the subsequent:

Theorem 3.4. *For each* $(M,\boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$*, define* $\boldsymbol{S}(M,\boldsymbol{g})$ *as the set of all states on* $\mathscr{A}(M,\boldsymbol{g})$ *whose GNS-representations are locally quasiequivalent to the GNS-representation of any quasifree Hadamard state on* $\mathscr{A}(M,\boldsymbol{g})$*. This assignment results in a state space which is locally quasi-equivalent and intermediate factorial, and* $\boldsymbol{S}(M,\boldsymbol{g})$ *contains in particular all quasifree Hadamard states on* $\mathscr{A}(M,\boldsymbol{g})$*.*

4. Dynamics

4.1. Relative Cauchy-evolution. For theories obeying the time-slice axiom one can define relative Cauchy-evolutions, as follows. Let $(M_1,\boldsymbol{g}_1)$ and $(M_2,\boldsymbol{g}_2)$ be in $\mathrm{Obj}(\mathfrak{Man})$. We suppose that there are globally hyperbolic sub-regions $N_j^\pm$ of M_j, $j=1,2$ containing Cauchy-surfaces of the respective spacetimes. Moreover, we assume that there are isometric (and orientation/time-orientation-preserving) diffeomorphisms $\iota^\pm : N_1^\pm \to N_2^\pm$ when the regions are endowed with the appropriate restrictions of the metrics $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$, respectively. Henceforth, we shall suppress the diffeomorphisms $\iota^\pm$ in our notation and identify $N_1^{\pm}$ and $N_2^{\pm}$ as being equal. The isometric embeddings of $N_j^{\pm}$ into M_j will be denoted by $\psi_j^{\pm}$. They are depicted in the following diagram:

$$\begin{array}{ccccc} N_1^+ & \xrightarrow{\psi_1^+} & M_1 & \xleftarrow{\psi_1^-} & N_1^- \\ \| & & & & \| \\ N_2^+ & \xrightarrow{\psi_2^+} & M_2 & \xleftarrow{\psi_2^-} & N_2^- \end{array}$$

By the functorial properties of a locally covariant quantum field theory $\mathscr{A}$, the previous diagram gives rise to the next:

$$\begin{array}{ccccc} \mathscr{A}(N_1^+) & \xrightarrow{\alpha_{\psi_1^+}} & \mathscr{A}(M_1) & \xleftarrow{\alpha_{\psi_1^-}} & \mathscr{A}(N_1^-) \\ \| & & & & \| \\ \mathscr{A}(N_2^+) & \xrightarrow{\alpha_{\psi_2^+}} & \mathscr{A}(M_2) & \xleftarrow{\alpha_{\psi_2^-}} & \mathscr{A}(N_2^-) \end{array}$$

where we have, for the sake of simplicity, suppressed the appearance of the spacetime metrics in our notation. If the theory $\mathscr{A}$ obeys the time-slice axiom, then all the morphisms in this diagram are onto and invertible, and hence one obtains from it an automorphism $\beta \in \hom_{\mathfrak{Alg}}(\mathscr{A}(M_1), \mathscr{A}(M_1))$ by setting

$$\beta = \alpha_{\psi_1^-} \circ \alpha_{\psi_2^-}^{-1} \circ \alpha_{\psi_2^+} \circ \alpha_{\psi_1^+}^{-1} .$$

Under certain circumstances (which may be expected to be generically fulfilled) it is possible to form the functional derivative of the relative Cauchy-evolution with respect to the metrics of the spacetimes involved in its construction. This functional derivative then has the meaning of an energy-momentum tensor. In fact, we will show below for the example of the Klein-Gordon field that the functional derivative of the relative Cauchy-evolution agrees with the action of the quantized energy-momentum tensor in representations of quasifree Hadamard states.

In order to give these ideas a more precise shape, we introduce the following

Geometric assumptions.

- We consider a globally hyperbolic spacetime $(M, \overset{\circ}{\boldsymbol{g}})$.
- We pick a Cauchy-surface C in $(M, \overset{\circ}{\boldsymbol{g}})$, and two open subregions $N_{\pm}$ of M with the properties:
  - $\overline{N_{\pm}} \subset \mathrm{int}\, J^{\pm}(C)$,
  - $(N_{\pm}, \overset{\circ}{\boldsymbol{g}}_{N_{\pm}})$ are contained in $\mathrm{Obj}(\mathfrak{Man})$,
  - $N_{\pm}$ contain Cauchy-surfaces for $(M, \overset{\circ}{\boldsymbol{g}})$.
- Let G be a set of Lorentzian metrics on M with the following properties:
  - Each $\boldsymbol{g} \in G$ deviates from $\overset{\circ}{\boldsymbol{g}}$ only on a compact subset of the region

$$M_{(+,-)} = M \backslash \mathrm{cl}[J^-(N_-) \cup J^+(N_+)] ,$$

  - each $(M, \boldsymbol{g})$, $\boldsymbol{g} \in G$, is a member of $\mathrm{Obj}(\mathfrak{Man})$,
  - C is a Cauchy-surface for $(M, \boldsymbol{g})$, $\boldsymbol{g} \in G$,

– The set of differences $\boldsymbol{g} - \overset{\circ}{\boldsymbol{g}}$ forms an open neighbourhood, U, with respect to the topology of $\mathcal{D}$ (cf. [10]), of the zero element in the space of all symmetric C^∞-sections in $T^*M \otimes T^*M$ having compact support in $M_{(+,-)}$.

Remark. A sufficiently small open neighbourhood, U, of the zero section may always be chosen such that G satisfies the other conditions listed above. Moreover, given any smooth, one-parametric family $\phi^{(s)}$, $s \in \mathbb{R}$, of diffeomorphisms of M acting trivially outside of $M_{(+,-)}$ and fulfilling $\phi^{(0)} = \mathrm{id}_M$, one can find for each $\boldsymbol{g} \in G$ an $s(\boldsymbol{g}) > 0$ so that $\phi_*^{(s)}\boldsymbol{g} \in G$ for $|s| < s(\boldsymbol{g})$.

These assumptions suggest that one may view the metrics $\boldsymbol{g}$ in G as "perturbations" around the metric $\overset{\circ}{\boldsymbol{g}}$ on $M_{(+,-)}$. Moreover, $(N_\pm, \overset{\circ}{\boldsymbol{g}}_{N_\pm})$ are also globally hyperbolic submanifolds of $(M, \boldsymbol{g})$ for each $\boldsymbol{g} \in G$. Hence there are isometric embeddings $\psi_{\boldsymbol{g}}^\pm \in \hom_{\mathfrak{Man}}((N_\pm, \overset{\circ}{\boldsymbol{g}}_{N_\pm}), (M, \boldsymbol{g}))$ for all $\boldsymbol{g} \in G$ as well as isometric embeddings $\psi_\circ^\pm \in \hom_{\mathfrak{Man}}((N_\pm, \overset{\circ}{\boldsymbol{g}}_{N_\pm}), (M, \overset{\circ}{\boldsymbol{g}}))$. To these embeddings one can associate the relative Cauchy-evolution $\beta_{\boldsymbol{g}} \in \hom_{\mathfrak{Alg}}(\mathscr{A}(M, \overset{\circ}{\boldsymbol{g}}), \mathscr{A}(M, \overset{\circ}{\boldsymbol{g}}))$ given by

$$\beta_{\boldsymbol{g}} = \alpha_{\psi_\circ^-} \circ \alpha_{\psi_{\boldsymbol{g}}^-}^{-1} \circ \alpha_{\psi_{\boldsymbol{g}}^+} \circ \alpha_{\psi_\circ^+}^{-1} \,. \tag{12}$$

Remarks. (A) One may view $\beta_{\boldsymbol{g}}$ as a "scattering morphism" describing the change that the propagation of a quantum field undergoes passing through the region with the "metric perturbation" $\boldsymbol{g} - \overset{\circ}{\boldsymbol{g}}$ compared to the background metric $\overset{\circ}{\boldsymbol{g}}$.

(B) There is some relation between the relative Cauchy-evolution and the evolution of Cauchy-data from one Cauchy-surface to another which e.g. in the case of the scalar Klein-Gordon field is also known to lead to C^*-algebraic endomorphisms [30, 42]. We refer to the references for more discussion.

(C) Hollands and Wald [26] consider for the case of the free Klein-Gordon field related operators $\tau_{\boldsymbol{g}}^{\mathrm{adv}}$ and $\tau_{\boldsymbol{g}}^{\mathrm{ret}}$, which would correspond to the operators $\alpha_{\psi_\circ^+} \circ \alpha_{\psi_{\boldsymbol{g}}^+}^{-1}$ and $\alpha_{\psi_\circ^-} \circ \alpha_{\psi_{\boldsymbol{g}}^-}^{-1}$.

As the theory $\mathscr{A}$ is locally covariant, it follows that the relative Cauchy-evolution is insensitive to changing $\boldsymbol{g}$ into $\phi_*\boldsymbol{g}$ when ϕ is a diffeomorphism of M that acts trivially outside of the intermediate region $M_{(+,-)}$. More precisely, one obtains:

Proposition 4.1. *Let ϕ be a diffeomorphism of M that acts trivially outside of $M_{(+,-)}$ (i.e. $\phi(x) = x$ for all x in the complement of $M_{(+,-)}$). Then for $\boldsymbol{g} \in G$ with $\phi_*\boldsymbol{g} \in G$ there holds*

$$\beta_{\boldsymbol{g}} = \beta_{\phi_*\boldsymbol{g}} \,.$$

Proof. It holds that ϕ is a morphism in $\hom_{\mathfrak{Man}}((M, \boldsymbol{g}), (M, \phi_*\boldsymbol{g}))$, and hence

$$\phi \circ \psi_{\boldsymbol{g}}^\pm = \psi_{\phi_*\boldsymbol{g}}^\pm$$

owing to the definition of $\psi_{\boldsymbol{g}}^{\pm}$ since ϕ acts trivially on $N_{\pm}$. On the other hand, it holds that

$$\begin{aligned}\beta_{\boldsymbol{g}} &= \alpha_{\psi_\circ^-} \circ \alpha^{-1}_{\psi_{\boldsymbol{g}}^-} \circ \alpha_{\psi_{\boldsymbol{g}}^+} \circ \alpha^{-1}_{\psi_\circ^+} \\ &= \alpha_{\psi_\circ^-} \circ \alpha^{-1}_{\psi_{\boldsymbol{g}}^-} \circ \alpha_{\phi}^{-1} \circ \alpha_{\phi} \circ \alpha_{\psi_{\boldsymbol{g}}^+} \circ \alpha^{-1}_{\psi_\circ^+} \\ &= \alpha_{\psi_\circ^-} \circ \alpha^{-1}_{\phi\circ\psi_{\boldsymbol{g}}^-} \circ \alpha_{\phi\circ\psi_{\boldsymbol{g}}^+} \circ \alpha^{-1}_{\psi_\circ^+} \\ &= \alpha_{\psi_\circ^-} \circ \alpha^{-1}_{\psi^-_{\phi_*\boldsymbol{g}}} \circ \alpha_{\psi^+_{\phi_*\boldsymbol{g}}} \circ \alpha^{-1}_{\psi_\circ^+} \\ &= \beta_{\phi_*\boldsymbol{g}} \,. \qquad \square\end{aligned}$$

We will now make assumptions that allow us to define the functional derivative of $\beta_{\boldsymbol{g}}$ with respect to $\boldsymbol{g} \in G$. To this end, we assume that π is a Hilbert-space representation of $\mathscr{A}(M, \mathring{\boldsymbol{g}})$, and that there is a dense subspace $\mathcal{V}$ of the representation-Hilbert-space $\mathcal{H}$ and a dense $*$-sub-algebra $\mathcal{B}$ of $\mathscr{A}(M, \mathring{\boldsymbol{g}})$ so that, for all smooth families $(-1, 1) \ni s \mapsto \boldsymbol{g}^{(s)} \in G$ with $\boldsymbol{g}^{(0)} = \mathring{\boldsymbol{g}}$, there holds

$$\frac{d}{ds}\langle\theta, \pi(\beta_{\boldsymbol{g}^{(s)}}(B))\theta\rangle\bigg|_{s=0} = \int_M b^{\mu\nu}(x)\delta\boldsymbol{g}_{\mu\nu}(x)\, d\mathring{\mu}(x) \tag{13}$$

for all $\theta \in \mathcal{V}$, $B \in \mathcal{B}$ with a suitable smooth section $x \mapsto b^{\mu\nu}(x)$ in $TM \otimes TM$ (depending on θ and B); we have written $\delta\boldsymbol{g} = d\boldsymbol{g}^{(s)}/ds\big|_{s=0}$, and $d\mathring{\mu}$ denotes the volume form induced by $\mathring{\boldsymbol{g}}$. Then we write

$$\langle\theta, \frac{\delta}{\delta\boldsymbol{g}_{\mu\nu}(x)}\pi(\beta_{\boldsymbol{g}}B)\theta\rangle = b^{\mu\nu}(x)\,,$$

and thus the functional derivative of the relative Cauchy-evolution $\beta_{\boldsymbol{g}}$ with respect to the metric $\boldsymbol{g}$,

$$\frac{\delta}{\delta\boldsymbol{g}_{\mu\nu}(x)}\pi(\beta_{\boldsymbol{g}}B)\,,$$

is defined in the representation π for all $B \in \mathcal{B}$ in the sense of quadratic forms on $\mathcal{V}$. (As announced before, these assumptions are realized for the free scalar Klein-Gordon field in representations of quasifree Hadamard states, see Sect. 4.2 below. Note that, as a consequence of the properties assumed of G, the set of all $\delta\boldsymbol{g}$ arising in the indicated way is total in the space of all symmetric smooth sections in $T^*M \otimes T^*M$ supported on $M_{(+,-)}$, so that $b^{\mu\nu}$ is uniquely determined by (13).) The functional derivative of $\beta_{\boldsymbol{g}}$ with respect to $\boldsymbol{g}$ describes the reaction of the quantum system to an infinitesimal local change of the spacetime metric. As known in classical field theory, this is described by the energy-momentum tensor, and we will find this corroborated in the quantum field case by Thm 4.3 below. It is mentioned in [26] that the functional derivative of $\tau_{\boldsymbol{g}}^{\mathrm{adv/ret}}$ with respect to $\boldsymbol{g}$ describes the advanced/retarded response of the quantum system upon infinitesimal metric changes.

When the indicated assumptions are fulfilled, then we find that the relative Cauchy-evolution is divergence-free.

Theorem 4.2. *For all $B \in \mathcal{B}$, one has*

$$\nabla_\mu \frac{\delta}{\delta \boldsymbol{g}_{\mu\nu}(x)} \pi(\beta_{\boldsymbol{g}}(B)) = 0\,, \quad x \in M\,,$$

in the sense of quadratic forms on $\mathcal{V}$, where ∇ is the covariant derivative with respect to $\overset{\circ}{\boldsymbol{g}}$.

Proof. Let X be a smooth vector field on M which vanishes outside of a compact subset of $M_{(+,-)}$, and let $\phi^{(s)}$, $s \in \mathbb{R}$, be the one-parametric group of diffeomorphisms that is generated by X. By Prop. 4.1, we have $\beta_{\overset{\circ}{\boldsymbol{g}}} - \beta_{\phi_*^{(s)}\overset{\circ}{\boldsymbol{g}}} = 0$ for all s with $|s| < s_0$, and hence one obtains that

$$\frac{d}{ds}\beta_{\phi_*^{(s)}\overset{\circ}{\boldsymbol{g}}} = 0\,.$$

On the other hand, using the notation $b^{\mu\nu}(x) = \langle \theta, \delta\pi(\beta_{\boldsymbol{g}}(B))/\delta \boldsymbol{g}_{\mu\nu}(x)\theta\rangle$ and recalling the definition of $\delta\beta_{\boldsymbol{g}}/\delta\boldsymbol{g}_{\mu\nu}(x)$, we have

$$0 = \frac{d}{ds}\langle\theta, \pi(\beta_{\phi_*^{(s)}\overset{\circ}{\boldsymbol{g}}}(B))\theta\rangle\Big|_{s=0} = \int_M b^{\mu\nu}(x)\,\frac{d}{ds}\Big|_{s=0}\phi_*^{(s)}\overset{\circ}{\boldsymbol{g}}_{\mu\nu}(x)\,d\overset{\circ}{\mu}(x)$$

for all $B \in \mathcal{B}$, $\theta \in \mathcal{V}$. Now one can conclude that $\nabla_\mu b^{\mu\nu} = 0$ as in the case of classical field theory (cf. [25], Sect. 3.3): It holds that $\frac{d}{ds}\big|_{s=0}\phi_*^{(s)}\overset{\circ}{\boldsymbol{g}}_{\mu\nu} = \pounds_X\overset{\circ}{\boldsymbol{g}}_{\mu\nu} = \nabla_\mu X_\nu + \nabla_\nu X_\mu$, where $\pounds_X$ denotes the Lie-derivative, and hence

$$\begin{aligned} 0 &= \int_M b^{\mu\nu}(x)\pounds_X\overset{\circ}{\boldsymbol{g}}_{\mu\nu}(x)\,d\overset{\circ}{\mu}(x) \\ &= 2\int_M (\nabla_\mu(b^{\mu\nu}X_\nu)(x) - (\nabla_\mu b^{\mu\nu}(x))X_\nu(x))\,d\overset{\circ}{\mu}(x)\,. \end{aligned}$$

The first term in the last expression is a divergence and can be converted to a surface integral which hence vanishes since X has compact support. As X was an arbitrary vectorfield supported inside $M_{(+,-)}$, one thus concludes that $\nabla_\mu b^{\mu\nu}(x) = 0$ for $x \in M_{(+,-)}$; on the other hand, $b^{\mu\nu}(x) = 0$ for all x outside of $M_{(+,-)}$ according to the definition of the functional derivative of the Cauchy-evolution. Thus $\nabla_\mu b^{\mu\nu} = 0$ on M, and this completes the proof. $\square$

4.2. Relative Cauchy-evolution for the Klein-Gordon field. In the present subsection we investigate the relation between the functional derivative of the relative Cauchy-evolution for the quantum Klein-Gordon field with respect to the spacetime metric, and the quantum field's energy-momentum tensor. This will be presented in Theorem 4.3 below. Before stating this result, we will discuss the form of the relative Cauchy-evolution for the generally covariant Klein-Gordon field in some detail.

Let $(M, \boldsymbol{g})$ be an object in $\mathrm{Obj}(\mathfrak{Man})$ and let $(N, \boldsymbol{g}_N)$ be a globally hyperbolic sub-spacetime of $(M, \boldsymbol{g})$, so that the identical injection $\iota_N : N \to M$, $\iota_N(x) = x$ is a morphism in $\mathrm{hom}_{\mathfrak{Man}}((N, \boldsymbol{g}_N), (M, \boldsymbol{g}))$, where $\boldsymbol{g}_N$ is $\boldsymbol{g}$ restricted to N. Furthermore, let $(\mathcal{R}, \sigma)$ denote the symplectic space of solutions of the Klein-Gordon equation (1) on $(M, \boldsymbol{g})$, and $(\mathcal{R}_N, \sigma_N)$ the corresponding symplectic space of solutions on $(N, \boldsymbol{g}_N)$. E

and E_N will denote the associated propagators, respectively. We have seen above that ι_N induces a C^*-monomorphism $\alpha_{\iota_N} : \mathfrak{W}(\mathcal{R}_N, \sigma_N) \to \mathfrak{W}(\mathcal{R}, \sigma)$ by

$$\alpha_{\iota_N}(W_N(\varphi)) = W(T_N\varphi), \quad \varphi \in \mathcal{R}_N,$$

where we have denoted by $W_N(\,.\,)$ the Weyl-generators of $\mathfrak{W}(\mathcal{R}_N, \sigma_N)$ and by $W(\,.\,)$ those of $(\mathcal{R}, \sigma)$. The map T_N assigns to each element $E_N f$, $f \in C_0^\infty(N, \mathbb{R})$, of $\mathcal{R}_N$ the element $Ef \in \mathcal{R}$.

Let us now consider the case where N contains a Cauchy-surface for $(M, \boldsymbol{g})$. In this case, Dimock [11] has shown that the map T_N is surjective, i.e. $T_N\mathcal{R}_N = \mathcal{R}$. T_N is also injective (since it is symplectic), and we want to derive the form of the inverse map T_N^{-1}. To this end, let $\varphi \in \mathcal{R}$, and let Σ be a Cauchy-surface for $(M, \boldsymbol{g})$ contained in N. There exists a pair of two other Cauchy-surfaces Σ^{adv} and Σ^{ret} for $(M, \boldsymbol{g})$ in N, where Σ^{adv} lies in the timelike future and Σ^{ret} in the timelike past of Σ, hence $U = \text{int}\, J^-(\Sigma^{\text{adv}}) \cap J^+(\Sigma^{\text{ret}})$ is an open neighbourhood of Σ whose closure in contained in N. Now we choose a partition of unity $\{\chi^{\text{adv}}, \chi^{\text{ret}}\}$ of M so that $\chi^{\text{adv}} = 0$ on $J^-(\Sigma^{\text{ret}})$ and $\chi^{\text{ret}} = 0$ on $J^+(\Sigma^{\text{adv}})$. Then the properties $\chi^{\text{adv}} + \chi^{\text{ret}} = 1$ and $(\nabla^\mu\nabla_\mu + \xi R + m^2)\varphi = 0$ imply

$$(\nabla^\mu\nabla_\mu + \xi R + m^2)(\chi^{\text{adv}}\varphi) = -(\nabla^a\nabla_a + \xi R + m^2)(\chi^{\text{ret}}\varphi). \tag{14}$$

Since the left-hand side vanishes on $J^-(\Sigma^{\text{ret}})$ and the right-hand side vanishes on $J^+(\Sigma^{\text{adv}})$ while $\varphi = Ef$ has support in $J(\text{supp}\, f)$ for some compactly supported f, one deduces that both the left- and right-hand side expressions of (14) are compactly supported in $\overline{U} \subset N$. Using the properties of the propagator E, one can moreover show (cf. [11])

$$E(\nabla^\mu\nabla_\mu + \xi R + m^2)(\chi^{\text{adv/ret}}\varphi) = \pm\varphi, \quad \varphi \in \mathcal{R}.$$

Since $E(\nabla^\mu\nabla_\mu + m^2 + \xi R)(\chi^{\text{adv/ret}}\varphi)$ is contained in $E(C_0^\infty(N, \mathbb{R}))$ and $Ef \mapsto E_N f$, $f \in C_0^\infty(N, \mathbb{R})$, is a symplectic map from $(\mathcal{R}, \sigma)$ onto $(\mathcal{R}_N, \sigma_N)$ owing to the uniqueness of advanced and retarded fundamental solutions of the Klein-Gordon equation in globally hyperbolic spacetimes, we can see that $T_N^{-1} : (\mathcal{R}, \sigma) \to (\mathcal{R}_N, \sigma_N)$ is given by

$$T_N^{-1}(\varphi) = \pm E_N(\nabla^\mu\nabla_\mu + \xi R + m^2)(\chi^{\text{adv/ret}}\varphi).$$

Now we wish to study the relative Cauchy-evolution for the scalar Klein-Gordon field. We assume that we are in the situation described in the previous subsection: We are given a globally spacetime $(M, \mathring{\boldsymbol{g}})$, with subregions $N_\pm$ and $M_{(+,-)}$ on the latter of which metrics $\boldsymbol{g}$ in a set G deviate from $\mathring{\boldsymbol{g}}$, where these data are subject to the geometric assumptions listed above.

For the generally covariant theory of the Klein-Gordon field, we see from our discussion above that $\beta_{\boldsymbol{g}}$ acts on the generators $\mathring{W}(\,.\,)$ of the CCR-algebra of the Klein-Gordon field on $(M, \mathring{\boldsymbol{g}})$ like

$$\beta_{\boldsymbol{g}}(\mathring{W}(\varphi)) = \mathring{W}(F_{\boldsymbol{g}}\varphi);$$

here, $F_{\boldsymbol{g}} : \mathring{\mathcal{R}} \to \mathring{\mathcal{R}}$ is the symplectic map

$$F_{\boldsymbol{g}} = T_{N_-,\circ} \circ T_{N_-,\boldsymbol{g}}^{-1} \circ T_{N_+,\boldsymbol{g}} \circ T_{N_+,\circ}^{-1}$$

with

$$T_{N_\pm,\boldsymbol{g}} : E_{N_\pm,\boldsymbol{g}} f \mapsto E_{\boldsymbol{g}} \iota_{N_\pm *} f\,, \quad f \in C_0^\infty(N_\pm, \mathbb{R})\,,$$
$$T_{N_\pm,\circ} : \overset{\circ}{E}_{N_\pm} f \mapsto \overset{\circ}{E} \iota_{N_\pm *} f\,, \quad f \in C_0^\infty(N_\pm, \mathbb{R})\,,$$
$$T^{-1}_{N_\pm,\boldsymbol{g}} : \phi \mapsto -E_{N_\pm,\boldsymbol{g}} K_{\boldsymbol{g}} (\chi_\pm^{\mathrm{ret}} \phi)\,, \quad \phi \in \mathcal{R}_{\boldsymbol{g}}\,,$$
$$T^{-1}_{N_\pm,\circ} : \varphi \mapsto -\overset{\circ}{E}_{N_\pm} \overset{\circ}{K} (\chi_\pm^{\mathrm{ret}} \varphi)\,, \quad \varphi \in \overset{\circ}{\mathcal{R}}\,,$$

where $\overset{\circ}{E}$, $\overset{\circ}{\mathcal{R}}$, $\overset{\circ}{\sigma}$, $\overset{\circ}{E}_{N_\pm}$, $\overset{\circ}{\mathcal{R}}_{N_\pm}$, $\overset{\circ}{\sigma}_{N_\pm}$, $E_{\boldsymbol{g}}$, $\mathcal{R}_{\boldsymbol{g}}$, $\sigma_{\boldsymbol{g}}$ and $E_{N_\pm,\boldsymbol{g}}$, $\mathcal{R}_{N_\pm,\boldsymbol{g}}$, $\sigma_{N_\pm,\boldsymbol{g}}$ denote the propagators, range-spaces and symplectic forms corresponding to the Klein-Gordon equation on the spacetimes $(M, \overset{\circ}{\boldsymbol{g}})$, $(N_\pm, \overset{\circ}{\boldsymbol{g}}_{N_\pm})$, $(M, \boldsymbol{g})$ and $(M, \overset{\circ}{\boldsymbol{g}})$, respectively. The functions $\chi_\pm^{\mathrm{adv/ret}}$ are defined relative to suitable pairs of Cauchy-surfaces $\Sigma_\pm^{\mathrm{adv/ret}}$ lying in $N_\pm$. By $K_{\boldsymbol{g}}$ and $\overset{\circ}{K}$ we denote the Klein-Gordon operator

$$\nabla^\mu \nabla_\mu + \xi R + m^2$$

on the spacetimes $(M, \boldsymbol{g})$ and $(M, \overset{\circ}{\boldsymbol{g}})$, respectively. Note that (up to identification) $E_{N_\pm,\boldsymbol{g}} = \overset{\circ}{E}_{N_\pm}$ for all $\boldsymbol{g} \in G$ according to our geometric assumptions, and thus also $\mathcal{R}_{N_\pm,\boldsymbol{g}} = \overset{\circ}{\mathcal{R}}_{N_\pm}$, $\sigma_{N_\pm,\boldsymbol{g}} = \overset{\circ}{\sigma}_{N_\pm}$. This entails

$$F_{\boldsymbol{g}} \varphi = \overset{\circ}{E} K_{\boldsymbol{g}} \chi_-^{\mathrm{ret}} E_{\boldsymbol{g}} \overset{\circ}{K} \chi_+^{\mathrm{ret}} \varphi\,, \quad \varphi \in \overset{\circ}{\mathcal{R}}\,, \tag{15}$$

where we have dropped the embedding identifications $\iota_{N_\pm *}$ from our notation. This relation will be the key ingredient in the proof of the next theorem. Prior to stating it, some further preparation is required.

Let us select some arbitrary quasifree Hadamard state ω on $\mathscr{A}(M, \overset{\circ}{\boldsymbol{g}}) = \mathfrak{W}(\overset{\circ}{\mathcal{R}}, \overset{\circ}{\sigma})$, the Weyl-algebra of the Klein-Gordon field on $(M, \overset{\circ}{\boldsymbol{g}})$. Then we will write

$$W_\omega(\varphi) = \pi_\omega(\overset{\circ}{W}(\varphi))\,, \quad \varphi \in \overset{\circ}{\mathcal{R}}\,,$$

for the Weyl-operators in the GNS-representation π_ω of ω; then we have

$$W_\omega(\varphi) = \mathrm{e}^{i\check{\Phi}_\omega(\varphi)}$$

with suitable selfadjoint operators $\check{\Phi}_\omega(\varphi)$ in the GNS-Hilbert-space $\mathcal{H}_\omega$, depending linearly on φ, and

$$w_2^{(\omega)}(f, h) = \langle \Omega_\omega, \check{\Phi}_\omega(\overset{\circ}{E} f) \check{\Phi}_\omega(\overset{\circ}{E} h) \Omega_\omega \rangle\,, \quad f, h \in C_0^\infty(M, \mathbb{R})\,,$$

with the GNS-vector Ω_ω. Let $\mathcal{V}_\omega$ be the set of all vectors θ in $\mathcal{H}_\omega$ which are of the form $\theta = B\Omega_\omega$ where B is an arbitrary polynomial in the variables $W_\omega(\varphi)$, $\check{\Phi}_\omega(\varphi')$ as φ and φ' vary over $\overset{\circ}{\mathcal{R}}$. One can show that each $\theta \in \mathcal{V}_\omega$ is in the domain of all operators $\check{\Phi}_\omega(\varphi)$ and that the wavefront sets $\mathrm{WF}(w_2^{[\theta]})$ of the two-point functions induced by $\theta \in \mathcal{V}_\omega$,

$$w_2^{[\theta]}(f, h) = \langle \theta, \check{\Phi}_\omega(\overset{\circ}{E} f) \check{\Phi}_\omega(\overset{\circ}{E} h) \theta \rangle\,, \quad f, h \in C_0^\infty(M, \mathbb{R})\,,$$

are of the same shape as those of the two-point functions of Hadamard states [17]. Furthermore, denoting by

$$\Phi_\omega(f) = \check{\Phi}_\omega(Ef)\,, \quad f \in C_0^\infty(M, \mathbb{R})\,,$$

the quantum field induced by $\check{\Phi}_\omega$, one can show that there is for each pair of vectors $\theta, \theta' \in \mathcal{V}_\omega$ a smooth function $x \mapsto \langle \theta, \Phi_\omega(x)\theta' \rangle$ on M so that

$$\langle \theta, \Phi_\omega(f)\theta' \rangle = \int_M \langle \theta, \Phi_\omega(x)\theta' \rangle f(x)\, d\mathring{\mu}(x),$$

where we recall that $\mathring{g}(x)$ is the determinant of $\mathring{\boldsymbol{g}}$ in the coordinates used for M. These assertions rest on the fact that (1) Ω_ω is an analytic vector for all $\check{\Phi}_\omega(\varphi)$, (2) $[\check{\Phi}_\omega(\varphi), W_\omega(\tilde{\varphi})] = -\sigma(\varphi, \tilde{\varphi}) W_\omega(\tilde{\varphi})$, and iterated use of this relation, (3) the distribution $f \mapsto w_2^{(\omega)}(f, h)$ is induced by a smooth function, and $w_2^{[\theta]}(f, h)$ can be reduced to a sum of products of such $w_2^{(\omega)}(f, h_j)$ (with suitable coefficients) since ω is quasifree.

After these preparations, we obtain:

Theorem 4.3. *Under the geometric assumptions listed above, there holds*

$$\frac{\delta}{\delta \boldsymbol{g}_{\mu\nu}(x)} \pi_\omega(\beta_{\boldsymbol{g}} \mathring{W}(\varphi)) = -\frac{i}{2}[T^{\mu\nu}(x), W_\omega(\varphi)]\,, \quad \varphi \in \mathring{\mathcal{R}},\ x \in M_{(+,-)}\,, \tag{16}$$

in the sense of quadratic forms on $\mathcal{V}_\omega$, where $T_{\mu\nu}$ is the generally covariant renormalized energy-momentum tensor of the quantized Klein-Gordon field on $(M, \mathring{\boldsymbol{g}})$ in the GNS-representation π_ω of ω, and ω is an arbitrary quasifree Hadamard state.

Remarks. (A) Note that the classical expression for $T_{\mu\nu}$ is $T_{\mu\nu} = \frac{2}{\sqrt{-g}} \frac{\delta}{\delta \boldsymbol{g}^{\mu\nu}} S_{\mathrm{KG}} \Big|_{\boldsymbol{g}=\mathring{\boldsymbol{g}}}$, where S_{KG} is the action integral of the Lagrangian density

$$\mathcal{L}_{\mathrm{KG}} = \frac{1}{2}\sqrt{-g}\left(\boldsymbol{g}^{\mu\nu}\nabla_\mu\varphi\nabla_\nu\varphi - (m^2 + \xi R)\varphi^2\right)\,.$$

Here we use the convention that $T_{\mu\nu}$ is defined in this way, and that $T^{\mu\nu} = \mathring{\boldsymbol{g}}^{\mu\alpha}\mathring{\boldsymbol{g}}^{\nu\beta} T_{\alpha\beta}$ and *not* $T^{\mu\nu} = \frac{2}{\sqrt{-g}} \frac{\delta}{\delta \boldsymbol{g}_{\mu\nu}} S_{\mathrm{KG}} \Big|_{\boldsymbol{g}=\mathring{\boldsymbol{g}}}$. The latter expression differs from the former, which we use, by a sign.

(B) Instead of the generally covariant renormalized energy-momentum tensor one may also use the energy-momentum tensor renormalized with respect to ω as reference state, since the two definitions differ by a term which is a multiple of the unit operator and hence is cancelled by the commutator on the right hand side of (16). In fact, one may even use (after point-split regularization) the "unrenormalized, formal expression" (cf. [49]) for the quantum energy-momentum tensor since only the commutator of the energy-momentum tensor appears.

(C) Similarly one can show that

$$\frac{\delta}{\delta \boldsymbol{g}_{\mu\nu}(x)} P_{\boldsymbol{g}} = -\frac{i}{2}[T^{\mu\nu}(x), P]$$

holds in the sense of quadratic forms on $\mathcal{V}_\omega$ for all polynomials

$$P = \sum_{j\le\ell,\, k_j\le n} \check{\Phi}_\omega(\varphi_{j,1})\cdots\check{\Phi}_\omega(\varphi_{j,k_j})$$

in the field operators, with

$$P_{\boldsymbol{g}} = \sum_{j\le\ell,\, k_j\le n} \check{\Phi}_\omega(F_{\boldsymbol{g}}\varphi_{j,1})\cdots\check{\Phi}_\omega(F_{\boldsymbol{g}}\varphi_{j,k_j})\,.$$

Proof. We will give the proof only for the case $\xi = 0$ in order to simplify notation; however, the case of arbitrary ξ can be carried out along the same lines. For any smooth family $(-1,1) \ni s \mapsto \boldsymbol{g}^{(s)} \in G$ with $\boldsymbol{g}^{(0)} = \overset{\circ}{\boldsymbol{g}}$ we write $\delta\boldsymbol{g} = d\boldsymbol{g}^{(s)}/ds\big|_{s=0}$, and $\delta y_{\boldsymbol{g}} = \frac{d}{ds}\big|_{s=0} y_{\boldsymbol{g}_s}$ for any function $y_{\boldsymbol{g}}$ depending on $\boldsymbol{g} \in G$.

Let $\theta \in \mathcal{V}_\omega$. Since $\beta_{\boldsymbol{g}}(\overset{\circ}{W}(\varphi)) = \overset{\circ}{W}(F_{\boldsymbol{g}}\varphi)$, one finds by a general argument (cf. e.g. [17]) that

$$\delta\pi_\omega(\beta_{\boldsymbol{g}}\overset{\circ}{W}(\varphi))\theta = \delta(W(F_{\boldsymbol{g}}\varphi))_\omega\theta = \frac{i}{2}\{\check{\Phi}_\omega(\delta F_{\boldsymbol{g}}\varphi),\, W_\omega(\varphi)\}\theta\,, \quad \varphi \in \overset{\circ}{\mathcal{R}}\,,$$

where $\{A, B\} = AB + BA$ denotes the anti-commutator. One must therefore derive an expression for $\delta F_{\boldsymbol{g}}\varphi$. It holds that (cf. (15))

$$\begin{aligned}\delta F_{\boldsymbol{g}}\varphi &= \delta(\overset{\circ}{E} K_{\boldsymbol{g}}\chi_-^{\mathrm{ret}} E_{\boldsymbol{g}}\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi)\\ &= \overset{\circ}{E}(\delta K_{\boldsymbol{g}})\chi_-^{\mathrm{ret}}\varphi + \overset{\circ}{E}\overset{\circ}{K}\chi_-^{\mathrm{ret}}(\delta E_{\boldsymbol{g}})\chi_+^{\mathrm{ret}}\varphi\,.\end{aligned}$$

Now $\delta K_{\boldsymbol{g}}$ is a partial differential operator whose coefficient functions are compactly supported within $M_{(+,-)}$ as a consequence of the geometric assumptions. Since $M_{(+,-)} \cap J^-(N_-) = \emptyset$, and $\mathrm{supp}\,\chi_-^{\mathrm{ret}} \subset J^-(N_-)$, it follows that $\overset{\circ}{E}(\delta K_{\boldsymbol{g}}\chi_-^{\mathrm{ret}})\varphi = 0$, and hence

$$\delta F_{\boldsymbol{g}}\varphi = \overset{\circ}{E}\overset{\circ}{K}\chi_-^{\mathrm{ret}}(\delta E_{\boldsymbol{g}})\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi\,.$$

On the other hand, it holds that

$$\chi_-^{\mathrm{ret}} E_{\boldsymbol{g}}\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi = \chi_-^{\mathrm{ret}} E_{\boldsymbol{g}}^{\mathrm{adv}}\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi - \chi_-^{\mathrm{ret}} E_{\boldsymbol{g}}^{\mathrm{ret}}\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi\,,$$

and since $E_{\boldsymbol{g}}^{\mathrm{adv}}\overset{\circ}{K}\chi_+^{\mathrm{ret}}$ has support in $J^+(N_+)$, while χ_-^{ret} has support in $J^-(N_-)$, the first term on the right hand side vanishes, leaving us with

$$\delta F_{\boldsymbol{g}}\varphi = -\overset{\circ}{E}\overset{\circ}{K}\chi_-^{\mathrm{ret}}(\delta E_{\boldsymbol{g}}^{\mathrm{ret}})\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi\,.$$

Then we deduce from $E_{\boldsymbol{g}}^{\mathrm{ret}} K_{\boldsymbol{g}} f = f$ for all $f \in C_0^\infty(M,\mathbb{R})$ that

$$\delta E_{\boldsymbol{g}}^{\mathrm{ret}} = -\overset{\circ}{E}{}^{\mathrm{ret}}(\delta K_{\boldsymbol{g}})\overset{\circ}{E}{}^{\mathrm{ret}}\,,$$

and thus we obtain

$$\delta F_{\boldsymbol{g}}\varphi = \overset{\circ}{E}\overset{\circ}{K}\chi_-^{\mathrm{ret}}\overset{\circ}{E}{}^{\mathrm{ret}}(\delta K_{\boldsymbol{g}})\overset{\circ}{E}{}^{\mathrm{ret}}\overset{\circ}{K}\chi_+^{\mathrm{ret}}\varphi\,.$$

Now we use the same support arguments as before to conclude that $\chi_-^{\text{ret}} \overset{\circ}{E}{}^{\text{adv}} \delta K_{\boldsymbol{g}} = 0$ and $\delta K_{\boldsymbol{g}} \overset{\circ}{E}{}^{\text{adv}} \overset{\circ}{K} \chi_+^{\text{ret}} \varphi = 0$, and hence it holds that

$$\delta F_{\boldsymbol{g}} \varphi = \overset{\circ}{E} \overset{\circ}{K} \chi_-^{\text{ret}} \overset{\circ}{E} (\delta K_{\boldsymbol{g}}) \overset{\circ}{E} \overset{\circ}{K} \chi_+^{\text{ret}} \varphi = \overset{\circ}{E} (\delta K_{\boldsymbol{g}}) \varphi$$

for all $\varphi \in \overset{\circ}{\mathcal{R}}$.

Therefore, our discussion so far shows that (16) is proved as soon as we have shown that, given any smooth family $\boldsymbol{g}^{(s)} \in G$, $s \in (-1, 1)$, with $\boldsymbol{g}^{(0)} = \overset{\circ}{\boldsymbol{g}}$,

$$\begin{aligned} &\int \langle \theta, \{\Phi_\omega(x), W_\omega(\varphi)\} \theta \rangle (\delta K_{\boldsymbol{g}} \varphi)(x) \, d\overset{\circ}{\mu}(x) \\ &= - \int \langle \theta, [T^{\mu\nu}(x), W_\omega(\varphi)] \theta \rangle \delta \boldsymbol{g}_{\mu\nu}(x) \, d\overset{\circ}{\mu}(x) \end{aligned} \tag{17}$$

holds for all $\varphi \in \overset{\circ}{\mathcal{R}}$ and all $\theta \in \mathcal{V}_\omega$; note that $\delta K_{\boldsymbol{g}}$ is a differential operator on $C^\infty(M, \mathbb{R})$ containing $\delta \boldsymbol{g}_{\mu\nu}$. To verify that (17) holds, we shall evaluate the integral on the left hand side in local coordinate patches. More precisely, we choose a locally finite covering of M by coordinate patches U_j on each of which we pick coordinates so that $|\overset{\circ}{g}(x)|$, the modulus of the metric determinant of $\overset{\circ}{\boldsymbol{g}}$ in those coordinates, is equal to 1. Then, on each U_j, the coordinate expression of $\delta K_{\boldsymbol{g}}$ assumes the form

$$\delta K_{\boldsymbol{g}} = \frac{1}{2} \overset{\circ}{\boldsymbol{g}}_{\mu\nu} (\partial^\mu (\overset{\circ}{\boldsymbol{g}}{}^{\alpha\beta} \delta \boldsymbol{g}_{\alpha\beta})) \partial^\nu - \partial^\mu \delta \boldsymbol{g}_{\mu\nu} \partial^\nu \quad (|\overset{\circ}{g}| = 1) \, .$$

Now let $\{\chi_j\}$ be a smooth partition of unity on M subordinate to the covering $\{U_j\}$. Using the coordinates with $|\overset{\circ}{g}| = 1$ on each patch and the coordinate expression for $\delta K_{\boldsymbol{g}}$ in these coordinates, one obtains by partial integration (observing that $d\overset{\circ}{\mu}(x) = dx$ in the chosen coordinates)

$$\begin{aligned} &\int \chi_j(x) \langle \theta, \{\Phi_\omega(x), W_\omega(\varphi)\} \theta \rangle (\delta K_{\boldsymbol{g}} \varphi)(x) \, d\overset{\circ}{\mu}(x) \\ &= \int \bigg(\langle \theta, \{\partial^\mu \Phi_\omega(x), W_\omega(\varphi)\} \theta \rangle \partial^\nu \varphi(x) - \frac{1}{2} \overset{\circ}{\boldsymbol{g}}{}^{\mu\nu}(x) \langle \theta, \{\partial^\alpha \Phi_\omega(x), W_\omega(\varphi)\} \theta \rangle \partial_\alpha \varphi(x) \\ &+ \frac{1}{2} \overset{\circ}{\boldsymbol{g}}{}^{\mu\nu}(x) m^2 \langle \theta, \{\Phi_\omega(x), W_\omega(\varphi)\} \theta \rangle \varphi(x) \bigg) \chi_j(x) \delta \boldsymbol{g}_{\mu\nu}(x) \, dx \\ &+ \int \langle \theta, \{\Phi_\omega(x), W_\omega(\varphi)\} \theta \rangle \bigg(\partial^\mu \chi_j(x) \partial^\nu \varphi(x) - \frac{1}{2} \overset{\circ}{\boldsymbol{g}}{}^{\mu\nu}(x) \partial^\alpha \chi_j(x) \partial_\alpha \varphi(x) \bigg) \delta \boldsymbol{g}_{\mu\nu}(x) \, dx \, . \end{aligned} \tag{18}$$

We shall next investigate the right hand side of (17). The commutator of $W_\omega(\varphi)$ with the formal, point-split expression for the bitensor $T^{\mu\nu}(x, x')$ is given by

$$\begin{aligned} \langle \theta, [T^{\mu\nu}(x, x'), W_\omega(\varphi)] \theta \rangle \; &= \langle \theta, [\partial^\mu \Phi_\omega(x) \partial^\nu \Phi_\omega(x'), W_\omega(\varphi)] \theta \rangle \\ &\quad - \frac{1}{2} \overset{\circ}{\boldsymbol{g}}{}^{\mu\rho}(x) Y_\rho{}^\nu(x, x') \langle \theta, [(\partial_\alpha \Phi_\omega(x) Y^\alpha{}_\beta(x, x') \partial^\beta \Phi_\omega(x') \\ &\quad - m^2 \Phi_\omega(x) \Phi_\omega(x')), W_\omega(\varphi)] \theta \rangle , \end{aligned}$$

where $Y^{\nu}{}_{\alpha}(x,x')$ denotes the bitensor of parallel transport of vectors in $T_{x'}M$ to T_xM. In order to be able to take the limit $x' \to x$, one uses the relations

$$[\Phi_\omega(h), W_\omega(\varphi)] = i[\Phi_\omega(h), \check{\Phi}_\omega(\varphi)]W_\omega(\varphi) \quad \text{and}$$
$$i[\Phi_\omega(x), \check{\Phi}_\omega(\varphi)] = -\varphi(x)\,, \quad h \in C_0^\infty(M,\mathbb{R}),\ \varphi \in \mathring{\mathcal{R}}\,;$$

the first relation holds generally in quasifree representations of the CCR-algebra as a consequence of the Weyl-relations, and the second relation is easily deduced from the equations

$$[\Phi_\omega(h), \check{\Phi}_\omega(\varphi)] = i\sigma(Eh,\varphi) = i\int h\,\varphi\,d\mathring{\mu}(x)\,,$$
$$\langle\theta, [\Phi_\omega(h), \check{\Phi}_\omega(\varphi)]\theta\rangle = \int\langle\theta, [\Phi_\omega(x), \check{\Phi}_\omega(\varphi)]\theta\rangle h(x)\,d\mathring{\mu}(x)$$

which hold for all $h \in C_0^\infty(M,\mathbb{R})$, $\theta \in \mathcal{V}_\omega$. Inserting these relations together with the identity $[AB,C] = [A,C]B + A[B,C]$ yields for all $\theta \in \mathcal{V}_\omega$,

$$\begin{aligned}
&\langle\theta, [T^{\mu\nu}(x,x'), W_\omega(\varphi)]\theta\rangle\\
&\quad = -\langle\theta, (\partial^\mu\Phi_\omega(x)W_\omega(\varphi)\partial^\nu\varphi(x') + \partial^\mu\varphi(x)W_\omega(\varphi)\partial^\mu\Phi_\omega(x'))\theta\rangle\\
&\qquad + \frac{1}{2}\mathring{\boldsymbol{g}}^{\mu\rho}(x)Y_\rho{}^\nu\langle\theta, Y^\alpha{}_\beta(\partial_\alpha\Phi_\omega(x)W_\omega(\varphi)\partial^\beta\varphi(x') + \partial_\alpha\varphi(x)W_\omega(\varphi)\partial^\beta\Phi_\omega(x'))\theta\rangle\\
&\qquad - \frac{1}{2}\mathring{\boldsymbol{g}}^{\mu\rho}(x)Y_\rho{}^\nu m^2\langle\theta, (\Phi_\omega(x)W_\omega(\varphi)\varphi(x') + \varphi(x)W_\omega(\varphi)\Phi_\omega(x'))\theta\rangle\,,
\end{aligned}$$

where we have abbreviated $Y_\rho{}^\nu(x,x')$ by $Y_\rho{}^\nu$, etc. In the last expressions, one can clearly take the limit $x' \to x$ without occurrence of any divergencies to obtain, upon observing $\delta\boldsymbol{g}_{\mu\nu} = \delta\boldsymbol{g}_{\nu\mu}$,

$$\begin{aligned}
&\langle\theta, [T^{\mu\nu}(x), W_\omega(\varphi)]\theta\rangle\delta\boldsymbol{g}_{\mu\nu}(x)\\
&\quad = -\ \langle\theta, \{\partial^\mu\Phi_\omega(x), W_\omega(\varphi)\}\theta\rangle\partial^\nu\varphi(x)\delta\boldsymbol{g}_{\mu\nu}(x)\\
&\qquad + \frac{1}{2}\mathring{\boldsymbol{g}}^{\mu\nu}(x)\langle\theta, \{\partial_\alpha\Phi_\omega(x), W_\omega(\varphi)\}\theta\rangle\partial^\alpha\varphi(x)\delta\boldsymbol{g}_{\mu\nu}(x)\\
&\qquad - \frac{1}{2}\mathring{\boldsymbol{g}}^{\mu\nu}(x)m^2\langle\theta, \{\Phi_\omega(x), W_\omega(\varphi)\}\theta\rangle\varphi(x)\delta\boldsymbol{g}_{\mu\nu}(x)\,.
\end{aligned} \tag{19}$$

Exploiting now (18) and (19), we obtain

$$\begin{aligned}
&\int \big(\langle\theta, \{\Phi_\omega(x), W_\omega(\varphi)\}\theta\rangle(\delta K_{\boldsymbol{g}}\varphi)(x) + \langle\theta, [T^{\mu\nu}(x), W_\omega(\varphi)]\theta\rangle\delta\boldsymbol{g}_{\mu\nu}(x)\big)\,d\mathring{\mu}(x)\\
&\quad = \sum_j\int \chi_j(x)\Big(\langle\theta, \{\Phi_\omega(x), W_\omega(\varphi)\}\theta\rangle(\delta K_{\boldsymbol{g}}\varphi)(x)\\
&\qquad\qquad + \langle\theta, [T^{\mu\nu}(x), W_\omega(\varphi)]\theta\rangle\delta\boldsymbol{g}_{\mu\nu}(x)\Big)\,d\mathring{\mu}(x)\\
&\quad = \sum_j\int \langle\theta, \{\Phi_\omega(x), W_\omega(\varphi)\}\theta\rangle\Big(\partial^\mu\chi_j(x)\partial^\nu\varphi(x)\\
&\qquad\qquad - \frac{1}{2}\mathring{\boldsymbol{g}}^{\mu\nu}(x)\partial^\alpha\chi_j(x)\partial_\alpha\varphi(x)\Big)\delta\boldsymbol{g}_{\mu\nu}(x)\,dx \ = \ 0\,,
\end{aligned}$$

since, owing to the fact that $\delta\boldsymbol{g}$ has compact support, only finitely many χ_j meet the support of $\delta\boldsymbol{g}$, where they add up to 1. This shows that Eq. (17) holds. □

5. Wick-Polynomials

The enlarged local algebras generated by the Wick polynomials defined in [7] also satisfy the condition of local covariance. This follows immediately from the fact that they are completions of the local algebras generated by the free field with respect to a locally covariant topology (see e.g. [26] where this is made very explicit). However, the Wick-polynomials themselves are in general not locally covariant quantum fields in the sense of Def. 2.4.

This point has been taken up recently by Hollands and Wald [26], who have shown that one may suitably define Wick-polynomials of the free scalar field which have the property to be locally covariant quantum fields in the sense of Def. 2.4. Here we show that this construction provides the solution of a cohomological problem.

Let $\mathscr{W}(M, \boldsymbol{g})$ denote the abstract algebra of Wick-polynomials on $(M, \boldsymbol{g}) \in \mathrm{Obj}(\mathfrak{Man})$ which was defined in [26] following the corresponding definition on Minkowski space in [15]. Let ω be a Hadamard state of the Klein-Gordon field on $(M, \boldsymbol{g})$. Then, heuristically, $A \in \mathscr{W}(M, \boldsymbol{g})$ has an expansion

$$A = \sum \int dx\, f_n(x) :\varphi(x_1) \cdots \varphi(x_n):_\omega , \ x = (x_1, \ldots , x_n)$$

into Wick-polynomials with respect to ω, and by Wick's Theorem, the product in $\mathscr{W}(M, \boldsymbol{g})$ can be expanded in terms of the coefficients f_n. Therefore, up to the ideal generated by the field equation, $\mathscr{W}(M, \boldsymbol{g})$ may be realized as a space of sequences of compactly supported distributions $f_n \in \mathcal{D}'(M^n)$ satisfying a condition on the wave front set and with a product depending on ω. A field corresponding to the Wick square of the free field is defined by

$$:\Phi^2:_{M,\omega} (f) = (0, 0, f\delta, 0, \ldots)$$

with $(f\delta)(x, y) = f(x)\delta(x, y)$. Here, $\delta(x, y)$ symbolizes the distribution concentrated on the diagonal:

$$\delta(H) = \int_M H(x, x) d\mu_{\boldsymbol{g}}(x) , \quad H \in C_0^\infty(M \times M) .$$

However, this definition of the Wick square does not lead to a locally covariant field. To see this, let $\psi \in \mathrm{hom}_{\mathfrak{Man}}((M', \boldsymbol{g}'), (M, \boldsymbol{g}))$ and let $\alpha_\psi : \mathscr{W}(M', \boldsymbol{g}') \to \mathscr{W}(M, \boldsymbol{g})$ denote the corresponding algebraic morphism. Then

$$\alpha_\psi(:\Phi^2:_{M',\omega\circ\alpha_\psi} (x)) =: \Phi^2 :_{M,\omega} (\psi(x)) ,$$

hence local covariance neccessitates $\omega \circ \alpha_\psi = \omega$. Since there is no locally covariant family of Hadamard states – as was discussed in Sect. 3.1 – the definition above does not yield a locally covariant field.

Let us indicate how this problem may be solved. If ω and ω' are two quasifree Hadamard states over the spacetime $(M, \boldsymbol{g})$, then there is a smooth function $B_{M,\omega,\omega'}$ on M so that $: \Phi^2 :_{M,\omega} (x) - \ : \Phi^2 :_{M,\omega'} (x) = B_{M,\omega,\omega'}(x)$. These functions satisfy the covariance condition

$$B_{M',\omega\alpha_\psi,\omega'\alpha_\psi}(x') = B_{M,\omega,\omega'}(\psi(x')) , \quad x' \in M' ,$$

for $\psi \in \mathrm{hom}_{\mathfrak{Man}}((M', \boldsymbol{g}'), (M, \boldsymbol{g}))$, and moreover, they fulfill a cocycle condition

$$B_{M,\omega,\omega'} + B_{M,\omega',\omega''} + B_{M,\omega'',\omega} = 0 .$$

The aim is now to trivialize this cocycle while preserving its covariance properties. In other words, we are seeking to associate with each quasifree Hadamard state ω over $(M, \boldsymbol{g})$ a smooth function $f_{M,\omega} \in C^\infty(M)$ so that the resulting family of smooth functions transforms covariantly, i.e.

$$f_{M',\omega\alpha_\psi}(x') = f_{M,\omega}(\psi(x')) , \quad \psi \in \hom_{\mathfrak{Man}}((M', \boldsymbol{g}'), (M, \boldsymbol{g})) ,$$

and trivializes the cocycle, i.e.

$$B_{M,\omega,\omega'}(x) = f_{M,\omega}(x) - f_{M,\omega'}(x) , \quad x \in M ,$$

for any pair of quasifree Hadamard states ω, ω' over $(M, \boldsymbol{g})$. Hence we would obtain a locally covariant Wick-square by setting

$$:\Phi^2:_{(M,\boldsymbol{g})}(x) = :\Phi^2:_{M,\omega}(x) - f_{M,\omega}(x)$$

for an arbitrary choice of quasifree Hadamard state ω over $(M, \boldsymbol{g})$.

It is not too difficult to find the solution to this cohomological problem. Recalling the definition of the Hadamard form by Kay and Wald [31], one finds that the diagonal values of the smooth, non-geometrical term H_ω (cf. Eq. (11)) of the two-point function of a quasifree Hadamard state ω have the required properties, i.e. a solution of the cohomological problem is provided by defining

$$f_{M,\omega}(x) = H_\omega(x, x) , \quad x \in M ,$$

for all quasifree Hadamard states ω over $(M, \boldsymbol{g})$. Actually, $H_\omega(x, y)$ is defined off the diagonal $x = y$ only up to a C^∞-function owing to the fact that the geometrical terms G_ϵ are affected by the like ambiguity. However, one can show that this ambiguity vanishes for $y \to x$ and that, consequently, $H_\omega(x, x)$ is well-defined, see the discussion in Sect. 5.2 of [26].

Higher order Wick-powers which are also locally covariant may then be obtained by differentiating the generating functional

$$:e^{\lambda\Phi(x)}:_{(M,\boldsymbol{g})} = e^{\frac{1}{2}\lambda^2 f_\omega(x)} :e^{\lambda\Phi(x)}:_\omega$$

with respect to the real parameter λ, where ω is any quasifree Hadamard state over $(M, \boldsymbol{g})$.

Finally we remark that we have only considered Wick-powers without derivatives. A discussion of Wick-powers with derivatives is contained in a recent work by Moretti [33].

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6. Appendix

a) *Proof of statement* (α) *in the proof of Thm. 3.2.*

It is clearly sufficient to prove that $\boldsymbol{F}(\pi_{\omega\circ\alpha}) \subset \boldsymbol{F}(\pi_\omega \circ \alpha)$ for all states ω on a C^*-algebra $\mathcal{B}$ and all C^*-algebraic morphisms $\alpha : \mathcal{A} \to \mathcal{B}$, where $\mathcal{A}$ is another C^*-algebra. Consider the GNS-representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ of $\mathcal{B}$ corresponding to the state ω. Define a new Hilbert-space $\mathcal{H}^\alpha$ as the closed subspace of $\mathcal{H}_\omega$ which is spanned by $\pi_\omega(\alpha(\mathcal{A}))\Omega_\omega$. Then we may clearly identify the GNS-representation $(\mathcal{H}_{\omega\circ\alpha}, \pi_{\omega\circ\alpha}, \Omega_{\omega\circ\alpha})$ of $\mathcal{A}$ induced by the state $\omega \circ \alpha$ with $(\mathcal{H}^\alpha, \pi_\omega \circ \alpha, \Omega_\omega)$ since this triple has all the properties of the GNS-triple corresponding to $\omega \circ \alpha$, and the GNS-triple is unique (up to unitary identifications). Hence, if $\omega' \in \boldsymbol{F}(\pi_{\omega\circ\alpha})$, then there is a density matrix $\rho' = \sum_j \mu_j |\phi_j\rangle\langle\phi_j|$ with unit vectors $\phi_j \in \mathcal{H}^\alpha$ such that

$$\omega'(A) = \mathrm{tr}(\rho' \pi_\omega \circ \alpha(A))$$

holds for all $A \in \mathcal{A}$. This density matrix is then also a density matrix on $\mathcal{H}_\omega \supset \mathcal{H}^\alpha$, and owing to the just displayed equality, then also $\omega' \in \boldsymbol{F}(\pi_\omega \circ \alpha)$ according to the definition of the folium of a representation.

b) *Proof of statement* (β) *in the proof of Thm. 3.2.*

We quote the following result which is proved as Prop. 5.3.5 in [13]: Let $\mathcal{B}$ be a C^*-algebra and π a representation of $\mathcal{B}$ on some Hilbert-space $\mathcal{H}$; moreover, let $\mathcal{H}'$ be a closed subspace of $\mathcal{H}$ which is left invariant by $\pi(\mathcal{B})$ and non-zero, and define the subrepresentation $\pi'(B) = \pi(B) \restriction \mathcal{H}'$, $B \in \mathcal{B}$, of π on $\mathcal{H}'$. Then π is quasi-equivalent to π' if the von Neumann algebra $\pi(\mathcal{B})''$ is a factor.

We apply this to prove statement (β) as follows: Let π be the identical representation of the factor $\mathcal{N}$ on the Hilbert-space $\mathcal{H}$, and let π' be the subrepresentation relative to $\mathcal{H}' = \mathcal{H}_\mathcal{N}$. According to the quoted result, $\boldsymbol{F}(\pi) = \boldsymbol{F}(\pi')$. And this just says that for each density matrix ρ on $\mathcal{H}$ there exists a density matrix $\rho^\mathcal{N}$ on $\mathcal{H}_\mathcal{H} = \mathcal{H}'$ so that

$$\mathrm{tr}(\rho \cdot N) = \mathrm{tr}(\rho \cdot \pi(N)) = \mathrm{tr}(\rho^\mathcal{N} \cdot \pi'(N)) = \mathrm{tr}(\rho^\mathcal{N} \cdot N)$$

holds for all $N \in \mathcal{N}$.

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