Chapter 2
Algebraic Quantum Field Theory on Curved Spacetimes

Abstract In this chapter, we review all background material on algebraic quantum field theory on curved spacetimes which is necessary for understanding the cosmological applications discussed in the next chapter. Starting with a brief account of globally hyperbolic curved spacetimes and related geometric notions, we then explain how the algebras of observables generated by products of linear quantum fields at different points are obtained by canonical quantization of spaces of classical observables. This discussion will be model-independent and will cover both Bosonic and Fermionic models with and without local gauge symmetries. Afterwards, we review the concept of Hadamard states which encompass all physically reasonable quantum states on curved spacetimes. The modern paradigm in QFT on curved spacetimes is that observables and their algebras should be constructed in a local and covariant way. We briefly review the theoretical formulation of this concept and explain how it is implemented in the construction of an extended algebra of observables of the free scalar field which also contains products of quantum fields at coinciding points. Finally, we discuss the quantum stress-energy tensor as a particular example of such an observable as well as the related semiclassical Einstein equation.

2.1 Globally Hyperbolic Spacetimes and Related Geometric Notions

The philosophy of algebraic quantum field theory in curved spacetimes is to set up a framework which is valid on all physically reasonable curved Lorentzian spacetimes and independent of their particular properties. Given this framework, one may then exploit particular properties of a given spacetime such as symmetries in order obtain specific results or to perform explicit calculations. A class of spacetimes which encompasses most cases which are of physical interest are *globally hyperbolic spacetimes*. These include Friedmann-Lemaître-Robertson-Walker spacetimes-in particular Minkowski spacetime-as well as Black Hole spacetimes such as Schwarzschild-and Kerr-spacetime, whereas prominent examples of spacetimes which are not globally hyperbolic are Anti de Sitter-spacetime (see e.g. [5, Chap. 3.5]) and a portion of Minkowski spacetime obtained by restricting one of the spatial coordinates to a

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finite interval such as the spacetimes relevant for discussing the Casimir effect. The constructions we shall review in the following are well-defined on all globally hyperbolic spacetimes. The physically relevant spacetime examples which are not globally hyperbolic are usually such that sufficiently small portions still have this property. Consequently, the algebraic constructions on globally hyperbolic spacetimes can be extended to these cases by patching together local constructions, see for instance [33, 85]. In this section we shall review the definition of globally hyperbolic spacetimes and a few related differential geometric notions which we shall use throughout this monograph.

To this end, in this work a *spacetime* (M, g) is meant to be a Hausdorff, connected, smooth manifold M, endowed with a Lorentzian metric g, the invariant volume measure of which shall be denoted by $d_g x \doteq \sqrt{|\det g|}dx$. We will mostly consider four-dimensional spacetimes. However, most notions and results can be formulated and obtained for Lorentzian spacetimes with a dimension d differing from four and we will try to point out how the spacetime dimension affects them whenever it seems interesting and possible. We will follow the monograph by Wald [122] regarding most conventions and notations and, hence, work with the metric signature $(-, +, +, +)$. It is often required that a spacetime be second countable, or, equivalently, paracompact, i.e. that its topology has a countable basis. Though, as proven by Geroch in [60], paracompactness already follows from the properties of (M, g) listed above. In addition to the attributes already required, we demand that the spacetime under consideration is orientable and time-orientable and that an orientation has been chosen in both respects. We will often omit the spacetime metric g and denote a spacetime by M in brief.

For a point $x \in M$, $T_x M$ denotes the tangent space of M at x and $T^*_x M$ denotes the respective cotangent space; the tangent and cotangent bundles of M shall be denoted by TM and T^*M, respectively. If $\chi : M_1 \to M_2$ is a diffeomorphism, we denote by χ^* the *pull-back* of χ and by χ_* the *push-forward* of χ. χ^* and χ_* map tensors on M_2 to tensors on M_1 and tensors on M_1 to tensors on M_2, respectively; they furthermore satisfy $\chi_* = (\chi^{-1})^*$ [122, Appendix C]. In case g_1 and g_2 are the chosen Lorentzian metrics on M_1 and M_2 and $\chi_* g_1 = g_2$, we call χ an *isometry*; if $\chi_* g_1 = \Omega^2 g_2$ with a strictly positive smooth function Ω, χ shall be called a *conformal isometry* and $\Omega^2 g$ a *conformal transformation* of g. Note that this definition differs from the one often used in the case of highly symmetric or flat spacetimes since one does not rescale coordinates, but the metric. A conformal transformation according to our definition is sometimes called *Weyl transformation* in the literature. If χ is an *embedding* $\chi : M_1 \hookrightarrow M_2$, i.e. $\chi(M_1)$ is a submanifold of M_2 and χ a diffeomorphism between M_1 and $\chi(M_1)$, it is understood that a push-forward χ_* of χ is only defined on $\chi(M_1) \subset M_2$. In case an embedding $\chi : M_1 \hookrightarrow M_2$ between the manifolds of two spacetimes (M_1, g_1) and (M_2, g_2) is an isometry between (M_1, g_1) and $(\chi(M_1), g_2|_{\chi(M_1)})$, we call χ an *isometric embedding*, whereas an embedding which is a conformal isometry between (M_1, g_1) and $(\chi(M_1), g_2|_{\chi(M_1)})$ shall be called a *conformal embedding*.

Some works make extensive use of the *abstract index notation*, i.e. they use Latin indices to denote tensorial identities which hold in any basis to distinguish them from identities which hold only in specific bases. As this distinction will not be necessary in the present work, we will not use abstract index notation, but shall use Greek indices to denote general tensor components in a coordinate basis $\{\partial_\mu\}_{\mu=0,\dots,3}$ and shall reserve Latin indices for other uses. We employ the Einstein summation convention, e.g. $A^\mu_\mu \doteq \sum_{\mu=0}^3 A^\mu_\mu$, and we shall lower Greek indices by means of $g_{\mu\nu} \doteq g(\partial_\mu, \partial_\nu)$ and raise them by $g^{\mu\nu} \doteq (g^{-1})_{\mu\nu}$.

Every smooth Lorentzian manifold admits a unique metric-compatible and torsion-free linear connection, the *Levi-Civita connection*, and we shall denote the associated *covariant derivative* along a vector field v, i.e. a smooth section of TM, by ∇_v. We will abbreviate ∇_{∂_μ} by ∇_μ and furthermore use the shorthand notation $T_{;\mu_1\cdots\mu_n} \doteq \nabla_{\mu_1}\cdots\nabla_{\mu_n} T$ for covariant derivatives of a tensor field T. Our definitions for the *Riemann tensor* $R_{\alpha\beta\gamma\delta}$, the *Ricci tensor* $R_{\alpha\beta}$, and the *Ricci scalar* R are

$$v_{\alpha;\beta\gamma} - v_{\alpha;\gamma\beta} \doteq R_\alpha{}^\lambda{}_{\beta\gamma} v_\lambda \,, \qquad R_{\alpha\beta} \doteq R_\alpha{}^\lambda{}_{\beta\lambda} \,, \qquad R \doteq R^\alpha{}_\alpha \,, \tag{2.1}$$

where v_α are the components of an arbitrary covector. The Riemann tensor possesses the symmetries

$$R_{\alpha\beta\gamma\delta} = -R_{\beta\alpha\gamma\delta} = R_{\gamma\delta\alpha\beta} \,, \qquad R_{\alpha\beta\gamma\delta} + R_{\alpha\delta\beta\gamma} + R_{\alpha\gamma\delta\beta} = 0 \tag{2.2}$$

and fulfils the *Bianchi identity*

$$R_{\alpha\beta\gamma\delta;\varepsilon} + R_{\alpha\beta\varepsilon\gamma;\delta} + R_{\alpha\beta\delta\varepsilon;\gamma} = 0 \,. \tag{2.3}$$

Moreover, its trace-free part, the *Weyl tensor*, is defined as

$$\begin{aligned} C_{\alpha\beta\gamma\delta} = R_{\alpha\beta\gamma\delta} &- \frac{1}{6}\left(g_{\alpha\delta}g_{\beta\gamma} - g_{\alpha\gamma}g_{\beta\delta}\right) R \\ &- \frac{1}{2}\left(g_{\beta\delta}R_{\alpha\gamma} - g_{\beta\gamma}R_{\alpha\delta} - g_{\alpha\delta}R_{\beta\gamma} + g_{\alpha\gamma}R_{\beta\delta}\right) , \end{aligned}$$

where the appearing coefficients differ in spacetimes with $d \neq 4$. In addition to the covariant derivative, we can define the notion of a *Lie derivative* along a vector field v: the integral curves $c(s)$ of v with respect to a curve parameter s define, in general only for small s and on an open neighbourhood of $c(0)$, a one-parameter group of diffeomorphisms χ^v_s [122, Chap. 2.2]. Given a tensor field T of arbitrary rank, we can thus define the Lie derivative of T along v as

$$\mathscr{L}_v T \doteq \lim_{s\to 0}\left(\frac{(\chi^v_{-s})^* T - T}{s}\right) .$$

If χ^v_s is a one-parameter group of isometries, we call v a *Killing vector field*, while in case of χ^v_s being a one-parameter group of conformal isometries, we shall call v a *conformal Killing vector field*. It follows that a Killing vector field v fulfils $\mathscr{L}_v g = 0$, while a conformal Killing vector field v fulfils $\mathscr{L}_v g = fg$ with some smooth function f [122, Appendix C.3].

In order to define what it means for a spacetime to be globally hyperbolic, we need a few additional standard notions related to Lorentzian spacetimes. To wit, following our sign convention, we call a vector $v_x \in T_x M$ *timelike* if $g(v_x, v_x) < 0$, *spacelike* if $g(v_x, v_x) > 0$, *lightlike* or *null* if $g(v_x, v_x) = 0$, and *causal* if it is either timelike or null. Extending this, we call a vector field $v : M \to TM$ spacelike, timelike, lightlike, or causal if it possesses this property at every point. Finally, we call a curve $c : \mathbb{R} \supset I \to M$, with I an interval, spacelike, timelike, lightlike, or causal if its tangent vector field bears this property. Note that, according to our definition, a trivial curve $c \equiv x$ is lightlike. As (M, g) is time orientable, we can split the lightcones in TM at all points in M into 'future' and 'past' in a consistent way and say that a causal curve is *future directed* if its tangent vector field at a point is always in the future lightcone at this point; *past directed* causal curves are defined analogously.

For the definition of global hyperbolicity, we need the notion of inextendible causal curves; these are curves that 'run off to infinity' or 'run into a singular point'. Hence, given a future directed curve c parametrised by s, we call x a *future endpoint* of c if, for every neighbourhood $\mathscr{O}$ of x, there is an s_0 such that $c(s) \in \mathscr{O}$ for all $s > s_0$. With this in mind, we say that a future directed causal curve is *future inextendible* if, for all possible parametrisations, it has *no* future endpoint and we define *past inextendible* past directed causal curves similarly. A related notion is the one of a *complete geodesic*. A geodesic c is called complete if, in its *affine parametrisation* defined by $\nabla_{dc/ds} \frac{dc}{ds} = 0$, the affine parameter s ranges over all $\mathbb{R}$. A manifold M is called *geodesically complete* if all geodesics on M are complete.

In the following, we are going to define the generalisations of flat spacetime lightcones in curved spacetimes. By $I^+(x, M)$ we denote the *chronological future* of a point x relative to M, i.e. all points in M which can be reached by a future directed timelike curve starting from x, while $J^+(x, M)$ denotes the *causal future* of a point x, *viz.* all points in M which can be reached by future directed causal curve starting from x. Notice that, generally, $x \in J^+(x, M)$ and $I^+(x, M)$ is an open subset of M while the situations $x \notin I^+(x, M)$ and $J^+(x, M)$ being a closed subset of M are not generic, but for instance present in globally hyperbolic spacetimes [122]. In analogy to the preceding definitions, we define the *chronological past* $I^-(x, M)$ and *causal past* $J^-(x, M)$ of a point x by employing past directed timelike and causal curves, respectively. We extend this definition to a general subset $\mathscr{O} \subset M$ by setting

$$I^\pm(\mathscr{O}, M) \doteq \bigcup_{x \in \mathscr{O}} I^\pm(x, M) \qquad J^\pm(\mathscr{O}, M) \doteq \bigcup_{x \in \mathscr{O}} J^\pm(x, M)\,;$$

additionally, we define $I(\mathscr{O}, M) \doteq I^+(\mathscr{O}, M) \cup I^-(\mathscr{O}, M)$ and $J(\mathscr{O}, M) \doteq J^+(\mathscr{O}, M) \cup J^-(\mathscr{O}, M)$. As the penultimate prerequisite for the definition of global hyperbolicity, we say that a subset $\mathscr{O}$ of M is *achronal* if $I^+(\mathscr{O}, M) \cap \mathscr{O}$ is empty, i.e. an achronal set is such that every timelike curve meets it at most once. Given a closed achronal set $\mathscr{O}$, we define its *future domain of dependence* $D^+(\mathscr{O}, M)$ as the set containing all points $x \in M$ such that every past inextendible causal curve through x intersects $\mathscr{O}$. By our definitions, $D^+(\mathscr{O}, M) \subset J^+(\mathscr{O}, M)$, but note that

$J^+(\mathscr{O}, M)$ is in general considerably larger than $D^+(\mathscr{O}, M)$. We define $D^-(\mathscr{O}, M)$ analogously and set $D(\mathscr{O}, M) \doteq D^+(\mathscr{O}, M) \cup D^-(\mathscr{O}, M)$. $D(\mathscr{O}, M)$ is sometimes also called the *Cauchy development* of $\mathscr{O}$. With this, we are finally in the position to state the definition of global hyperbolicity (valid for all spacetime dimensions).

Definition 2.1 A *Cauchy surface* is a closed achronal set $\Sigma \subset M$ with $D(\Sigma, M) = M$. A spacetime (M, g) is called *globally hyperbolic* if it contains a Cauchy surface.

Although the geometric intuition sourced by our knowledge of Minkowski spacetime can fail us in general Lorentzian spacetimes, it is essentially satisfactory in globally hyperbolic spacetimes. According to Definition 2.1, a Cauchy surface is a 'non-timelike' set on which every 'physical signal' or 'worldline' must register exactly once. This is reminiscent of a constant time surface in flat spacetime and one can indeed show that this is correct. In fact, Geroch has proved in [61] that globally hyperbolic spacetimes are topologically $\mathbb{R} \times \Sigma$ and Bernal and Sanchez [9–11] have been able to improve on this and to show that every globally hyperbolic spacetime has a *smooth* Cauchy surface Σ and is, hence, even diffeomorphic to $\mathbb{R} \times \Sigma$. This implies in particular the existence of a (non-unique) smooth global *time function* $t : M \to \mathbb{R}$, i.e. t is a smooth function with a timelike and future directed gradient field ∇t; t is, hence, strictly increasing along any future directed timelike curve. In the following, we shall always consider smooth Cauchy surfaces, even in the cases where we do not mention it explicitly.

In the remainder of this chapter, we will gradually see that globally hyperbolic curved spacetimes have many more nice properties well-known from flat spacetime and, hence, seem to constitute the perfect compromise between a spacetime which is generically curved and one which is physically sensible. Particularly, it will turn out that second order, linear, hyperbolic partial differential equations have well-defined global solutions on a globally hyperbolic spacetime. Hence, whenever we speak of a spacetime in the following and do not explicitly demand it to be globally hyperbolic, this property shall be understood to be present implicitly.

On globally hyperbolic spacetimes, there can be no closed timelike curves, otherwise we would have a contradiction to the existence of a smooth and strictly increasing time function. There is a causality condition related to this which can be shown to be weaker than global hyperbolicity, namely, *strong causality*. A spacetime is called strongly causal if it can not contain almost closed timelike curves, i.e. for every $x \in M$ and every neighbourhood $\mathscr{O}_1 \ni x$, there is a neighbourhood $\mathscr{O}_2 \subset \mathscr{O}_1$ of x such that no causal curve intersects $\mathscr{O}_2$ more than once. One might wonder if this weaker condition can be filled up to obtain full global hyperbolicity and indeed some references, e.g. [5, 66], define a spacetime (M, g) to be globally hyperbolic if it is strongly causal and $J^+(x) \cap J^-(y)$ is compact for all $x, y \in M$. One can show that the latter definition is equivalent to Definition 2.1 [5, 122] which is, notwithstanding, the more intuitive one in our opinion.

We close this section by introducing a few additional sets with special causal properties. To this avail, we denote by $\exp_x$ the exponential map at $x \in M$. A set $\mathscr{O} \subset M$ is called *geodesically starshaped* with respect to $x \in \mathscr{O}$ if there is an open subset $\mathscr{O}'$ of $T_x M$ which is starshaped with respect to $0 \in T_x M$ such that $\exp_x : \mathscr{O}' \to \mathscr{O}$ is a diffeomorphism. We call a subset $\mathscr{O} \subset M$ *geodesically convex* if it is geodesically starshaped with respect to all its points. This entails in particular that each two points x, y in $\mathscr{O}$ are connected by a unique geodesic which is completely contained in $\mathscr{O}$. A related notion are *causal domains*, these are subsets of geodesically convex sets which are in addition globally hyperbolic. Finally, we would like to introduce *causally convex regions*, a generalisation of geodesically convex sets. They are open, non-empty subsets $\mathscr{O} \subset M$ with the property that, for all $x, y \in \mathscr{O}$, all causal curves connecting x and y are entirely contained in $\mathscr{O}$. One can prove that every point in a spacetime lies in a geodesically convex neighbourhood and in a causal domain [57] and one might wonder if the case of a globally hyperbolic spacetime which is geodesically convex is not quite generic. However, whereas Friedmann-Lemaître–Robertson-Walker spacetimes with flat spatial sections are geodesically convex, even de Sitter spacetime, which is both globally hyperbolic and maximally symmetric and could, hence, be expected to share many properties of Minkowski spacetime, is not.

2.2 Linear Classical Fields on Curved Spacetimes

As outlined in Sect. 1.1, the 'canonical' route to quantize linear classical field theories on curved spacetimes in the algebraic language is to first construct the canonical covariant classical Poisson bracket (or a symmetric equivalent in the case of Fermionic theories) and then to quantize the model by enforcing canonical (anti)commutation relations defined by this bracket. In this section, we shall first review how this is done for free field theories without gauge symmetry before discussing the case where local gauge symmetries are present.

2.2.1 Models Without Gauge Symmetry

We shall start our discussion of classical field theories without local gauge symmetries by looking at the example of the free Klein-Gordon field, which is the 'harmonic oscillator' of QFT on curved spacetimes. In discussing this example it will become clear what the basic ingredients determining a linear field theoretic model are and how they enter the definition and construction of this model in the algebraic framework.

2.2.1.1 The Free Neutral Klein-Gordon Field

In Physics, we are used to describe dynamics by (partial) differential equations and initial conditions. The relevant equation for the neutral scalar field is the free Klein-Gordon equation

$$(-\Box + f)\phi \doteq (-\nabla_\mu \nabla^\mu + f)\phi = 0$$

with the *d'Alembert operator* $\Box$ and some scalar function f of mass dimension 2. The function f determines the 'potential' $V(\phi) = \frac{1}{2} f \phi^2$ of the Klein-Gordon field and may be considered as a background field just like the metric g. Usually one considers the case $f = m^2 + \xi R$, i.e.

$$P\phi \doteq \left(-\Box + \xi R + m^2\right)\phi = 0 \tag{2.4}$$

such that f is entirely determined in terms of a constant mass $m \geq 0$ and the Ricci scalar R where the dimensionless constant ξ parametrises the strength of the coupling of ϕ to R. In principle one could consider more non-trivial coupling terms with the correct mass dimension such as $f = (R^{\alpha\beta} R_{\alpha\beta})^2/(m^4 R)$, however these may be ruled out by either invoking Occam's razor or by demanding analytic dependence of f on the metric and m like in [70, Sect. 5.1].

The case (2.4) with $\xi = 0$ is usually called *minimal coupling*, whereas, in four dimensions, the case $\xi = 1/6$ is called *conformal coupling*. While the former name refers to the fact that the Klein-Gordon field is coupled to the background metric only via the covariant derivative, the reason for the latter is rooted in the behaviour of this derivative under conformal transformations. Namely, if we consider the conformally related metrics g and $\widetilde{g} \doteq \Omega^2 g$ with a strictly positive smooth function Ω, denote by ∇, $\Box$, and R the quantities associated to g and by $\widetilde{\nabla}$, $\widetilde{\Box}$, and $\widetilde{R}$ the quantities associated to $\widetilde{g}$, then the respective metric compatibility of the covariant derivatives ∇ and $\widetilde{\nabla}$ and their agreement on scalar functions imply [122, Appendix D]

$$\left(-\widetilde{\Box} + \frac{1}{6}\widetilde{R}\right)\frac{1}{\Omega} = \frac{1}{\Omega^3}\left(-\Box + \frac{1}{6}R\right). \tag{2.5}$$

This entails that a function ϕ solving $(-\Box + \frac{1}{6}R)\phi = 0$ can be mapped to a solution $\widetilde{\phi}$ of $(-\widetilde{\Box} + \frac{1}{6}\widetilde{R})\widetilde{\phi} = 0$ by multiplying it with the conformal factor Ω to the power of the *conformal weight* -1, i.e. $\widetilde{\phi} = \Omega^{-1}\phi$. We shall therefore call a scalar field ϕ with an equation of motion $(-\Box + \frac{1}{6}R)\phi = 0$ *conformally invariant*. In other spacetimes dimensions $d \neq 4$, the conformal weight and the magnitude of the conformal coupling are different, see [122, Appendix D].

Having a partial differential equation for a free scalar field at hand, one would expect that giving sufficient initial data would determine a unique solution on all M. However, this is, in case of the Klein-Gordon operator at hand, in general only true for globally hyperbolic spacetimes. To see a simple counterexample, let us consider Minkowski spacetime with a compactified time direction and the massless case, i.e. the equation $(\partial_t^2 - \partial_x^2 - \partial_y^2 - \partial_z^2)\phi = 0$. Giving initial conditions $\phi|_{t=0} = 0$, $\partial_t \phi|_{t=0} = 1$, a possible *local* solution is $\phi \equiv t$. But this can of course never be a global solution, since one would run into contradictions after a full revolution around the compactified time direction.

In what follows, the *fundamental solutions* or *Green's functions* of the Klein-Gordon equation shall play a distinguished role. Before stating their existence, as well as the existence of general solutions, let us define the function spaces we shall be working with in the following, as well as their topological duals, see e.g. [22, Chap. VI] for an introduction.

Definition 2.2 By $\Gamma(M) \doteq C^\infty(M, \mathbb{R})$ we denote the *smooth (infinitely often continuously differentiable), real-valued functions* on M equipped with the usual *locally convex topology*, i.e. a sequence of functions $f_n \in \Gamma(M)$ is said to converge to $f \in \Gamma(M)$ if all derivatives of f_n converge to the ones of f uniformly on all compact subsets of M.

The space $\Gamma_0(M) \doteq C_0^\infty(M, \mathbb{R})$ is the subset of $\Gamma(M)$ constituted by the *smooth, real-valued functions with compact support*. We equip $\Gamma_0(M)$ with the locally convex topology determined by saying that a sequence of functions $f_n \in \Gamma_0(M)$ converges to $f \in \Gamma_0(M)$ if there is a compact subset $K \subset M$ such that all f_n and f are supported in K and all derivatives of f_n converge to the ones of f uniformly in K.

By $\Gamma_0^{\mathbb{C}}(M) \doteq \Gamma_0(M) \otimes_{\mathbb{R}} \mathbb{C}$, $\Gamma^{\mathbb{C}}(M) \doteq \Gamma(M) \otimes_{\mathbb{R}} \mathbb{C}$ we denote the complexifications of $\Gamma_0(M)$ and $\Gamma(M)$ respectively.

The spaces $\Gamma_{\mathrm{sc}}(M)$ and $\Gamma_{\mathrm{tc}}(M)$ denote the subspaces of $\Gamma(M)$ consisting of functions with *spacelike-compact* and *timelike-compact support* respectively. I.e. $\mathrm{supp}\, f \cap \Sigma$ is compact for all Cauchy surfaces Σ of (M, g) and all $f \in \Gamma_{\mathrm{sc}}(M)$, whereas for all $f \in \Gamma_{\mathrm{tc}}(M)$ there exist two Cauchy surfaces Σ_1, Σ_2 with $\mathrm{supp}\, f \subset J^-(\Sigma_1, M) \cap J^+(\Sigma_2, M)$.

By $\Gamma_0'(M)$ we denote the space of *distributions*, i.e. the topological dual of $\Gamma_0(M)$ provided by continuous, linear functionals $\Gamma_0(M) \to \mathbb{R}$, whereas $\Gamma'(M)$ denotes the topological dual of $\Gamma(M)$, i.e. the space of *distributions with compact support*. $\Gamma'^{\mathbb{C}}(M)$ and $\Gamma_0'^{\mathbb{C}}(M)$ denote the complexified versions of the real-valued spaces.

For $f \in \Gamma(M)$ and $u \in \Gamma_0'(M) \supset \Gamma(M) \supset \Gamma_0(M)$ with compact overlapping support, we shall denote the (symmetric and non-degenerate) *dual pairing* of f and u by

$$\langle u, f \rangle \doteq \int_M d_g x \; u(x) f(x) \,.$$

The physical relevance of the above spaces is that functions in $\Gamma_0(M)$, so-called *test functions*, should henceforth essentially be viewed as encoding the localisation of some observable in space and time, reflecting the fact that a detector is of finite spatial extent and a measurement is made in a finite time interval. From the point of view of dynamics, initial data for a partial differential equation may be encoded by distributions or functions with both compact and non-compact support, whereas solutions of hyperbolic partial differential equations like the Klein-Gordon one are typically distributions or smooth functions which do *not* have compact support on account of the causal propagation of initial data; having a solution with compact support in time would entail that data 'is lost somewhere'. Moreover, fundamental solutions of differential equations will always be singular distributions, as can be expected from the fact that they are solutions with a singular δ-distribution as source.

Finally, since (anti)commutation relations of quantum fields are usually formulated in terms of fundamental solutions, the quantum fields and their expectation values will also turn out to be singular distributions quite generically. Physically this stems from the fact that a quantum field has infinitely many degrees of freedom.

Let us now state the theorem which guarantees us existence and properties of solutions and fundamental solutions (also termed Green's functions or propagators) of the Klein-Gordon operator P. We refer to the monograph [5] for the proofs.

Theorem 2.1 *Let* $P : \Gamma(M) \to \Gamma(M)$ *be a* normally hyperbolic operator *on a globally hyperbolic spacetime* (M, g)*, i.e. in each coordinate patch of* M*,* P *can be expressed as*

$$P = -g^{\mu\nu}\partial_\mu\partial_\nu + A^\mu\partial_\mu + B$$

with smooth functions A^μ*,* B *and the* metric principal symbol $-g^{\mu\nu}\partial_\mu\partial_\nu$*. Then, the following results hold.*

1. *Let* $f \in \Gamma_0(M)$*, let* Σ *be a smooth Cauchy surface of* M*, let* $(u_0, u_1) \in \Gamma_0(\Sigma) \times \Gamma_0(\Sigma)$*, and let* N *be the future directed timelike unit normal vector field of* Σ*. Then, the* Cauchy problem

$$Pu = f, \qquad u|_\Sigma \equiv u_0, \qquad \nabla_N u|_\Sigma \equiv u_1$$

   has a unique solution $u \in \Gamma(M)$*. Moreover,*

$$\text{supp } u \subset J\left(\text{supp } f \cup \text{supp } u_0 \cup \text{supp } u_1, M\right).$$

   A unique solution to the Cauchy problem also exists if the assumptions on the compact support of f*,* u_0 *and* u_1 *are dropped.*
2. *There exist unique* retarded E_R *and* advanced E_A fundamental solutions (Green's functions, propagators) *of* P*. Namely, there are unique continuous maps* $E_{R/A} : \Gamma_0(M) \to \Gamma(M)$ *satisfying* $P \circ E_{R/A} = E_{R/A} \circ P = \mathrm{id}_{\Gamma_0(M)}$ *and* supp $E_{R/A} f \subset J^\pm(\text{supp } f, M)$ *for all* $f \in \Gamma_0(M)$*.*
3. *Let* $f, g \in \Gamma_0(M)$*. If* P *is* formally selfadjoint*, i.e.* $\langle f, Pg\rangle = \langle Pf, g\rangle$*, then* E_R *and* E_A *are the formal adjoints of one another, namely,* $\langle f, E_{R/A} g\rangle = \langle E_{A/R} f, g\rangle$*.*
4. *The* causal propagator (Pauli-Jordan function) *of* P *defined as* $E \doteq E_R - E_A$ *is a continuous map* $\Gamma_0(M) \to \Gamma_{\mathrm{sc}}(M) \subset \Gamma(M)$ *satisfying: for all solutions* u *of* $Pu = 0$ *with compactly supported initial conditions on a Cauchy surface there is an* $f \in \Gamma_0(M)$ *such that* $u = Ef$*. Moreover, for every* $f \in \Gamma_0(M)$ *satisfying* $Ef = 0$ *there is a* $g \in \Gamma_0(M)$ *such that* $f = Pg$*. Finally if* P *is formally self-adjoint, then* E *is formally skew-adjoint, i.e.* $\langle f, Eg\rangle = -\langle Ef, g\rangle$*.*

The Klein-Gordon operator P is manifestly normally hyperbolic. Moreover, one can check by partial integration that P is also formally self-adjoint. Hence, all above-mentioned results hold for P.

By continuity and the fact that $\Gamma(M) \subset \Gamma_0'(M)$, the operators $E_{R/A}$ and E define bi-distributions $E_{R/A}, E \in \Gamma_0'(M^2)$ which we denote by the same symbol via e.g.

$$E_{R/A}(f, g) \doteq \langle f, E_{R/A} g \rangle = \int_{M^2} d_g x \, d_g y \; E_{R/A}(x, y) f(x) g(y) \, .$$

In terms of integral kernels of these distributions, some of the identities stated in Theorem 2.1 read

$$P_x E_{R/A}(x, y) = \delta(x, y) \, , \qquad E_A(x, y) = E_R(y, x) \, , \qquad E(y, x) = -E(x, y) \, .$$

The support properties of $E_{R/A}$ entail that $E(f, g)$ vanishes if the supports of f and g are spacelike separated. On the level of distribution kernels, this implies that $E(x, y)$ vanishes for spacelike separated x and y. In anticipation of the quantization of the free Klein-Gordon field, this qualifies $E(x, y)$ as a *commutator function*. In the classical theory instead, $E(x, y)$ defines a *Poisson bracket* or *symplectic form*. To see this, we first need to specify the vector space on which this bracket should be evaluated.

Definition 2.3 By Sol ($\mathrm{Sol}_{\mathrm{sc}}$) we denote the space of real (spacelike-compact) solutions of the Klein-Gordon equation

$$\mathrm{Sol} \doteq \{\phi \in \Gamma(M) \mid P\phi = 0\} \, , \qquad \mathrm{Sol}_{\mathrm{sc}} \doteq \mathrm{Sol} \cap \Gamma_{\mathrm{sc}}(M) \, .$$

By $\mathscr{E}$ we denote the quotient space

$$\mathscr{E} \doteq \Gamma_0(M) / P[\Gamma_0(M)] \, ,$$

which is the *labelling space of linear on-shell observables of the free neutral Klein-Gordon field.*

The fact that $\mathscr{E}$ is the labelling space of (classical) linear on-shell observables of the free neutral Klein-Gordon field follows from the observation that each equivalence class $[f] \in \mathscr{E}$ defines a linear functional on Sol by

$$\mathrm{Sol} \ni \phi \mapsto \mathscr{O}_{[f]}(\phi) \doteq \langle f, \phi \rangle \, ,$$

where we note that, in the classical theory, Sol plays the role of the space of pure states of the model. As ϕ is a solution of the Klein-Gordon equation $\mathscr{O}_{[f]}(\phi)$ does not depend on the representative $f \in [f]$ and is well-defined. The observable $\langle f, \phi \rangle$ may be interpreted as the 'smeared classical field' $\phi(f) \simeq \langle f, \phi \rangle$. The classical observable $\phi(x)$, i.e. the observable that gives the value of a configuration ϕ at the point x, may be obtained by formally considering $\phi(f)$ with $f = \delta_x$.

We know that every $\phi \in \mathrm{Sol}$ is in one-to-one correspondence with initial data given on an arbitrary but fixed Cauchy surface Σ of (M, g). Analogously the support of a representative $f \in [f] \in \mathscr{E}$ can be chosen to lie in an arbitrarily small neighbourhood of an arbitrary Cauchy surface.

Lemma 2.1 *Let $[f] \in \mathscr{E}$ be arbitrary and let Σ be any Cauchy surface of (M, g). Then, for any bounded neighbourhood $\mathscr{O}(\Sigma)$ of Σ, we can find a $g \in \Gamma_0(M)$ with* $\mathrm{supp}\, g \subset \mathscr{O}(\Sigma)$ *and* $g \in [f]$.

Proof Let us assume that $\mathscr{O}(\Sigma)$ lies in the future of $\mathrm{supp}\, f$, i.e. $J^-(\mathrm{supp}\, f, M) \cap \mathscr{O}(\Sigma) = \emptyset$, the other cases can be treated analogously. Let us consider two auxiliary Cauchy surfaces Σ_1 and Σ_2 which are both contained in $\mathscr{O}(\Sigma)$ and which are chosen such that Σ_2 lies in the future of Σ whereas Σ_1 lies in the past of Σ. Moreover, let us take a smooth function $\chi \in \Gamma(M)$ which is identically vanishing in the future of Σ_2 and fulfils $\chi \equiv 1$ in the past of Σ_1 and let us define $g \doteq f - P\chi E_R f$. By construction and on account of the properties of both a globally hyperbolic spacetime (M, g) and a retarded fundamental solution E_R on M, $\chi E_R f$ has compact support, hence $g \in [f]$. Finally, $\mathrm{supp}\, g$ is contained in a compact subset of $J^+(\mathrm{supp}\, f, M) \cap \mathscr{O}(\Sigma)$.

We now observe that the causal propagator E induces a meaningful Poisson bracket on $\mathscr{E}$.

Proposition 2.1 *The tuple $(\mathscr{E}, \tau)$ with $\tau : \mathscr{E} \times \mathscr{E} \to \mathbb{R}$ defined by*

$$\tau([f], [g]) \doteq \langle f, Eg \rangle$$

is a symplectic space. *In particular*

1. *τ is well-defined and independent of the chosen representatives,*
2. *τ is antisymmetric,*
3. *τ is (weakly) non-degenerate, i.e. $\tau([f], [g]) = 0$ for all $[g] \in \mathscr{E}$ implies $[f] = [0]$.*

Proof τ is independent of the chosen representatives because $P \circ E = 0$. τ is antisymmetric because E is formally skew-adjoint, cf. the last item of Theorem 2.1, and because $\langle \cdot, \cdot \rangle$ is symmetric. The non-degeneracy of τ follows again from the last item of Theorem 2.1 and the fact that $\langle \cdot, \cdot \rangle$ is non-degenerate.

In standard treatments on scalar field theory, one usually defines Poisson brackets at 'equal times', but as realised by Peierls in [97], one can give a covariant version of the Poisson bracket which does not depend on a splitting of spacetime into space and time, and this is what we have given above. To relate the covariant form τ to an equal-time version, we need the definition of a 'future part' of a function $f \in \Gamma(M)$.

Definition 2.4 We consider a temporal cutoff function χ of the form discussed in the proof of Lemma 2.1, i.e. a smooth function χ which is identically vanishing in the future of some Cauchy surface Σ_2 and identically one in the past of some Cauchy surface Σ_1 in the past of Σ_2. Given such a χ, we define for an arbitrary $f \in \Gamma(M)$ the *future part* f^+ and the *past part* f^- by

$$f^+ \doteq (1-\chi)f\,, \qquad f^- = \chi f\,.$$

The relation of the covariant picture to the equal time-picture can be now shown in several steps.

Theorem 2.2 *Let $\langle\cdot,\cdot\rangle_{\mathrm{Sol}}$ be defined on tuples of solutions with compact overlapping support by*

$$\mathrm{Sol}\times\mathrm{Sol} \ni (\phi_1,\phi_2) \mapsto \langle\phi_1,\phi_2\rangle_{\mathrm{Sol}} \doteq \left\langle P\phi_1^+,\phi_2\right\rangle\,.$$

Moreover, let Σ be an arbitrary Cauchy surface of (M,g) with future-pointing unit normal vectorfield N and canonical measure $d\Sigma$ induced by $d_g x$.

1. *The causal propagator $E : \Gamma_0(M) \to \Gamma_{\mathrm{sc}}(M)$ descends to a bijective map $E : \mathscr{E} \to \mathrm{Sol}_{\mathrm{sc}}$.*
2. *$\langle\cdot,\cdot\rangle_{\mathrm{Sol}}$ is antisymmetric and well-defined on all tuples of solutions with compact overlapping support, in particular this bilinear form does not depend on the choice of cutoff χ entering the definition of the future part.*
3. *For all $f \in \Gamma_0(M)$ and all $\phi \in \mathrm{Sol}$, $\langle f,\phi\rangle = \langle Ef,\phi\rangle_{\mathrm{Sol}}$. In particular, $\langle\cdot,\cdot\rangle_{\mathrm{Sol}}$ is well-defined on all tuples of solutions with spacelike-compact overlapping support.*
4. *For all $f, g \in \Gamma_0(M)$, $\tau([f],[g]) = \langle Ef, Eg\rangle_{\mathrm{Sol}}$, thus the causal propagator $E : \Gamma_0(M) \to \Gamma_{\mathrm{sc}}(M)$ descends to an isomorphism between the symplectic spaces $(\mathscr{E},\tau)$ and $(\mathrm{Sol}_{\mathrm{sc}},\langle\cdot,\cdot\rangle_{\mathrm{Sol}})$.*
5. *For all $\phi_1,\phi_2 \in \mathrm{Sol}$ with spacelike-compact overlapping support,*

$$\langle\phi_1,\phi_2\rangle_{\mathrm{Sol}} = \int\limits_{\Sigma} d\Sigma\; N^\mu j_\mu(\phi_1,\phi_2)\,, \qquad j_\mu(\phi_1,\phi_2) \doteq \phi_1\nabla_\mu\phi_2 - \phi_2\nabla_\mu\phi_1\,.$$

6. *For all $f \in \Gamma_0(\Sigma)$ it holds*

$$\nabla_N Ef|_\Sigma = f\,, \qquad Ef|_\Sigma = 0\,.$$

On the level of distribution kernels, this entails that

$$\nabla_N E(x,y)|_{\Sigma\times\Sigma} = \delta_\Sigma(x,y)\,, \qquad E(x,y)|_{\Sigma\times\Sigma} \equiv 0\,,$$

where δ_Σ is the δ-distribution with respect to the canonical measure on Σ.

Proof We sketch the proof. The first statement follows from the last item of Theorem 2.1. The fact that $\langle\cdot,\cdot\rangle_{\mathrm{Sol}}$ is well-defined follows from the observation that two different definitions ϕ^+, $\phi^{+\prime}$ of the future part differ by a compactly supported smooth function $f = \phi_1^+ - \phi_1^{+\prime}$; consequently the supposedly different definitions of the bilinear form differ by $\langle\phi_1,\phi_2\rangle_{\mathrm{Sol}} - \langle\phi_1,\phi_2\rangle'_{\mathrm{Sol}} = \langle Pf,\phi_2\rangle = \langle f, P\phi_2\rangle = 0$. Note that this partial integration is only possible because f has compact support, in particular, $\langle\cdot,\cdot\rangle_{\mathrm{Sol}}$ is non-vanishing in general. The antisymmetry of $\langle\cdot,\cdot\rangle_{\mathrm{Sol}}$ follows by similar arguments and $P\phi^+ = P(\phi-\phi^-) = -P\phi^-$. The third statement follows from the fact that $E_R f$ is a valid future part of Ef, thus $\langle Ef,\phi\rangle_{\mathrm{Sol}} = \langle PE_R f,\phi\rangle = \langle f,\phi\rangle$. The fourth statement follows immediately from the first and third one, whereas the fifth one follows from $\nabla^\mu j_\mu(\phi_1,\phi_2) = \phi_2 P\phi_1 - \phi_1 P\phi_2$ by an application of Stokes theorem, see e.g. [38], where also a proof of the last statement can be found.

We now interpret the previous results. As argued above, elements $[f]\in\mathscr{E}$ label linear on-shell observables $\phi(f)\simeq\langle f,\phi\rangle$, i.e. the classical field ϕ smeared with the test function f. The causal propagator E induces a non-degenerate symplectic form τ on $\mathscr{E}$, which we may interpret as $\{\phi(f),\phi(g)\}\simeq\tau([f],[g]) = \langle f, Eg\rangle$, or, formally, as $\{\phi(x),\phi(y)\} = E(x,y)$. On the other hand, since $(\mathscr{E},\tau)$ and $(\mathrm{Sol}_{\mathrm{sc}},\langle\cdot,\cdot\rangle_{\mathrm{Sol}})$ are symplectically isomorphic, we can equivalently label linear on-shell observables by $\mathrm{Sol}_{\mathrm{sc}}\ni u$, i.e. by $\langle u,\phi\rangle_{\mathrm{Sol}}$, the classical field 'symplectically smeared' with the test solution u, where this symplectic smearing consists of integrating a particular expression at equal times. The last result of the above theorem implies that the covariant Poisson bracket $\{\phi(x),\phi(y)\} = E(x,y)$ has the well-known equal-time equivalent

$$\{\nabla_N\phi(x)|_\Sigma,\phi(y)|_\Sigma\} = \nabla_N E(x,y)|_{\Sigma\times\Sigma} = \delta_\Sigma(x,y)\,,$$

$$\{\phi(x)|_\Sigma,\phi(y)|_\Sigma\} = E(x,y)|_{\Sigma\times\Sigma} = 0\,,$$

which may be interpreted as equal-time Poisson brackets of the field $\phi(x)$ and its 'canonical momentum' $\nabla_N\phi(x)$. Further details on the relation between the equal-time and covariant picture can be found e.g. in [123, Chap. 3].

2.2.1.2 General Models Without Gauge Symmetry

The previous discussion of the classical free neutral Klein-Gordon field revealed the essential ingredients defining this model. Following e.g. [6, 107], this can be generalised to define an arbitrary linear field-theoretic model on a curved spacetime.

Definition 2.5 A real Bosonic linear field-theoretic model without local gauge symmetries on a curved spacetime is defined by the data $(M,\mathscr{V},P)$, where

1. $M\simeq(M,g)$ is a globally hyperbolic spacetime,
2. $\mathscr{V}$ is a real vector bundle over M, the space of smooth sections $\Gamma(\mathscr{V})$ of $\mathscr{V}$ is endowed with a symmetric and non-degenerate bilinear form $\langle\cdot,\cdot\rangle_{\mathscr{V}}$ which is well-defined on sections with compact overlapping support and given by the integral of a fibrewise symmetric and non-degenerate bilinear form $\langle\langle\cdot,\cdot\rangle\rangle_{\mathscr{V}}$: $\Gamma(\mathscr{V})\times\Gamma(\mathscr{V})\to\Gamma(M)$,
3. $P:\Gamma(\mathscr{V})\to\Gamma(\mathscr{V})$ is a Green-hyperbolic partial differential operator, i.e. there exist unique advanced E^P_R and retarded E^P_A fundamental solutions of P which

satisfy $P \circ E^P_{R/A} = E^P_{R/A} \circ P = \mathrm{id}|_{\Gamma_0(\mathscr{V})}$ and supp $E^P_{R/A} f \subset J^\pm(\text{supp } f, M)$ for all $f \in \Gamma_0(\mathscr{V})$; moreover P is formally self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\mathscr{V}}$.

A real Fermionic linear field-theoretic model without local gauge symmetries on a curved spacetime is defined analogously with the only difference being that $\langle\langle \cdot, \cdot \rangle\rangle_{\mathscr{V}}$ and $\langle \cdot, \cdot \rangle_{\mathscr{V}}$ are not symmetric but antisymmetric. Complex theories can be obtained from the real ones by complexification.

The relevance of the given data is as follows. Classical configurations Φ of the linear field model under consideration are smooth sections $\Phi \in \Gamma(\mathscr{V})$ of the vector bundle $\mathscr{V}$. We recall that $\mathscr{V}$ is locally of the form $M \times V$ with a real vector space V which implies that locally Φ is a smooth function from M to V, see e.g. [82, 94] for background material on vector bundles. We shall denote by $\Gamma_0(\mathscr{V})$, $\Gamma_{\mathrm{tc}}(\mathscr{V})$, $\Gamma_{\mathrm{sc}}(\mathscr{V})$ the subspaces of $\Gamma_0(\mathscr{V})$ consisting of smooth sections of $\mathscr{V}$ with compact, timelike-compact and spacelike-compact support, respectively.

The operator P specifies the equation of motion for the field model, the formal self-adjointness of P is motivated by the fact that equations of motion arising as Euler-Lagrange equations of a Lagrangean are generally given by a formally self-adjoint P. In fact the (formal) action $S(\Phi) = \frac{1}{2} \langle \Phi, P\Phi \rangle_{\mathscr{V}}$ leads to the Euler-Lagrange equation $P\Phi = 0$.

In the Klein-Gordon case we are dealing with an operator which is normally hyperbolic, i.e. the leading order term is of the form $-g^{\mu\nu}\partial_\mu\partial_\nu$. As reviewed in Theorem 2.1, this operator has a well-defined Cauchy problem, i.e. it is *Cauchy-hyperbolic*, and consequently unique advance and retarded fundamental solutions exist such that the operator is *Green-hyperbolic*. Example of partial differential operators which are Cauchy-hyperbolic, but not normally hyperbolic are the Dirac operator and the Proca operator which defines the equation of motion for a massive vector field, see e.g. [6]. On the other hand, the distinction between Cauchy-hyperbolic operators and Green-hyperbolic operators does not matter in most examples although one can construction operators which are Green-hyperbolic but not Cauchy-hyperbolic, cf. [6] for details.

Based on the data given in Definition 2.5, a symplectic space (Bosonic case) or inner product space (Fermionic case) can be constructed in full analogy to the Klein-Gordon case, in particular, the following can be shown.

Theorem 2.3 *Under the assumptions of Definition 2.5, let $E^P \doteq E^P_R - E^P_A$ denote the causal propagator of P, and let* Sol $\subset \Gamma(\mathscr{V})$, Sol$_{\mathrm{sc}} \subset \Gamma_{\mathrm{sc}}(\mathscr{V})$ *denote the space of smooth (smooth and spacelike-compact) solutions of $P\Phi = 0$.*

1. The tuple $(\mathscr{E}, \tau)$, where

$$\mathscr{E} \doteq \Gamma_0(\mathscr{V})/P[\Gamma_0(\mathscr{V})],$$

$$\tau : \mathscr{E} \times \mathscr{E} \to \mathbb{R}, \qquad \tau([f],[g]) \doteq \left\langle f, E^P g \right\rangle_{\mathscr{V}},$$

is a well-defined symplectic (Bosonic case) or inner product (Fermionic case) space. In particular τ is well-defined and independent of the chosen represen-

tatives and moreover non-degenerate and antisymmetric (Bosonic case) or symmetric (Fermionic case).

2. *Let* $[f] \in \mathscr{E}$ *be arbitrary and let* Σ *be any Cauchy surface of* (M, g). *Then, for any bounded neighbourhood* $\mathscr{O}(\Sigma)$ *of* Σ, *we can find a* $g \in \Gamma_0(\mathscr{V})$ *with* $\operatorname{supp} g \subset \mathscr{O}(\Sigma)$ *and* $g \in [f]$.
3. *The causal propagator* $E^P : \Gamma_0(\mathscr{V}) \to \Gamma_{sc}(\mathscr{V})$ *descends to a bijective map* $\mathscr{E} \to \mathrm{Sol}_{sc}$ *and for all* $f \in \Gamma_0(\mathscr{V})$ *and all* $\Phi \in \mathrm{Sol}$,

$$\langle f, \Phi \rangle_{\mathscr{V}} = \left\langle E^P f, \Phi \right\rangle_{\mathrm{Sol}} ,$$

where for all $\Phi_1, \Phi_2 \in \mathrm{Sol}$ *with spacelike-compact overlapping support, the bilinear form* $\langle \cdot, \cdot \rangle_{\mathrm{Sol}}$ *is defined as*

$$\langle \Phi_1, \Phi_2 \rangle_{\mathrm{Sol}} \doteq \left\langle P \Phi_1^+, \Phi_2 \right\rangle_{\mathscr{V}} .$$

4. $\langle \cdot, \cdot \rangle_{\mathrm{Sol}}$ *may be computed as a suitable integral over an arbitrary but fixed Cauchy surface* Σ *of* (M, g) *with future-pointing normal vector field* N *and induced measure* $d\Sigma$. *If there exists a 'current'* $j : \Gamma(\mathscr{V}) \times \Gamma(\mathscr{V}) \to T^*M$ *such that* $\nabla^\mu j_\mu(\Phi_1, \Phi_2) = \langle\langle \Phi_1, P\Phi_2 \rangle\rangle_{\mathscr{V}} - \langle\langle \Phi_2, P\Phi_1 \rangle\rangle_{\mathscr{V}}$ *for all* $\Phi_1, \Phi_2 \in \Gamma(\mathscr{V})$, *then*

$$\langle \Phi_1, \Phi_2 \rangle_{\mathrm{Sol}} = \int_\Sigma d\Sigma \; N^\mu j_\mu(\Phi_1, \Phi_2) .$$

5. *The tuple* $(\mathrm{Sol}_{sc}, \langle \cdot, \cdot \rangle_{\mathrm{Sol}})$ *is a well-defined symplectic (Bosonic case) or inner product (Fermionic case) space which is isomorphic to* $(\mathscr{E}, \tau)$.

As with the Klein-Gordon field, the last statement implies in physical terms that the symplectic respectively inner product space can be constructed both in a covariant and in an equal-time fashion, and that the two constructions give equivalent results. In many cases, the equal-time point of view is better suited for practical computations and for proving particular further properties of the bilinear form τ, cf. the following discussion of theories with local gauge invariance.

2.2.2 Models with Gauge Symmetry

The discussion of linear field theoretic models with local gauge symmetries on curved spacetimes is naturally more involved than the case where such symmetries are absent. However, as in this monograph we will only be dealing with linear models and simple observables, it will not be necessary to introduce auxiliary fields like in the BRST/BV formalism [50, 68]. Instead, we shall review an approach which has been developed in [39] for the Maxwell field, used for linearised gravity in [42] and then further generalised to arbitrary linear gauge theories in [63]. For linear models and simple observables this approach and the BRST/BV formalism give equivalent results, however, non-linear models and more general observables are not tractable in the way we shall review in the following.

2.2.2.1 A Toy Model

We outline the essential ideas of this approach at the example of a toy model. We consider as a gauge field $\Phi = (\phi_1, \phi_2)^t \subset \Gamma(\mathscr{V})$ a tuple of two scalar fields on a spacetime (M, g) satisfying the equation of motion

$$P\Phi = \begin{pmatrix} -\Box & \Box \\ \Box & -\Box \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = 0\,,$$

where $\mathscr{V}$ is the (trivial) vector bundle $\mathscr{V} \doteq M \times \mathbb{R}^2$. The gauge transformations are given by the following translations on configuration space $\Phi \mapsto \Phi + K\varepsilon$, where the gauge transformation operator $K : \Gamma(M) \to \Gamma(\mathscr{V})$ is the linear operator defined by $K\varepsilon \doteq (\varepsilon, \varepsilon)^t$ for a smooth function $\varepsilon \in \Gamma(M)$. One may check that $P \circ K = 0$ holds which is equivalent to the gauge-invariance of the action $S(\Phi) \doteq \frac{1}{2}\langle \Phi, P\Phi\rangle_{\mathscr{V}}$ with $\langle \Phi, \Phi'\rangle_{\mathscr{V}} \doteq \int_M d_g x\ (\phi_1\phi_1' + \phi_2\phi_2')$.

Clearly, the linear combination $\psi \doteq \phi_1 - \phi_2$ is gauge-invariant and satisfies $-\Box\psi = 0$, and it would be rather natural to quantize Φ by directly quantizing ψ as a massless, minimally coupled scalar field. This would be much in the spirit of the usual quantization of perturbations in Inflation, where gauge-invariant linear combinations of the gauge field components, e.g. the Bardeen-Potentials or the Mukhanov-Sasaki variable, are taken as the fundamental fields for quantization, see the last chapter of this monograph. However, in general it is rather difficult to directly identify a gauge-invariant fundamental field like ψ whose classical and quantum theory is equivalent to the classical and quantum theory of the original gauge field. Notwithstanding, an indirect characterisation of such a gauge-invariant linear combination of gauge-field components, which can serve as a fundamental field for quantization, is still possible. In the toy model under consideration we consider a tuple $f = (f_1, f_2) \in \Gamma_0(\mathscr{V})$ of test functions $f_i \in \Gamma_0(M)$. We ask that $K^\dagger f \doteq f_1 + f_2 = 0$, where $K^\dagger : \Gamma(\mathscr{V}) \to \Gamma(M)$ is the adjoint of the gauge transformation operator K i.e. $\int_M d_g x\ \varepsilon K^\dagger f = \langle K\varepsilon, f\rangle_{\mathscr{V}}$. Clearly, any f satisfying this condition is of the form $f = (h, -h)^t$ for a test function h. We now observe that the pairing between a gauge field configuration Φ and such an f is gauge-invariant, i.e. $\langle \Phi + K\varepsilon, f\rangle_{\mathscr{V}} = \langle f, \Phi\rangle_{\mathscr{V}} + \int_M d_g x\ \varepsilon K^\dagger f = \langle \Phi, f\rangle_{\mathscr{V}}$. Thus we can consider the 'smeared field' $\Phi(f) \simeq \langle f, \Phi\rangle_{\mathscr{V}}$, with $f = (h, -h)^t$ and arbitrary h, as a gauge-invariant linear combination of gauge-field components which is suitable for playing the role of a fundamental field for quantization. We can compute $\langle f, \Phi\rangle_{\mathscr{V}} = \int_M d_g x\ \ \psi h$, and observe that, up to the 'smearing' with h, this indirect choice of gauge-invariant fundamental field is exactly the one discussed in the beginning. If one chooses h to be the delta distribution $\delta(x, y)$ rather than a test function, one even finds $\langle f, \Phi\rangle = \psi(x)$, whereas for general h, $\langle f, \Phi\rangle$ can be interpreted as a weighted, gauge-invariant measurement of the field configuration Φ.

Moreover, as already anticipated, in general gauge theories with more complicated gauge transformation operators K it usually extremely difficult to classify all solutions of $K^\dagger f = 0$, which would be equivalent to a direct characterisation of one or several fundamental gauge-invariant fields such as ψ, whereas working implicitly with the condition $K^\dagger f = 0$ is always possible.

2.2.2.2 General Models

From the previous discussion we can already infer most of the additional data which is needed in addition to the data mentioned in Definition 2.5 in order to specify a linear field theoretic model with local gauge symmetries on curved spacetimes.

Definition 2.6 A real Bosonic linear field-theoretic model with local gauge symmetries on a curved spacetime is defined by the data $(M, \mathscr{V}, \mathscr{W}, P, K)$, where

1. $M \simeq (M, g)$ is a globally hyperbolic spacetime,
2. $\mathscr{V}$ and $\mathscr{W}$ are real vector bundles over M, the spaces of smooth sections $\mathscr{V}$ and $\mathscr{W}$ are endowed with symmetric and non-degenerate bilinear forms $\langle\cdot,\cdot\rangle_{\mathscr{V}}$ and $\langle\cdot,\cdot\rangle_{\mathscr{W}}$ which are well-defined on sections with compact overlapping support and given by the integral of fibrewise symmetric and non-degenerate bilinear forms $\langle\langle\cdot,\cdot\rangle\rangle_{\mathscr{V}} : \Gamma(\mathscr{V}) \times \Gamma(\mathscr{V}) \to \Gamma(M)$ and $\langle\langle\cdot,\cdot\rangle\rangle_{\mathscr{W}} : \Gamma(\mathscr{W}) \times \Gamma(\mathscr{W}) \to \Gamma(M)$,
3. $P : \Gamma(\mathscr{V}) \to \Gamma(\mathscr{V})$ is a partial differential operator which is formally self-adjoint with respect to $\langle\cdot,\cdot\rangle_{\mathscr{V}}$,
4. $K : \Gamma(\mathscr{W}) \to \Gamma(\mathscr{V})$ is a partial differential operator such that $P \circ K = 0$; moreover $R \doteq K^\dagger \circ K : \Gamma(\mathscr{W}) \to \Gamma(\mathscr{W})$ is Cauchy-hyperbolic and there exists an operator $T : \Gamma(\mathscr{W}) \to \Gamma(\mathscr{V})$ such that a) $\widetilde{P} \doteq P + T \circ K^\dagger$ is Green-hyperbolic and b) $Q \doteq K^\dagger \circ T$ is Cauchy-hyperbolic.

A real Fermionic linear field-theoretic model with local gauge symmetries on a curved spacetime is defined analogously with the only difference being that $\langle\langle\cdot,\cdot\rangle\rangle_{\mathscr{V}}$, $\langle\cdot,\cdot\rangle_{\mathscr{V}}$, $\langle\langle\cdot,\cdot\rangle\rangle_{\mathscr{W}}$ and $\langle\cdot,\cdot\rangle_{\mathscr{W}}$ are not symmetric but antisymmetric. Complex theories can be obtained from the real ones by complexification.

These data have the following meaning. Sections of $\mathscr{V}$ are configurations of the gauge field Φ, whereas local gauge transformations are parametrised via the gauge transformation operator K by sections of $\mathscr{W}$. The differential operator P defines the equation of motion for the gauge field Φ via $P\Phi = 0$. The formal self-adjointness of P is motivated by P being the Euler-Lagrange operator of a local action $S(\Phi)$, e.g. $S(\Phi) = \frac{1}{2}\langle\Phi, P\Phi\rangle_{\mathscr{V}}$, whereas the gauge-invariance condition $P \circ K = 0$ implies gauge-invariance of the action $S(\Phi)$. This condition implies (for $K \neq 0$) that P can *not* be Cauchy-hyperbolic, because any 'pure gauge configuration' $\Phi_\varepsilon = K\varepsilon$ with $\varepsilon \in \Gamma_0(\mathscr{W})$ of compact support solves the equation of motion $P\Phi_\varepsilon = 0$ with vanishing initial data in the distant past, whereas for Cauchy-hyperbolic P the unique solution with vanishing initial data is identically zero.

The Cauchy-hyperbolicity of $R = K^\dagger \circ K$ implies that for every $\Phi \in \Gamma(\mathscr{V})$ there exists an $\varepsilon \in \Gamma(\mathscr{W})$ such that $\Phi' \doteq \Phi + K\varepsilon$ satisfies the 'canonical gauge-fixing condition' $K^\dagger \Phi' = 0$. The existence of the gauge-fixing operator T such that the gauge-fixed equation of motion operator $\widetilde{P} = P + T \circ K^\dagger$ is Green-hyperbolic implies that every solution of $P\Phi = 0$ in fact satisfies $\widetilde{P}\Phi = 0$ up to gauge-equivalence; consequently, the dynamics of the 'physical degrees of freedom' is ruled by a hyperbolic equation of motion even if P is not hyperbolic. Finally, the condition that $Q = K^\dagger \circ T$ is Cauchy-hyperbolic implies that the gauge-fixing $K^\dagger \Phi = 0$ is compatible with the hyperbolic dynamics of $\widetilde{P}\Phi = 0$. T is in general not canonical and the following constructions will not depend on the particular choice of T in case several T with the required properties exist, thus we do not consider the gauge-fixing operator T as part of the data specifying the model.

Apart from the toy model discussed above, a simple example of a linear gauge theory which fits into Definition 2.6 is the Maxwell field (on a trivial principal $U(1)$-bundle) which after all was the inspiration for the formulation of this definition. This model is specified by (in differential form notation)

$$\mathscr{W} = M \times \mathbb{R}\,, \qquad \mathscr{V} = \mathscr{W} \otimes T^*M = T^*M\,,$$

$$\langle \varepsilon_1, \varepsilon_2 \rangle_{\mathscr{W}} \doteq \int_M \varepsilon_1 \wedge *\varepsilon_2\,, \qquad \langle \Phi_1, \Phi_2 \rangle_{\mathscr{V}} \doteq \int_M \Phi_1 \wedge *\Phi_2\,,$$

$$P = d^\dagger d\,, \qquad K = T = d\,,$$

$$\widetilde{P} = d^\dagger d + dd^\dagger\,, \qquad K^\dagger K = K^\dagger T = d^\dagger d = \Box\,.$$

We would like to construct a (pre-)symplectic or (pre-)inner product space corresponding to the data given in Definition 2.6 by following as much as possible the logic of the case without gauge symmetry. To this avail we need a few further definitions of section spaces.

Definition 2.7 As before, we denote by $\mathrm{Sol} \subset \Gamma(\mathscr{V})$ ($\mathrm{Sol}_{\mathrm{sc}} \subset \Gamma_{\mathrm{sc}}(\mathscr{V})$) the spaces of smooth solutions of the equation $P\Phi = 0$ (with spacelike-compact support). By $\mathscr{G}$ and $\mathscr{G}_{\mathrm{sc}}$ we denote the space of gauge configurations (with spacelike-compact support), by $\mathscr{G}_{\mathrm{sc},0}$ we denote the gauge configurations induced by spacelike-compact gauge transformation parameters

$$\mathscr{G} \doteq K\left[\Gamma(\mathscr{W})\right]\,, \qquad \mathscr{G}_{\mathrm{sc}} \doteq \mathscr{G} \cap \Gamma_{\mathrm{sc}}(\mathscr{W})\,, \qquad \mathscr{G}_{\mathrm{sc},0} \doteq K\left[\Gamma_{\mathrm{sc}}(\mathscr{W})\right]\,.$$

In general, $\mathscr{G}_{\mathrm{sc},0} \subsetneq \mathscr{G}_{\mathrm{sc}}$. By $\ker_0(K^\dagger)$ we denote the space of gauge-invariant test-sections and by $\mathscr{E}$ the *labelling space of linear gauge-invariant on-shell observables*

$$\ker_0(K^\dagger) \doteq \{f \in \Gamma_0(\mathscr{V}) \mid K^\dagger f = 0\}\,, \qquad \mathscr{E} \doteq \ker_0(K^\dagger)/P\left[\Gamma_0(\mathscr{V})\right]\,.$$

Our discussion of the toy model in the previous subsection already indicated why $\mathscr{E}$ defined above is a good candidate for a labelling space of linear gauge-invariant on-shell observables. First of all we observe that $\mathscr{E}$ is well-defined because

$P\,[\Gamma_0(\mathscr{V})] \subset \ker_0(K^\dagger)$ owing to $P \circ K = 0$. Moreover, we have by construction for arbitrary $\Phi \in \mathrm{Sol}$, $\varepsilon \in \Gamma(\mathscr{W})$, $f \in \ker_0(K^\dagger)$ and $g \in \Gamma_0(\mathscr{V})$

$$\langle f + Pg, \Phi + K\varepsilon\rangle_{\mathscr{V}} = \langle f, \Phi\rangle_{\mathscr{V}} \ .$$

Consequently, every element $[f]$ of $\mathscr{E}$ induces a well-defined linear functional on $\mathrm{Sol}/\mathscr{G}$, i.e. on gauge-equivalence classes of on-shell configurations, by $\mathrm{Sol}/\mathscr{G} \ni [\Phi] \mapsto \mathscr{O}_{[f]}([\Phi]) \doteq \langle f, \Phi\rangle_{\mathscr{V}}$. Being gauge-invariant, these functionals correspond to meaningful (physical) observables. On the level of classical observables, the fact that the physical degrees of freedom of the gauge field propagate in a causal fashion is reflected in the following generalisation of Lemma 2.1 which is proved in [63].

Lemma 2.2 *Let $[f] \in \mathscr{E}$ be arbitrary and let Σ be any Cauchy surface of (M, g). Then, for any bounded neighbourhood $\mathscr{O}(\Sigma)$ of Σ, we can find a $g \in \ker_0(K^\dagger)$ with* $\mathrm{supp}\, g \subset \mathscr{O}(\Sigma)$ *and $g \in [f]$.*

In constructing the classical bracket for models without gauge symmetry the last statement of Theorem 2.1, which in fact holds for the causal propagator E^P of any Green-hyperbolic operator P on an arbitrary vector bundle $\mathscr{V}$, has been crucial. In the following, we review results obtained in [63, Theorem 3.12+Theorem 5.2] which essentially imply that, although P is not hyperbolic, the causal propagator $E^{\widetilde{P}}$ of the gauge-fixed equation of motion operator $\widetilde{P} = P + T \circ K^\dagger$ is effectively a causal propagator for P up to gauge-equivalence. The crucial observation here is that P and $\widetilde{P}$ coincide on $\ker_0(K^\dagger)$ which implies that $E^{\widetilde{P}}$ restricted to $\ker_0(K^\dagger)$ is independent of the particular form of the gauge fixing operator T.

Theorem 2.4 *The causal propagator $E^{\widetilde{P}}$ of $\widetilde{P} = P + T \circ K^\dagger$ satisfies the following relations.*

1. *$h \in \ker_0(K^\dagger)$ and $E^{\widetilde{P}} h \in \mathscr{G}_{\mathrm{sc},0}$ if and only if $h \in P[\Gamma_0(\mathscr{V})]$, with $\mathscr{G}_{\mathrm{sc},0}$ defined in Definition 2.7.*
2. *Every $h \in \mathrm{Sol}_{\mathrm{sc}}$ can be split as $h = h_1 + h_2$ with $h_1 \in E^{\widetilde{P}}\left[\ker_0(K^\dagger)\right]$ and $h_2 \in \mathscr{G}_{\mathrm{sc},0}$.*
3. *$E^{\widetilde{P}}$ descends to a bijective map $\mathscr{E} \to \mathrm{Sol}_{\mathrm{sc}}/\mathscr{G}_{\mathrm{sc},0}$.*
4. *$E^{\widetilde{P}}$ is formally skew-adjoint w.r.t. $\langle\cdot,\cdot\rangle_{\mathscr{V}}$ on $\ker_0(K^\dagger)$, i.e.*

$$\left\langle h_1, E^{\widetilde{P}} h_2\right\rangle_{\mathscr{V}} = -\left\langle E^{\widetilde{P}} h_1, h_2\right\rangle_{\mathscr{V}}$$

for all $h_1, h_2 \in \ker_0(K^\dagger)$.

5. *Let $T' : \Gamma(\mathscr{W}) \to \Gamma(\mathscr{V})$ be any differential operator satisfying the properties required for the operator T in Definition 2.6 and let $E^{\widetilde{P}'}$ be the causal propagator of $\widetilde{P}' \doteq P + T' \circ K^\dagger$. Then $E^{\widetilde{P}'}$ satisfies the four properties above.*

Given these results, we can now construct a meaningful bracket on $\mathscr{E}$ by generalising Proposition 2.1.

Proposition 2.2 *The tuple* $(\mathscr{E}, \tau)$ *with* $\tau : \mathscr{E} \times \mathscr{E} \to \mathbb{R}$ *defined by*

$$\tau([f], [g]) \doteq \left\langle f, E^{\widetilde{P}} g \right\rangle_{\mathscr{V}}$$

is a pre-symplectic space *(Bosonic case) or* pre-inner product space *(Fermionic case). In particular,*

1. τ *is well-defined and independent of the chosen representatives,*
2. τ *is antisymmetric (Bosonic case) or symmetric (Fermionic case).*
3. *Let* $T' : \Gamma(\mathscr{W}) \to \Gamma(\mathscr{V})$ *be any differential operator satisfying the properties required for the operator* T *in Definition 2.6 and define* τ' *in analogy to* τ *but with the causal propagator* $E^{\widetilde{P}'}$ *of* $\widetilde{P}' \doteq P + T' \circ K^\dagger$ *instead of* $E^{\widetilde{P}}$. *Then* $\tau' = \tau$.

We stress that τ is in general *not* weakly non-degenerate, cf. the last statement of Theorem 2.5. This is a particular feature of gauge theories, cf. e.g. [8, 110] for a discussion of the physical interpretation of this non-degeneracy in the case of the Maxwell field. The last statement above indicates that τ is independent of the gauge-fixing operator T and in this sense, gauge-invariant. Indeed, we shall see in what follows that τ can be rewritten in a manifestly gauge-invariant form. The form of τ given here can be derived directly from the action $S(\Phi) = \frac{1}{2} \langle \Phi, P\Phi \rangle_{\mathscr{V}}$ by Peierls' method in analogy to the derivation for electromagnetism in [110], see also [79, 80]) for a broader context.

As in the case without local gauge symmetries it is interesting and useful to observe that the covariant pre-symplectic or pre-inner product space $(\mathscr{E}, \tau)$ can be understood equivalently in an equal-time fashion. In fact the following statements have been proved in [63, Proposition 5.1+Theorem 5.2] (or can be proved by slightly generalising the arguments used there).

Theorem 2.5 *Under the assumptions of Definition 2.6, let* $\langle \cdot, \cdot \rangle_{\mathrm{Sol}}$ *be the bilinear form on* Sol *defined for* $\Phi_1, \Phi_2 \in \mathrm{Sol}$ *with spacelike-compact overlapping support by*

$$\langle \Phi_1, \Phi_2 \rangle_{\mathrm{Sol}} \doteq \left\langle P\Phi_1^+, \Phi_2 \right\rangle_{\mathscr{V}} ,$$

where Φ^+ *denotes the future part of* Φ, *see Definition 2.4. This bilinear form has the following properties.*

1. $\langle \Phi_1, \Phi_2 \rangle_{\mathrm{Sol}}$ *is well-defined for all* $\Phi_1, \Phi_2 \in \mathrm{Sol}$ *with spacelike-compact overlapping support. In particular, it is independent of the choice of future part entering its definition.*
2. $\langle \cdot, \cdot \rangle_{\mathrm{Sol}}$ *is antisymmetric (Bosonic case) or symmetric (Fermionic case).*
3. $\langle \cdot, \cdot \rangle_{\mathrm{Sol}}$ *is gauge-invariant, i.e.*

$$\langle \Phi_1, \Phi_2 + K\varepsilon \rangle_{\mathrm{Sol}} = \langle \Phi_1, \Phi_2 \rangle_{\mathrm{Sol}}$$

for all $\Phi_1, \Phi_2 \in \mathrm{Sol}$, $\varepsilon \in \Gamma(\mathscr{W})$ *s.t.* Φ_1 *and* ε *have spacelike-compact overlapping support.*

4. $\langle \cdot, \cdot \rangle_{\mathrm{Sol}}$ *may be computed as a suitable integral over an arbitrary but fixed Cauchy surface* Σ *of* (M, g) *with future-pointing normal vector field* N *and induced measure* $d\Sigma$*. If there exists a 'current'* $j : \Gamma(\mathscr{V}) \times \Gamma(\mathscr{V}) \to T^*M$ *such that* $\nabla^\mu j_\mu(\Phi_1, \Phi_2) = \langle\langle \Phi_1, P\Phi_2 \rangle\rangle_{\mathscr{V}} - \langle\langle \Phi_2, P\Phi_1 \rangle\rangle_{\mathscr{V}}$ *for all* $\Phi_1, \Phi_2 \in \Gamma(\mathscr{V})$*, then*

$$\langle \Phi_1, \Phi_2 \rangle_{\mathrm{Sol}} = \int\limits_{\Sigma} d\Sigma\; N^\mu j_\mu(\Phi_1, \Phi_2)\,.$$

5. *For all* $\Phi \in \mathrm{Sol}$ *and all* $h \in \ker_0(K^\dagger)$*,*

$$\left\langle E^{\widetilde{P}} h, \Phi \right\rangle_{\mathrm{Sol}} = \langle h, \Phi \rangle_{\mathscr{V}}\;.$$

6. $E^{\widetilde{P}}$ *descends to an isomorphism of pre-symplectic (Bosonic case) or pre-inner product spaces (Fermionic case)* $E^{\widetilde{P}} : (\mathscr{E}, \tau) \to (\mathrm{Sol}_{\mathrm{sc}}/\mathscr{G}_{\mathrm{sc},0}, \langle \cdot, \cdot \rangle_{\mathrm{Sol}})$.
7. *If* $\mathscr{G}_{\mathrm{sc},0} \subsetneq \mathscr{G}_{\mathrm{sc}}$*, then* τ *is degenerate, i.e. there exists* $[0] \neq [h] \in \mathscr{E}$ *s.t.* $\tau([h], \mathscr{E}) = 0$.

The fourth and fifth statement in the above theorem show that one can view the observable $\mathrm{Sol}/\mathscr{G} \ni [\Phi] \mapsto \langle h, \Phi \rangle_{\mathscr{V}} \simeq \Phi(h)$, i.e. the 'covariantly smeared classical field', equivalently as an 'equal-time smeared classical field' $\mathrm{Sol}/\mathscr{G} \ni [\Phi] \mapsto \langle H, \Phi \rangle_{\mathrm{Sol}}$ with $H = E^{\widetilde{P}} h \in [H] \in \mathrm{Sol}_{\mathrm{sc}}/\mathscr{G}_{\mathrm{sc},0}$.

2.3 Linear Quantum Fields on Curved Spacetimes

Given the (pre-)symplectic or (pre-)inner product spaces of classical linear observables constructed in the previous section for Bosonic and Fermionic theories with or without local gauge symmetries, there are several 'canonical' ways to construct corresponding algebras of observables in the associated quantum theories; these constructions differ mainly in technical terms.

In the Bosonic case, one can consider the *Weyl algebra* corresponding to the pre-symplectic space $(\mathscr{E}, \tau)$, which essentially means to quantize exponentials $\exp(i\,\langle f, \Phi \rangle_{\mathscr{V}})$ of the smeared classical field $\Phi(f) \simeq \langle f, \Phi \rangle_{\mathscr{V}}$ rather than the smeared classical field itself. This mainly has the technical advantage that one is dealing with a C^*-algebra corresponding to bounded operators on a Hilbert space, i.e. to operators with a bounded spectrum. However, sometimes it is also advisable in physical terms to consider exponential observables rather than linear ones as fundamental building blocks, e.g. in case one is dealing with *finite* gauge transformations, cf. [8]. The Weyl algebra is initially constructed under the assumption that the form τ is non-degenerate such that the pre-symplectic space $(\mathscr{E}, \tau)$ is in fact symplectic. However, the construction of the Weyl algebra is also well-defined in the degenerate case [12] and even in case $\mathscr{E}$ is not a vector space, but only an Abelian group [8]. In the Fermionic case it is not necessary to consider exponential observables in order to access the advantages of a C^*-algebraic framework, as a C^*-algebra can already be constructed based on linear observables due to the anticommutation relations of Fermionic quantum fields, see e.g. [14].

As in this monograph we shall not make use of the C^*-algebraic framework, it will be sufficient to consider the algebra of quantum observables constructed by directly quantizing the smeared classical fields $\Phi(f) \simeq \langle f, \Phi\rangle_{\mathscr{V}}$ themselves both in the Bosonic case and in the Fermionic case. We shall first construct the *Borchers-Uhlmann algebra* $\mathscr{A}(M)$ corresponding to the linear model defined by the data $(M, \mathscr{V}, \mathscr{W}, P, K)$ cf. Definition 2.6, where we can consider a model $(M, \mathscr{V}, P)$ without gauge invariance as the subclass $(M, \mathscr{V}, \mathscr{W} = \mathscr{V}, P, K = 0)$. The algebra $\mathscr{A}(M)$ contains only the most simple observables, in particular it does not contain observables which correspond to pointwise powers of the field such as $\Phi(x)^2$ or the stress-energy tensor. We shall discuss a larger algebra which contains also these observables in Sect. 2.6.1.

In order to construct the Borchers-Uhlmann algebra, we recall that the labelling space $\mathscr{E}$ consists of equivalence classes of test sections $[f]$ corresponding to the classical observables $\Phi(f) \simeq \langle f, \Phi\rangle_{\mathscr{V}}$ with $\Phi \in [\Phi] \in \mathrm{Sol}/\mathscr{G}$ (= Sol in the absence of gauge symmetries, i.e. for $K = 0$) and $f \in [f] \in \mathscr{E} = \ker_0(K^\dagger)/P[\Gamma_0(\mathscr{V})]$ $(= \Gamma_0(\mathscr{V})/P[\Gamma_0(\mathscr{V})]$ for $K = 0)$. We recall that omitting the equivalence classes in the notation $\Phi(f) \simeq \langle f, \Phi\rangle_{\mathscr{V}}$ is meaningful because the latter expression is independent of the chosen representatives of the equivalence classes. For the quantum theory, we need complex expressions and therefore consider the complexification $\mathscr{E}_{\mathbb{C}} \doteq \mathscr{E} \otimes_{\mathbb{R}} \mathbb{C}$ of the labelling space $\mathscr{E}$.

With this in mind, we represent the quantum product of two smeared fields $\Phi(f_1)\Phi(f_2)$ by the tensor product $[f_1] \otimes [f_2]$. On the long run, we would like to represent $\Phi(f)$ as an operator on a Hilbert space, we therefore need an operation which encodes 'taking the adjoint with respect to a Hilbert space inner product' on the abstract algebraic level. We define such a $*$-operation by setting $[\Phi(f)]^* \doteq \Phi(\overline{f})$, corresponding to $[f_1]^* \doteq [\overline{f_1}]$, and $[\Phi(f_1)\cdots\Phi(f_n)]^* = [\Phi(f_n)]^*\cdots[\Phi(f_1)]^*$. Observables would then be polynomials $\mathscr{P}$ of smeared fields (tensor polynomials of elements of $\mathscr{E}_{\mathbb{C}}$) which fulfil $\mathscr{P}^* = \mathscr{P}$ (in the Fermionic case we need further conditions e.g. $\mathscr{P}$ has to be an even polynomial). To promote $\Phi(f)$ to a proper quantum field with the correct (anti)commutation relations, we define

$$[\Phi(f), \Phi(g)]_\mp \doteq \Phi(f)\Phi(g) \mp \Phi(g)\Phi(f) = i\tau([f],[g])\mathbb{I} = i\left\langle f, E^{\widetilde{P}}, g\right\rangle_{\mathscr{V}} \mathbb{I}, \quad (2.6)$$

where we recall that $E^{\widetilde{P}}$ is the causal propagator of the gauge-fixed equation of motion operator $\widetilde{P} = P + T\circ K^\dagger$ (= P in the absence of gauge symmetries $K = 0$), $\mathbb{I}$ is the identity and the $-$ $(+)$ sign applies for the Bosonic (Fermionic) case. Recall that $\tau([f],[g])$ vanishes if the supports of f and g are spacelike separated, the above *canonical (anti)commutation relations* (CCR/CAR) therefore assure that observables commute at spacelike separations. In the case without gauge symmetries, one can write the CCR/CAR formally as

$$[\Phi(x), \Phi(y)]_\mp = iE^P(x,y)\mathbb{I}.$$

Recall that this is nothing but the covariant version of the well-known equal-time CCR/CAR. In the case where gauge symmetries are present, this expression does not make sense because the equality holds only when smeared with 'gauge-invariant' test sections $f \in \ker_0(K^\dagger)$. Finally, we remark that dynamics is already encoded by the fact that $\mathscr{E}_\mathbb{C}$ consists of equivalence classes with $[Pg] = [0] \in \mathscr{E}_\mathbb{C}$ for all $g \in \Gamma_0^\mathbb{C}(\mathscr{V})$ and that it is convenient to have a topology on the algebra $\mathscr{A}(M)$ in order to be able to quantify to which extent two abstract observables are 'close', i.e. similar in physical terms. We subsume the above discussion in the following definition.

Definition 2.8 Consider a linear Bosonic or Fermionic (gauge) field theory defined by $(M, \mathscr{V}, \mathscr{W}, P, K)$ (with $\mathscr{W} = \mathscr{V}$ and $K = 0$ in the absence of gauge symmetries), cf. Definitions 2.5 and 2.6 and let $(\mathscr{E}, \tau)$ be the corresponding (pre-)symplectic or (pre-)inner product space constructed as in Theorem 2.3 and Proposition 2.2. The *Borchers-Uhlmann algebra* $\mathscr{A}(M)$ of the model $(M, \mathscr{V}, \mathscr{W}, P, K)$ is defined as

$$\mathscr{A}(M) \doteq \mathscr{A}_0(M)/\mathscr{I} \,,$$

where $\mathscr{A}_0(M)$ is the direct sum

$$\mathscr{A}_0(M) \doteq \bigoplus_{n=0}^{\infty} \mathscr{E}_\mathbb{C}^{\otimes n}$$

($\mathscr{E}_\mathbb{C}^{\otimes 0} \doteq \mathbb{C}$) equipped with a product defined by the linear extension of the tensor product of $\mathscr{E}_\mathbb{C}^{\otimes n}$, a $*$-operation defined by the antilinear extension of $([f_1] \otimes \cdots \otimes [f_n])^* = [\overline{f_n}] \otimes \cdots \otimes [\overline{f_1}]$, and it is required each element of $\mathscr{A}_0(M)$ is a linear combination of elements of $\mathscr{E}_\mathbb{C}^{\otimes n}$ with $n \leq n_{\max} < \infty$. Additionally, we equip $\mathscr{A}_0(M)$ with the topology induces by the locally convex topology of $\Gamma_0(\mathscr{V})$. Moreover, $\mathscr{I}$ is the closed $*$-ideal generated by elements of the form $-i\tau([f],[g]) \oplus ([f] \otimes [g] \mp [g] \otimes [f])$, where $-$ $(+)$ stands for the Bosonic (Fermionic) case, and $\mathscr{A}(M)$ is thought to be equipped with the product, $*$-operation, and topology descending from $\mathscr{A}_0(M)$. If $\mathscr{O}$ is an open subset of M, $\mathscr{A}(\mathscr{O})$ denotes the algebra obtained by allowing only test sections with support in $\mathscr{O}$.

$\mathscr{A}(M)$, in contrast to $\mathscr{A}_0(M)$, depends explicitly on the metric g of a spacetime (M, g) via the causal propagator and the equation of motion. However, now and in the following we shall omit this dependence in favour of notational simplicity.

We recall that, by Lemma 2.2, every equivalence class $[f] \in \mathscr{E}_\mathbb{C}$ is so large that it contains elements with support in an arbitrarily small neighbourhood of any Cauchy surface of M. This implies the following well-known result, which on physical grounds entails the predictability of observables.

Lemma 2.3 *The Borchers-Uhlmann algebra $\mathscr{A}(M)$ fulfils the* time-slice axiom. *Namely, let Σ be a Cauchy surface of (M, g) and let $\mathscr{O}$ be an arbitrary neighbourhood of Σ. Then $\mathscr{A}(\mathscr{O}) = \mathscr{A}(M)$.*

We now turn our attention to states. Let $\mathfrak{A}$ be a topological, unital $*$-algebra, i.e. $\mathfrak{A}$ is endowed with an operation * which fulfils $(AB)^* = B^*A^*$ and $(A^*)^* = A$ for all elements A, B in $\mathfrak{A}$. A *state* ω on $\mathfrak{A}$ is defined to be a continuous linear functional $\mathfrak{A} \to \mathbb{C}$ which is normalised, i.e. $\omega(\mathbb{I}) = 1$ and positive, namely, $\omega(A^*A) \geq 0$ must hold for any $A \in \mathfrak{A}$. Considering the special topological and unital $*$-algebra $\mathscr{A}(M)$, a state on $\mathscr{A}(M)$ is determined by its n-point correlation functions

$$\omega_n(f_1, \ldots, f_n) \doteq \omega\left(\Phi(f_1) \cdots \Phi(f_n)\right) .$$

which are distributions in $\Gamma_0'^{\mathbb{C}}(M^n)$. Given a state ω on $\mathfrak{A}$, one can represent $\mathfrak{A}$ on a Hilbert space $\mathscr{H}_\omega$ by the so-called *GNS construction* (after Gel'fand, Naimark, and Segal), see for instance [4, 65]. By this construction, algebra elements $A \in \mathfrak{A}$ are represented as operators $\pi_\omega(A)$ on a common dense and invariant subspace of $\mathscr{H}_\omega$, while ω is represented as a vector of $|\Omega_\omega\rangle \in \mathscr{H}_\omega$ such that for all $A \in \mathfrak{A}$

$$\omega(A) = \langle \Omega_\omega | \pi_\Omega(A) | \Omega_\omega \rangle .$$

Conversely, every vector in a Hilbert space $\mathscr{H}$ gives rise to an algebraic state on the algebra of linear operators on $\mathscr{H}$.

Among the possible states on $\mathscr{A}(M)$ there are several special classes, which we collect in the following definition. Some of the definitions are sensible for general $*$-algebras, as we point out explicitly.

Definition 2.9 Let $\mathfrak{A}$ denote a general $*$-algebra and let $\mathscr{A}(M)$ denote the Borchers-Uhlmann algebra of a linear Bosonic or Fermionic (gauge) field theory.

1. A state ω on $\mathfrak{A}$ is called *mixed*, if it is a convex linear combination of states, i.e. $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$, where $\lambda < 1$ and $\omega_i \neq \omega$ are states on $\mathfrak{A}$. A state is called *pure* if it is not mixed.
2. A state ω on $\mathscr{A}(M)$ is called *even*, if it is invariant under $\Phi(f) \mapsto -\Phi(f)$, i.e. it has vanishing n-point functions for all odd n.
3. An even state on $\mathscr{A}(M)$ is called *quasifree* or *Gaussian* if, for all even n,

$$\omega_n(f_1, \ldots, f_n) = \sum_{\pi_n \in S_n'} \prod_{i=1}^{n/2} \omega_2\left(f_{\pi_n(2i-1)}, f_{\pi_n(2i)}\right) .$$

   Here, S_n' denotes the set of ordered permutations of n elements, namely, the following two conditions are satisfied for $\pi_n \in S_n'$:

$$\pi_n(2i-1) < \pi_n(2i) \quad \text{for} \quad 1 \leq i \leq n/2 ,$$

$$\pi_n(2i-1) < \pi_n(2i+1) \quad \text{for} \quad 1 \leq i < n/2 .$$

4. Let α_t denote a one-parameter group of $*$-automorphisms on $\mathfrak{A}$, i.e. for arbitrary elements A, B of $\mathfrak{A}$,

$$\alpha_t\left(A^* B\right) = (\alpha_t(A))^* \alpha_t(B)\,, \qquad \alpha_t(\alpha_s(A)) = \alpha_{t+s}(A)\,, \qquad \alpha_0(A) = A\,.$$

A state ω on $\mathfrak{A}$ is called α_t*-invariant* if $\omega(\alpha_t(A)) = \omega(A)$ for all $A \in \mathfrak{A}$.

5. An α_t-invariant state ω on $\mathfrak{A}$ is said to satisfy the *KMS condition* for an inverse temperature $\beta = T^{-1} > 0$ if, for arbitrary elements A, B of $\mathfrak{A}$, the two functions

$$F_{AB}(t) \doteq \omega\left(B\alpha_t(A)\right)\,, \qquad G_{AB}(t) \doteq \omega\left(\alpha_t(A)B\right)$$

extend to functions $F_{AB}(z)$ and $G_{AB}(z)$ on the complex plane which are analytic in the strips $0 < \operatorname{Im} z < \beta$ and $-\beta < \operatorname{Im} z < 0$ respectively, continuous on the boundaries $\operatorname{Im} z \in \{0, \beta\}$, and fulfil

$$F_{AB}(t + i\beta) = G_{AB}(t)\,.$$

The KMS condition (after Kubo, Martin, and Schwinger) holds naturally for Gibbs states of *finite* systems in quantum statistical mechanics, i.e. for states that are given as $\omega_\beta(A) = \mathrm{Tr}\rho A$ with a density matrix $\rho = \exp(-\beta H)(\mathrm{Tr}\exp(-\beta H))^{-1}$, H the Hamiltonian operator of the system, and Tr denoting the trace over the respective Hilbert space. This follows by setting

$$\alpha_t(A) = e^{itH} A e^{-itH}\,,$$

making use of the cyclicity of the trace, and considering that $\exp(-\beta H)$ is bounded and has finite trace in the case of a finite system. In the thermodynamic limit, $\exp(-\beta H)$ does not possess these properties any more, but the authors of [64] have shown that the KMS condition is still a reasonable condition in this infinite-volume limit. Physically, KMS states are states which are in (thermal) equilibrium with respect to the time evolution encoded in the automorphism α_t. In general curved spacetimes, there is no 'time evolution' which acts as an automorphism on $\mathscr{A}(M)$. One could be tempted to introduce a time evolution by a canonical time-translation with respect to some time function of a globally hyperbolic spacetime. However, the causal propagator E^P will in general not be invariant under this time translation if the latter does not correspond to an isometry of (M, g). Hence, such time-translation would not result in an automorphism of $\mathscr{A}(M)$. There have been various proposals to overcome this problem and to define generalised notions of thermal equilibrium in curved spacetimes, see [119] for a review. Ground states (vacuum states) may be thought of as KMS states with inverse temperature $\beta = T^{-1} = \infty$.

Quasifree or Gaussian states which are in addition pure are closely related to the well-known Fock space picture in the sense that the GNS representation of a pure quasifree state is an irreducible representation on Fock space, see e.g. [78, Sect. 3.2]. In this sense, a pure quasifree state is in one-to-one correspondence to a specific definition of a 'particle'.

For the remainder of this chapter and most of the remainder of this monograph, the only model we shall discuss is the free neutral Klein-Gordon field for simplicity. However, all concepts we shall review will be applicable to more general models.

2.4 Hadamard States

The power of the algebraic approach lies in its ability to separate the algebraic relations of quantum fields from the Hilbert space representations of these relations and thus in some sense to treat *all* possible Hilbert space representations at once. However, the definition of an algebraic state reviewed in the previous subsection is too general and thus further conditions are necessary in order to select the physically meaningful states among all possible ones on $\mathscr{A}(M)$.

To this avail it seems reasonable to look at the situation in Minkowski spacetime. Physically interesting states there include the Fock vacuum state and associated multiparticle states as well as coherent states and states describing thermal equilibrium situations. All these states share the same ultraviolet (UV) properties, *i.e.* the same high-energy behaviour, namely they satisfy the so-called *Hadamard condition*, which we shall review in a few moments. A closer look at the formulation of quantum field theory in Minkowski spacetime reveals that the Hadamard condition is indeed essential for the mathematical consistency of QFT in Minkowski spacetime, as we would like to briefly explain now. In the following we will only discuss real scalar fields for simplicity. Analyses of Hadamard states for fields of higher spin can be found e.g. in [34, 43, 67, 107].

The Borchers-Uhlmann algebra $\mathscr{A}(M)$ of the free neutral Klein-Gordon field ϕ contains only very basic observables, namely, linear combinations of products of free fields at separate points, e.g. $\phi(x)\phi(y)$. However, if one wants to treat interacting fields in perturbation theory, or the backreaction of quantum fields on curved spacetimes via their stress-energy tensor, ones needs a notion of normal ordering, i.e. a way to define field monomials like $\phi^2(x)$ at the same point. To see that this requires some work, let us consider the massless scalar field in Minkowski spacetime. Its two point function reads

$$\omega_2(x, y) = \omega(\phi(x)\phi(y)) = \lim_{\varepsilon \downarrow 0} \frac{1}{4\pi^2} \frac{1}{(x-y)^2 + 2\,i\varepsilon(x_0 - y_0) + \varepsilon^2}\,, \tag{2.7}$$

where $(x-y)^2$ denotes the Minkowskian product induced by the Minkowski metric and the limit has to be understood as being performed after integrating ω_2 with at least one test function (weak limit). $\omega_2(x, y)$ is a smooth function if x and y are spacelike or timelike separated. It is singular at $(x-y)^2 = 0$, but the singularity is 'good enough' to give a finite result when smearing $\omega_2(x, y)$ with two test functions. Hence, ω_2 is a well-defined (tempered) distribution. Loosely speaking, this shows once more that the product of fields $\phi(x)\phi(y)$ is 'well-defined' at non-null related points. However, if we were to define $\phi^2(x)$ by some 'limit' like

$$\phi^2(x) \doteq \lim_{x \to y} \phi(x)\phi(y)\,,$$

the expectation value of the resulting object would 'blow up' and would not be any meaningful object. The well-known solution to this apparent problem is to define field monomials by appropriate regularising subtractions. For the squared field, this is achieved by setting

$$:\phi^2(x): \doteq \lim_{x\to y} \left(\phi(x)\phi(y) - \omega_2(x,y)\mathbb{I}\right) ,$$

where of course one would have to specify in which sense the limit should be taken. Omitting the details of this procedure, it seems still clear that the *Wick square* $:\phi^2(x):$ is a meaningful object, as it has a sensible expectation value, i.e. $\omega(:\phi^2(x):) = 0$. In the standard Fock space picture, one heuristically writes the field (operator) in terms of creation and annihilation operators in momentum space, i.e.

$$\phi(x) = \frac{1}{\sqrt{2\pi}^3} \int\limits_{\mathbb{R}^3} \frac{d\vec{k}}{\sqrt{2k_0}} \left(a^\dagger_{\vec{k}}\, e^{ikx} + a_{\vec{k}}\, e^{-ikx}\right) ,$$

and defines $:\phi^2(x):$ by writing the mode expansion of the product $\phi(x)\phi(y)$, 'normal ordering' the appearing products of creation and annihilation operators such that the creation operators are standing on the left hand side of the annihilation operators, and then finally taking the limit $x \to y$. It is easy to see that this procedure is equivalent to the above defined subtraction of the vacuum expectation value. However, having defined the Wick polynomials is not enough. We would also like to multiply them, i.e., we would like them to constitute an algebra. Using the mode-expansion picture, one can straightforwardly compute

$$:\phi^2(x)::\phi^2(y): = :\phi^2(x)\phi^2(y): + 4 :\phi(x)\phi(y): \omega_2(x,y) + 2\left(\omega_2(x,y)\right)^2 ,$$

which is a special case of the well-known *Wick theorem*, see for instance [76]. The right hand side of the above equation is a sensible object if the appearing square of the two-point function $\omega_2(x, y)$ is well-defined. In more detail, we know that $\omega_2(x, y)$ has singularities, and that these are integrable with test functions. Obviously, $(\omega_2(x, y))^2$ has singularities as well, and the question is whether the singularities are still good enough to be integrable with test functions. In terms of a mode decomposition, one could equivalently wonder whether the momentum space integrals appearing in the definition of $:\phi^2(x)\phi^2(y):$ via normal ordering creation and annihilation operators converge in a sensible way. The answer to these questions is 'yes' because of the energy positivity property of the Minkowskian vacuum state, and this is the reason why one usually never worries about whether normal ordering is well-defined in quantum field theory on Minkowski spacetime. In more detail, the Fourier decomposition of the massless two-point function ω_2 reads

$$\omega_2(x,y) = \lim_{\varepsilon\downarrow 0} \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^4} dk\ \Theta(k_0)\delta(k^2)\ e^{ik(x-y)} e^{-\varepsilon k_0} , \tag{2.8}$$

where $\Theta(k_0)$ denotes the Heaviside step function. We see that the Fourier transform of ω_2 has only support on the forward lightcone (or the positive mass shell in the massive case); this corresponds to the fact that we have associated the positive frequency modes to the creation operator in the above mode expansion of the quantum field. This insight allows to determine (or rather, define) the square of $\omega_2(x, y)$ by a convolution in Fourier space

$$
\begin{aligned}
(\omega_2(x, y))^2 &= \lim_{\varepsilon \downarrow 0} \frac{1}{(2\pi)^6} \int\limits_{\mathbb{R}^4} dq \int\limits_{\mathbb{R}^4} dp \ \Theta(q_0)\ \delta(q^2)\ \Theta(p_0)\ \delta(p^2)\ e^{i(q+p)(x-y)} e^{-\varepsilon(q_0+p_0)} \\
&= \lim_{\varepsilon \downarrow 0} \frac{1}{(2\pi)^6} \int\limits_{\mathbb{R}^4} dk \int\limits_{\mathbb{R}^4} dq \ \Theta(q_0)\ \delta(q^2)\ \Theta(k_0 - q_0)\ \delta((k-q)^2)\ e^{ik(x-y)} e^{-\varepsilon k_0} \,.
\end{aligned}
$$

Without going too much into details here, let us observe that the above expression can only give a sensible result (a distribution) if the integral over q converges, i.e. if the integrand is rapidly decreasing in q. To see that this is the case, note that for an arbitrary but fixed k and large q where here 'large' is meant in the Euclidean norm on $\mathbb{R}^4$, the integrand is vanishing on account of $\delta(q^2)$ and $\Theta(k_0 - q_0)$ as $k_0 - q_0 < 0$ for large q. Loosely speaking, we observe the following: by the form of a convolution, the Fourier transform of ω_2 is multiplied by the same Fourier transform, but with negative momentum. Since the ω_2 has only Fourier support in one 'energy direction', namely the positive one, the intersection of its Fourier support and the same support evaluated with negative momentum is compact, and the convolution therefore well-defined. Moreover, as this statement only relies on the large momentum behaviour of Fourier transforms, it holds equally in the case of massive fields, as the mass shell approaches the light cone for large momenta.

The outcome of the above considerations is the insight that, if we want to define a sensible generalisation of normal ordering in curved spacetimes, we have to select states whose two-point functions are singular, but regular enough to allow for point-wise multiplication. Even though general curved spacetimes are not translationally invariant and therefore do not allow to define a global Fourier transform and a related global energy positivity condition, one could think that this task can be achieved by some kind of a 'local Fourier transform' and a related 'local energy positivity condition' because only the 'large momentum behaviour' is relevant. In fact, as showed in the pioneering work of Radzikowski [103, 104], this heuristic idea can be made precise in terms of *microlocal analysis*, a modern branch of Mathematics. Microlocal analysis gives a rigorous way to define the 'large momentum behaviour' of a distribution in a coordinate-independent manner and in the aforementioned works [103, 104], it has been shown that so-called *Hadamard states*, which have already been known to allow for a sensible renormalisation of the stress-energy tensor [120, 121, 123], indeed fulfil a local energy positivity condition in the sense that their two-point function has a specific *wave front set*. Based on this, Brunetti, Fredenhagen, Köhler, Hollands, and Wald [18, 19, 70–72] have been able to show that one can as a matter of fact define normal ordering and perturbative interacting quantum field theories based on Hadamard states essentially in the same way as on Minkowski spacetimes.

Though, it turned out that there is a big conceptual difference to flat spacetime quantum field theories, namely, new regularisation freedoms in terms of curvature terms appear. Although these are finitely many, and therefore lead to the result that theories which are perturbatively renormalisable in Minkowski spacetime retain this property in curved spacetimes [19, 70], the appearance of this additional renormalisation freedom may have a profound impact on the backreaction of quantum fields on curved spacetimes, as we will discuss in the last chapter of this monograph.

As we have already seen at the example of the massless Minkowski vacuum, Hadamard states can be approached from two angles. One way to discuss them is to look at the concrete realisation of their two-point function in 'position space'. This treatment has lead to the insight that Hadamard states are the sensible starting point for the definition of a regularised stress-energy tensor [120, 121, 123], and it is well-suited for actual calculations in particular. On the other hand, the rather abstract study of Hadamard states based on microlocal analysis is useful in order to tackle and solve conceptual problems. Following our discussion of the obstructions in the definition of normal ordering, we shall start our treatment by considering the microlocal aspects of Hadamard states. A standard monograph on microlocal analysis is the book of Hörmander [75], who has also contributed a large part to this field of Mathematics [40, 74]. Introductory treatments can be found in [19, 83, 112, 115].

Let us start be introducing the notion of a wave front set. To motivate it, let us recall that a smooth function on $\mathbb{R}^m$ with compact support has a rapidly decreasing Fourier transform. If we take an distribution u in $\Gamma_0'(\mathbb{R}^m)$ and multiply it by an $f \in \Gamma_0(\mathbb{R}^m)$ with $f(x_0) \neq 0$, then uf is an element of $\Gamma'(\mathbb{R}^m)$, i.e., a distribution with compact support. If fu were smooth, then its Fourier transform $\widehat{fu}$ would be smooth and rapidly decreasing. The failure of fu to be smooth in a neighbourhood of x_0 can therefore be quantitatively described by the set of directions in Fourier space where $\widehat{fu}$ is not rapidly decreasing. Of course it could happen that we choose f badly and therefore 'cut' some of the singularities of u at x_0. To see the full singularity structure of u at x_0, we therefore need to consider all test functions which are non-vanishing at x_0. With this in mind, one first defines the wave front set of distributions on $\mathbb{R}^m$ and then extends it to curved manifolds in a second step.

Definition 2.10 A neighbourhood Γ of $k_0 \in \mathbb{R}^m$ is called *conic* if $k \in \Gamma$ implies $\lambda k \in \Gamma$ for all $\lambda \in (0, \infty)$. Let $u \in \Gamma_0'(\mathbb{R}^m)$. A point $(x_0, k_0) \in \mathbb{R}^m \times (\mathbb{R}^m \setminus \{0\})$ is called a regular directed point of u if there is an $f \in \Gamma_0(\mathbb{R}^m)$ with $f(x_0) \neq 0$ such that, for every $n \in \mathbb{N}$, there is a constant $C_n \in \mathbb{R}$ fulfilling

$$|\widehat{fu}(k)| \leq C_n(1 + |k|)^{-n}$$

for all k in a conic neighbourhood of k_0. The *wave front set* $\mathrm{WF}(u)$ is the complement in $\mathbb{R}^m \times (\mathbb{R}^m \setminus \{0\})$ of the set of all regular directed points of u.

We immediately state a few important properties of wave front sets, the proofs of which can be found in [75] (see also [112]).

Theorem 2.6 *Let $u \in \Gamma_0'(\mathbb{R}^m)$.*

(a) If u is smooth, then $\mathrm{WF}(u)$ *is empty.*
(b) Let P be an arbitrary partial differential operator. It holds

$$\mathrm{WF}(Pu) \subset \mathrm{WF}(u)\,.$$

(c) Let $U, V \subset \mathbb{R}^m$, let $u \in \Gamma_0'(V)$, and let $\chi : U \to V$ be a diffeomorphism. The pull-back $\chi^*(u)$ of u defined by $\chi^* u(f) = u(\chi_* f)$ for all $f \in \Gamma_0(U)$ fulfils

$$\mathrm{WF}(\chi^* u) = \chi^* \mathrm{WF}(u) \doteq \left\{(\chi^{-1}(x), \chi^* k) \mid (x, k) \in \mathrm{WF}(u)\right\}\,,$$

where $\chi^* k$ denotes the push-forward of χ in the sense of cotangent vectors. *Hence, the wave front set transforms covariantly under diffeomorphisms as an element of $T^*\mathbb{R}^m$, and we can extend its definition to distributions on general curved manifolds M by patching together wave front sets in different coordinate patches of M. As a result, for $u \in \Gamma_0'(M)$,* $\mathrm{WF}(u) \subset T^*M \setminus \{\mathbf{0}\}$, *where* $\mathbf{0}$ *denotes the zero section of T^*M.*
(d) Let $u_1, u_2 \in \Gamma_0'(M)$ and let

$$\mathrm{WF}(u_1) \oplus \mathrm{WF}(u_2) \doteq \{(x, k_1 + k_2) \mid (x, k_1) \in \mathrm{WF}(u_1),\ (x, k_2) \in \mathrm{WF}(u_2)\}\,.$$

If $\mathrm{WF}(u_1) \oplus \mathrm{WF}(u_2)$ *does not intersect the zero section, then one can define the product $u_1 u_2$ in such a way that it yields a well-defined distribution in $\Gamma_0'(M)$ and that it reduces to the standard pointwise product of smooth functions if u_1 and u_2 are smooth. Moreover, the wave front set of such product is bounded in the following way*

$$\mathrm{WF}(u_1 u_2) \subset \mathrm{WF}(u_1) \cup \mathrm{WF}(u_2) \cup (\mathrm{WF}(u_1) \oplus \mathrm{WF}(u_2))\,.$$

Note that the wave front set transforms as a subset of the cotangent bundle on account of the covector nature of k in $\exp(ikx)$. The last of the above statements is exactly the criterion for pointwise multiplication of distributions we have been looking for. Namely, from (2.8) and (2.7) one can infer that the wave front set of the Minkowskian two-point function (for $m \geq 0$) is [115]

$$\mathrm{WF}(\omega_2) = \left\{(x, y, k, -k) \in T^*\mathbb{M}^2 \mid x \neq y,\ (x-y)^2 = 0,\ k||(x-y),\ k_0 > 0\right\} \tag{2.9}$$
$$\cup \left\{(x, x, k, -k) \in T^*\mathbb{M}^2 \mid k^2 = 0,\ k_0 > 0\right\}\,,$$

particularly, it is the condition $k_0 > 0$ which encodes the energy positivity of the Minkowskian vacuum state. We can now rephrase our observation that the pointwise square of $\omega_2(x, y)$ is a well-defined distribution by noting that $\mathrm{WF}(\omega_2) \oplus \mathrm{WF}(\omega_2)$ does not contain the zero section. In contrast, we know that the δ-distribution $\delta(x)$ is singular at $x = 0$ and that its Fourier transform is a constant. Hence, its wave front set reads

$$\mathrm{WF}(\delta) = \{(0, k) \mid k \in \mathbb{R} \setminus \{0\}\} ,$$

and we see that the δ-distribution does not have a 'one-sided' wave front set and, hence, can not be squared. The same holds if we view δ as a distribution $\delta(x, y)$ on $\Gamma_0(\mathbb{R}^2)$. Then

$$\mathrm{WF}(\delta(x, y)) = \{(x, x, k, -k) \mid k \in \mathbb{R} \setminus \{0\}\} .$$

The previous discussion suggests that a generalisation of (2.9) to curved spacetimes is the sensible requirement to select states which allow for the construction of Wick polynomials. We shall now define such a generalisation.

Definition 2.11 Let ω be a state on $\mathscr{A}(M)$. We say that ω fulfils the *Hadamard condition* and is therefore a *Hadamard state* if its two-point function ω_2 fulfils

$$\mathrm{WF}(\omega_2) = \left\{(x, y, k_x, -k_y) \in T^*M^2 \setminus \{\mathbf{0}\} \mid (x, k_x) \sim (y, k_y),\ k_x \rhd 0\right\} .$$

Here, $(x, k_x) \sim (y, k_y)$ implies that there exists a null geodesic c connecting x to y such that k_x is coparallel and cotangent to c at x and k_y is the parallel transport of k_x from x to y along c. Finally, $k_x \rhd 0$ means that the covector k_x is future-directed.

Having discussed the rather abstract aspect of Hadamard states, let us now turn to their more concrete realisations. To this avail, let us consider a geodesically convex set $\mathscr{O}$ in (M, g), see Sect. 2.1. By definition, there are open subsets $\mathscr{O}'_x \subset T_xM$ such that the exponential map $\exp_x : \mathscr{O}'_x \to \mathscr{O}$ is well-defined for all $x \in \mathscr{O}$, i.e. we can introduce Riemannian normal coordinates on $\mathscr{O}$. For any two points $x, y \in \mathscr{O}$, we can therefore define the *half squared geodesic distance* $\sigma(x, y)$ as

$$\sigma(x, y) \doteq \frac{1}{2} g\left(\exp_x^{-1}(y), \exp_x^{-1}(y)\right) .$$

This entity is sometimes also called *Synge's world function* and is both smooth and symmetric on $\mathscr{O} \times \mathscr{O}$. Moreover, one can show that it fulfils the following identity

$$\sigma_{;\mu}\sigma_{;}^{\ \mu} = 2\sigma , \tag{2.10}$$

where the covariant derivatives are taken with respect to x (even though this does not matter by the symmetry of σ), see for instance [57, 102]. Let us introduce a couple of standard notations related to objects on $\mathscr{O} \times \mathscr{O}$ such as σ. If $\mathscr{V}$ and $\mathscr{W}$ are vector bundles over M with typical fibers constituted by the vector spaces V and W respectively, then we denote by $\mathscr{V} \boxtimes \mathscr{W}$ the *exterior tensor product* of $\mathscr{V}$ and $\mathscr{W}$. $\mathscr{V} \boxtimes \mathscr{W}$ is defined as the vector bundle over $M \times M$ with typical fibre $V \otimes W$. The more familiar notion of the tensor product bundle $\mathscr{V} \otimes \mathscr{W}$ is obtained by considering the pull-back bundle of $\mathscr{V} \boxtimes \mathscr{W}$ with respect to the map $M \ni x \mapsto (x, x) \in M^2$.

Typical exterior product bundles are for instance the tangent bundles of Cartesian products of M, e.g. $T^*M \boxtimes T^*M = T^*M^2$. A section of $\mathscr{V} \boxtimes \mathscr{W}$ is called a *bitensor*. We introduce the *Synge bracket notation* for the coinciding point limits of a bitensor. Namely, let B be a smooth section of $\mathscr{V} \boxtimes \mathscr{W}$. We define

$$[B](x) \doteq \lim_{y \to x} B(x, y) .$$

With this definition, $[B]$ is a section of $\mathscr{V} \otimes \mathscr{W}$. In the following, we shall denote by unprimed indices tensorial quantities at x, while primed indices denote tensorial quantities at y. As an example, let us state the well-known *Synge rule*, proved for instance in [23, 102].

Lemma 2.4 *Let B be an arbitrary smooth bitensor. Its covariant derivatives at x and y are related by* Synge's rule. *Namely,*

$$[B_{;\mu'}] = [B]_{\mu} - [B_{;\mu}] .$$

Particularly, let $\mathscr{V}$ be a vector bundle, let f_a be a local frame of $\mathscr{V}$ defined on $\mathscr{O} \subset M$ and let $x, y \in \mathscr{O}$. If B is symmetric*, i.e. the coefficients $B_{ab'}(x, y)$ of*

$$B(x, y) \doteq B^{ab'}(x, y)\ f_a(x) \otimes f_{b'}(y)$$

fulfil

$$B^{ab'}(x, y) = B^{b'a}(y, x) ,$$

then

$$[B_{;\mu'}] = [B_{;\mu}] = \frac{1}{2}[B]_{;\mu} .$$

The half squared geodesic distance is a prototype of a class of bitensors of which we shall encounter many in the following. Namely, σ fulfils a partial differential equation (2.10) which relates its higher order derivatives to lower order ones. Hence, given the initial conditions

$$[\sigma] = 0 , \qquad [\sigma_{;\mu}] = 0 , \qquad [\sigma_{;\mu\nu}] = g_{\mu\nu}$$

which follow from the very definition of σ, one can compute the coinciding point limits of its higher derivatives by means of an inductive procedure, see for instance [23, 37, 56, 102]. As an example, in the case of $[\sigma_{;\mu\nu\rho}]$, one differentiates (2.10) three times and then takes the coinciding point limit. Together with the already known relations, one obtains

$$[\sigma_{;\mu\nu\rho}] = 0 .$$

At a level of fourth derivative, the same procedure yields a linear combination of three coinciding fourth derivatives, though with different index orders. To relate those, one has to commute derivatives to rearrange the indices in the looked-for fashion, and this ultimately leads to the appearance of Riemann curvature tensors and therefore to

$$[\sigma_{;\mu\nu\rho\tau}] = -\frac{1}{3}(R_{\mu\rho\nu\tau} + R_{\mu\tau\nu\rho})\,.$$

A different bitensor of the abovementioned kind we shall need in the following is the *bitensor of parallel transport* $g^{\mu}_{\rho'}(x, y)$. Namely, given a geodesically convex set $\mathscr{O}$, $x, y \in \mathscr{O}$, and a vector $v = v^{\mu'}\partial_{\mu'}$ in T_yM, the parallel transport of v from y to x along the unique geodesic in $\mathscr{O}$ connecting x and y is given by the vector $\tilde{v}$ in T_xM with components

$$\tilde{v}^{\mu} = g^{\mu}_{\rho'}v^{\rho'}\,.$$

This definition of the bitensor of parallel transport entails

$$[g^{\mu}_{\rho'}] = \delta^{\mu}_{\rho}\,, \qquad g^{\mu}_{\rho';\alpha}\sigma_{;}^{\ \alpha} = 0\,, \qquad g^{\mu}_{\rho'}\sigma_{;}^{\ \rho'} = -\sigma_{;}^{\ \mu}\,.$$

In fact, the first two identities can be taken as the defining partial differential equation of $g^{\mu}_{\rho'}$ and its initial condition (one can even show that the mentioned partial differential equation is an ordinary one). Out of these, one can obtain by the inductive procedure outlined above

$$[g^{\mu}_{\rho';\alpha}] = 0\,, \qquad [g^{\mu}_{\rho';\alpha\beta}] = \frac{1}{2}R^{\mu}_{\ \ \nu\alpha\beta}\,.$$

With these preparations at hand, let us now provide the explicit form of Hadamard states.

Definition 2.12 Let ω_2 be the two-point function of a state on $\mathscr{A}(M)$, let t be a time function on (M, g), let

$$\sigma_\varepsilon(x, y) \doteq \sigma(x, y) + 2i\varepsilon(t(x) - t(y)) + \varepsilon^2\,,$$

and let λ be an arbitrary length scale. We say that ω_2 if of *local Hadamard form* if, for every $x_0 \in M$ there exists a geodesically convex neighbourhood $\mathscr{O}$ of x_0 such that $\omega_2(x, y)$ on $\mathscr{O} \times \mathscr{O}$ is of the form

$$\begin{aligned}\omega_2(x, y) &= \lim_{\varepsilon\downarrow 0}\frac{1}{8\pi^2}\left(\frac{u(x, y)}{\sigma_\varepsilon(x, y)} + v(x, y)\log\left(\frac{\sigma_\varepsilon(x, y)}{\lambda^2}\right) + w(x, y)\right)\\ &\doteq \lim_{\varepsilon\downarrow 0}\frac{1}{8\pi^2}\left(h_\varepsilon(x, y) + w(x, y)\right)\,.\end{aligned}$$

Here, the *Hadamard coefficients* u, v, and w are smooth, real-valued biscalars, where v is given by a series expansion in σ as

$$v = \sum_{n=0}^{\infty} v_n \sigma^n$$

with smooth biscalar coefficients v_n. The bidistribution h_ε shall be called *Hadamard parametrix*, indicating that it solves the Klein-Gordon equation up to smooth terms.

Note that the above series expansion of v does not necessarily converge on general smooth spacetimes, however, it is known to converge on analytic spacetimes [58]. One therefore often truncates the series at a finite order n and asks for the w coefficient to be only of regularity C^n, see [78]. Moreover, the local Hadamard form is special case of the *global Hadamard form* defined for the first time in [78]. The definition of the global Hadamard form in [78] assures that there are no (spacelike) singularities in addition to the lightlike ones visible in the local form and, moreover, that the whole concept is independent of the chosen time function t. However, as proven by Radzikowski in [104] employing the microlocal version of the Hadamard condition, the local Hadamard form already implies the global Hadamard form on account of the fact that ω_2 must be positive, have the causal propagator E as its antisymmetric part, and fulfil the Klein-Gordon equation in both arguments. It is exactly this last fact which serves to determine the Hadamard coefficients u, v, and w by a recursive procedure.

To see this, let us omit the subscript ε and the scale λ in the following, since they do not influence the result of the following calculations, and let us denote by P_x the Klein-Gordon operator $P = -\Box + \xi R + m^2$ acting on the x-variable. Applying P_x to h, we obtain potentially singular terms proportional to σ^{-n} for $n = 1, 2, 3$ and to $\log \sigma$, as well as smooth terms proportional to positive powers of σ. We know, however, that the total result is smooth because $P_x(h + w) = 0$ since ω_2 is a bisolution of the Klein-Gordon equation and w is smooth. Consequently, the potentially singular terms in $P_x h$ have to vanish identically at each order in σ and $\log \sigma$. This immediately implies

$$P_x v = 0 \,. \tag{2.11}$$

and, further, the following recursion relations

$$- P_x u + 2 v_{0;\mu} \sigma^\mu + (\Box_x \sigma - 2) v_0 = 0 \,, \tag{2.12}$$

$$2 u_{;\mu} \sigma^\mu + (\Box_x \sigma - 4) u = 0 \,, \tag{2.13}$$

$$- P_x v_n + 2(n+1) v_{n+1;\mu} \sigma_{;}^{\ \mu} + (n+1) \left(\Box_x \sigma + 2n\right) v_{n+1} = 0 \,, \quad \forall n \geq 0 \,. \tag{2.14}$$

To solve these recursive partial differential equations, let us now focus on (2.13). Since the only derivative appearing in this equation is the derivative along the geodesic connecting x and y, (2.13) is in fact an ordinary differential equation with respect to the affine parameter of the mentioned geodesic. u is therefore uniquely determined once a suitable initial condition is given. Comparing the Hadamard form with the Minkowskian two-point function (2.7), the initial condition is usually chosen as

$$[u] = 1\,,$$

which leads to the well-known result that u is given by the square root of the so-called *Van Vleck-Morette* determinant, see for instance [23, 37, 56, 102]. Similarly, given u, the differential equation (2.12) is again an ordinary one with respect to the geodesic affine parameter, and it can be immediately integrated since taking the coinciding point limit of (2.12) and inserting the properties of σ yields the initial condition

$$[v_0] = \frac{1}{2}[P_x u]\,.$$

It is clear how this procedure can be iterated to obtain solutions for all v_n. Particularly, one obtains the initial conditions

$$[v_{n+1}] = \frac{1}{2(n+1)(n+2)}[P_x v_n]$$

for all $n > 0$. Moreover, one finds that u depends only on the local geometry of the spacetime, while the v_n and, hence, v depend only on the local geometry and the parameters appearing in the Klein-Gordon operator P, namely, the mass m and the coupling to the scalar curvature ξ. These observations entail that the state dependence of ω_2 is encoded in the smooth biscalar w, which furthermore has to be symmetric because it is bound to vanish in the difference of two-point functions yielding the antisymmetric causal propagator E, *viz.*

$$\omega_2(x, y) - \overline{\omega_2(x, y)} = \omega_2(x, y) - \omega_2(y, x) = iE(x, y)\,.$$

More precisely, this observation ensues from the following important result obtained in [89, 90].

Theorem 2.7 *The Hadamard coefficients v_n are symmetric biscalars.*

This theorem proves the folklore knowledge that the causal propagator E is locally given by

$$iE = \lim_{\varepsilon \downarrow 0} \frac{1}{8\pi^2}(h_\varepsilon - h_{-\varepsilon})\,.$$

Even though we can in principle obtain the v_n as unique solutions of ordinary differential equations, we shall only need their coinciding point limits and coinciding points limit of their derivatives in what follows. In this respect, the symmetry of the v_n will prove very valuable in combination with Lemma 2.4. In fact, employing the Hadamard recursion relations, we find the following results [91].

Lemma 2.5 *The following identities hold for the Hadamard parametrix $h(x, y)$*

$$[P_x h] = [P_y h] = -6[v_1]\,, \quad [(P_x h)_{;\mu}] = [(P_y h)_{;\mu'}] = -4[v_1]_{;\mu}\,,$$

$$[(P_x h)_{;\mu'}] = [(P_y h)_{;\mu}] = -2[v_1]_{;\mu}\,.$$

It is remarkable that these rather simple computations will be essentially sufficient for the construction of a conserved stress-energy tensor of a free scalar quantum field [91]. Particularly, the knowledge of the explicit form of, say, $[v_1]$ is not necessary to accomplish such a task. However, if one is interested in computing the actual backreaction of a scalar field on curved spacetimes, one needs the explicit form of $[v_1]$. One can compute this straightforwardly by the inductive procedure already mentioned at several occasions and the result is [36, 91]

$$\begin{aligned}[v_1] &= \frac{m^4}{8} + \frac{(6\xi-1)\,m^2 R}{24} + \frac{(6\xi-1)\,R^2}{288} + \frac{(1-5\xi)\Box R}{120} \\ &\quad - \frac{R_{\alpha\beta}R^{\alpha\beta}}{720} + \frac{R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}}{720} \\ &= \frac{m^4}{8} + \frac{(6\xi-1)\,m^2 R}{24} + \frac{(6\xi-1)\,R^2}{288} + \frac{(1-5\xi)\Box R}{120} \\ &\quad + \frac{C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} + R_{\alpha\beta}R^{\alpha\beta} - \frac{R^2}{3}}{720}\,.\end{aligned} \tag{2.15}$$

The Hadamard coefficients are related to the so-called *DeWitt-Schwinger* coefficients, see for instance [35, 89, 90], which stem from an *a priori* completely different expansion of two-point functions. The latter have been computed for the first time in [23, 24] and can also be found in many other places like, e.g. [35, 56].

Having discussed the Hadamard form to a large extent, let us state the already anticipated equivalence result obtained by Radzikowski in [103]. See also [107] for a slightly different proof, which closes a gap in the proof of [103].

Theorem 2.8 *Let ω_2 be the two-point function of a state on $\mathscr{A}(M)$. ω_2 fulfils the Hadamard condition of Definition 2.11 if and only if it is of global Hadamard form.*

By the result of [104], that a state which is locally of Hadamard form is already of global Hadamard form, we can safely replace 'global' by 'local' in the above theorem. Moreover, from the above discussion it should be clear that the two-point functions of two Hadamard states differ by a smooth and symmetric biscalar.

In past works on (algebraic) quantum field theory in curved spacetimes, one has often considered only on quasifree Hadamard states. For non-quasifree states, a more general *microlocal spectrum condition* has been proposed in [18] which requires certain wave front set properties of the higher order n-point functions of a non-quasifree state. However, as shown in [108, 109], the Hadamard condition of the two-point function of a non-quasifree state alone already determines the singularity structure of all higher order n-point functions by the CCR. It is therefore sufficient to specify the singularity structure of ω_2 also in the case of non-quasifree states. Note however, that certain technical results on the structure of Hadamard states have up to now only been proven for the quasifree case [117].

We close the general discussion of Hadamard states by providing examples and non-examples.

Examples of Hadamard states

1. Given a Hadamard state ω on $\mathscr{A}(M)$, any 'finite excitation of ω' is again Hadamard, i.e. for all $A \in \mathscr{A}(M)$, ω_A defined for all $B \in \mathscr{A}(M)$ by $\omega_A(B) \doteq \omega(A^* B A)/\omega(A^* A)$ is Hadamard [109].
2. All vacuum states and KMS (thermal equilibrium) states on ultrastatic spacetimes (i.e. spacetimes with a metric $ds^2 = -dt^2 + h_{ij} dx^i dx^j$, with h_{ij} not depending on time) are Hadamard states [55, 106].
3. Based on the previous statement, it has been proven in in [55] that Hadamard states exist on *any* globally hyperbolic spacetime by means of a spacetime deformation argument.
4. The *Bunch-Davies state* on de Sitter spacetime is a Hadamard state [2, 30, 31]. It has been shown in [30, 31] that this result can be generalised to asymptotically de Sitter spacetimes, where distinguished Hadamard states can be constructed by means of a holographic argument; these states are generalisations of the Bunch-Davies state in the sense that the aforementioned holographic construction yields the Bunch-Davies state in de Sitter spacetime.
5. Similar holographic arguments have been used in [28, 34, 92, 93] to construct distinguished Hadamard states on asymptotically flat spacetimes, to rigorously construct the Unruh state in Schwarzschild spacetimes and to prove that it is Hadamard in [29], to construct asymptotic vacuum and thermal equilibrium states in certain classes of Friedmann-Robertson-Walker spacetimes in-see [27] and the next chapter—and to construct Hadamard states in bounded regions of any globally hyperbolic spacetime in [32].
6. A interesting class of Hadamard states in general Friedmann-Robertson-Walker are the *states of low energy* constructed in [95]. These states minimise the energy density integrated in time with a compactly supported weight function and thus loosely speaking minimise the energy in the time interval specified by the support of the weight function. This construction has been generalised to encompass almost equilibrium states in [84] and to expanding spacetimes with less symmetry in [114]. We shall review the construction of these states in the next chapter.
7. A construction of Hadamard states which is loosely related to states of low energy has been given in [15]. There the authors consider for a given spacetime (M, g) with the spacetime (N, g) where N is a finite-time slab of M. Given a smooth timelike-compact function f on M which is identically 1 on N, one considers $A \doteq i f E f$ which can be shown to be a bounded and self-adjoint operator on $L^2(N, d_g x)$. The positive part A^+ of A constructed with standard functional calculus defines a two-point function of a quasifree state ω on $\mathscr{A}(N)$ via $\omega_2(f, g) \doteq \langle f, A^+ g \rangle$ which can be shown to be Hadamard (at least on

classes of spacetimes) [15]. Taking for f the characteristic function of N gives the Sorkin-Johnston states proposed in [1] which are in general not Hadamard [45].

8. Hadamard states which possess an approximate local thermal interpretation have been constructed in [111], see [119] for a review.
9. Given a Hadamard state ω on the algebra $\mathscr{A}(M)$ and a smooth solution Ψ of the field equation $P\Psi = 0$, one can construct a coherent state by redefining the quantum field $\phi(x)$ as $\phi(x) \mapsto \phi(x) + \Psi(x)\mathbb{I}$. The thus induced coherent state has the two-point function $\omega_{\Psi,2}(x, y) = \omega_2(x, y) + \Psi(x)\Psi(y)$, which is Hadamard since $\Psi(x)$ is smooth.
10. A construction of Hadamard states via pseudodifferential calculus was developed in [59].

Non-examples of Hadamard states

1. The so-called *α-vacua* in de Sitter spacetime [2] violate the Hadamard condition as shown in [20].
2. As already mentioned the *Sorkin-Johnston states* proposed in [1] are in general not Hadamard [45].
3. A class of states related to Hadamard states, but in general not Hadamard, is constituted by *adiabatic states*. These have been introduced in [96] and put on rigorous grounds by [86]. Effectively, they are states which approximate ground states if the curvature of the background spacetime is only slowly varying. In [77], the concept of adiabatic states has been generalised to arbitrary curved spacetimes. There, it has also been displayed in a quantitative way how adiabatic states are related to Hadamard states. Namely, an adiabatic state of a specific order n has a certain *Sobolev wave front set* (in contrast to the C^∞ wave front set introduced above) and hence, loosely speaking, it differs from a Hadamard state by a biscalar of finite regularity C^n. In this sense, Hadamard states are adiabatic states of 'infinite order'. We will review the concept of adiabatic states in the next chapter.

Finally, let us remark that one can define the Hadamard form also in spacetimes with dimensions differing from 4, see for instance [91, 107]. Moreover, the proof of the equivalence of the concrete Hadamard form and the microlocal Hadamard condition also holds in arbitrary spacetime dimensions, as shown in [107]. A recent detailed exposition of Hadamard states may be found in [81].

2.5 Locality and General Covariance

And important aspect of QFT on curved spacetimes is the backreaction of quantum fields in curved spacetimes, i.e. the effect of quantum matter-energy on the curvature of spacetime. This of course necessitates the ability to define quantum field theory on a curved spacetime *without knowing the curved spacetime beforehand*. It is therefore advisable to employ only generic properties of spacetimes in the construction of quantum fields. This entails that we have to formulate a quantum field theory in a *local* way, i.e. only employing local properties of the underlying curved manifold. In addition, we would like to take into account the diffeomorphism-invariance of General Relativity and therefore construct *covariant* quantum fields. This concept of a *locally covariant quantum field theory* goes back to many works, of which the first one could mention is [38], followed by many others such as [123, Chap. 4.6] and [70, 118]. Building on these works, the authors of [21] have given the first complete definition of a locally covariant quantum field theory.

As shown in [21], giving such a definition in precise mathematical terms requires the language of *category theory*, a branch of mathematics which basically aims to unify *all* mathematical structures into one coherent picture. A category is essentially a class $\mathfrak{C}$ of *objects* denoted by $obj(\mathfrak{C})$, with the property that, for each two objects A, B in $\mathfrak{C}$ there is (at least) one *morphism* or *arrow* $\phi : A \to B$ relating A and B. The collection of all such arrows is denoted by $hom_{\mathfrak{C}}(A, B)$. Morphisms relating a chain of three objects are required to be associative with respect to compositions, and one demands that each object has an *identity morphism* $id_A : A \to A$ which leaves all morphisms $\phi : A \to B$ starting from A invariant upon composition, i.e. $\phi \circ id_A = \phi$. An often cited simple example of a category is the category of sets $\mathfrak{Set}$. The objects of $\mathfrak{Set}$ are sets, while the morphism are maps between sets, the identity morphism of an object just being the identity map of a set. Given two categories $\mathfrak{C}_1$ and $\mathfrak{C}_2$, a *functor* $F : \mathfrak{C}_1 \to \mathfrak{C}_2$ is a map between two categories which maps objects to objects and morphisms to morphisms such that identity morphisms in $\mathfrak{C}_1$ are mapped to identity morphism in $\mathfrak{C}_2$ and the composition of morphisms is preserved under the mapping. This paragraph was only a very brief introduction to category theory and we refer the reader to the standard monograph [87] and to the introduction in [113, Sect. 1.7] for further details. A locally covariant quantum field theory according to [21] should be a functor from a category of spacetimes to a category of suitable algebras. The first step in understanding such a construction if of course the definition of a suitable category of spacetimes.

We have already explained in the previous sections of this chapter that four-dimensional, oriented and time-oriented, globally hyperbolic spacetimes are the physically sensible class of spacetimes among all curved Lorentzian manifolds. It is therefore natural to take them as the objects of a potential category of spacetimes. Regarding the morphisms, one could think of various possibilities to select them among all possible maps between the spacetimes under consideration. However, to be able to emphasise the local nature of a quantum field theory, we shall take embeddings between spacetimes. This will allow us to require locality by asking that a quantum field theory on a 'small' spacetime can be easily embedded into a larger spacetime without 'knowing anything' about the remainder of the larger spacetime. Moreover, a sensible quantum field theory will depend on the orientation and time-orientation and the causal structure of the underlying manifold, we should therefore only consider embeddings that preserve these structures. To this avail, the authors in [21] have chosen isometric embeddings with causally convex range (see Sect. 2.1 regarding an explanation of these notions), but since the causal structure of a spacetime is left invariant by conformal transformations, one could also choose conformal embeddings, as done in [98]. We will nevertheless follow the choice of [21], since it will be sufficient for our purposes. Let us now subsume the above considerations in a definition.

Definition 2.13 The *category of spacetimes* $\mathfrak{Man}$ is the category having as its class of objects *obj*($\mathfrak{Man}$) the globally hyperbolic, four-dimensional, oriented and time-oriented spacetimes (M, g). Given two spacetimes (M_1, g_1) and (M_2, g_2) in *obj*($\mathfrak{Man}$), the considered morphisms $hom_{\mathfrak{Man}}((M_1, g_1), (M_2, g_2))$ are isometric embeddings $\chi : (M_1, g_1) \hookrightarrow (M_2, g_2)$ preserving the orientation and time-orientation and having causally convex range $\chi(M_1)$. Moreover, the identity morphism $id_{(M,g)}$ of a spacetime in *obj*($\mathfrak{Man}$) is just the identity map of M and the composition of morphisms is defined as the usual composition of embeddings.

The just defined category is sufficient to discuss locally covariant Bosonic quantum field theories. However, for Fermionic quantum field theories, one needs a category which incorporates spin structures as defined in [108, 118]. At this point we briefly remark that our usage of the words 'Boson' and 'Fermion' for integer and half-integer spin fields respectively is allowed on account of the spin-statistics theorem in curved spacetimes proved in [118], see also [41] for a more recent and general work.

To introduce the notion of a locally covariant quantum field theory and the related concept of a locally covariant quantum field, we need a few categories in addition to the one introduced above. By $\mathfrak{TAlg}$ we denote the category of unital topological $*$-algebras, where for two $\mathscr{A}_1$, $\mathscr{A}_2$ in obj($\mathfrak{TAlg}$), the considered morphisms $\hom_{\mathfrak{TAlg}}(\mathscr{A}_1, \mathscr{A}_2)$ are continuous, unit-preserving, injective $*$-homomorphisms. In addition, we introduce the category $\mathfrak{Test}$ of test function spaces $\Gamma_0(M)$ of objects (M, g) in $\mathfrak{Man}$, where here the morphisms $\hom_{\mathfrak{Test}}(\Gamma_0(M_1), \Gamma_0(M_2))$ are push-forwards χ_* of the isometric embeddings $\chi : M_1 \hookrightarrow M_2$. In fact, by $\mathscr{D}$ we shall denote the functor between $\mathfrak{Man}$ and $\mathfrak{Test}$ which assigns to a spacetime (M, g) in $\mathfrak{Man}$ its test function space $\Gamma_0(M)$ and to a morphism in $\mathfrak{Man}$ its push-forward. For reasons of nomenclature, we consider $\mathfrak{TAlg}$ and $\mathfrak{Test}$ as subcategories of the category $\mathfrak{Top}$ of all topological spaces with morphisms given by continuous maps. Let us now state the first promised definition.

Definition 2.14 A *locally covariant quantum field theory* is a (covariant) functor $\mathscr{A}$ between the two categories $\mathfrak{Man}$ and $\mathfrak{TAlg}$. Namely, let us denote by α_χ the mapping $\mathscr{A}(\chi)$ of a morphism χ in $\mathfrak{Man}$ to a morphism in $\mathfrak{TAlg}$ and by $\mathscr{A}(M, g)$ the mapping of an object in $\mathfrak{Man}$ to an object in $\mathfrak{TAlg}$, see the following diagram.

$$\begin{array}{ccc}
(M_1,g_1) & \xrightarrow{\chi} & (M_2,g_2) \\
\mathscr{A}\big\downarrow & & \big\downarrow\mathscr{A} \\
\mathscr{A}(M_1,g_1) & \xrightarrow{\alpha_\chi} & \mathscr{A}(M_2,g_2)
\end{array}$$

Then, the following relations hold for all morphisms $\chi_{ij} \in \hom_{\mathfrak{Man}}((M_i, g_i), (M_j, g_j))$:

$$\alpha_{\chi_{23}} \circ \alpha_{\chi_{12}} = \alpha_{\chi_{23} \circ \chi_{12}}\,, \qquad \alpha_{id_M} = id_{\mathscr{A}(M,g)}\,.$$

A locally covariant quantum field theory is called *causal* if in all cases where $\chi_i \in \hom_{\mathfrak{Man}}((M_i, g_i), (M, g))$ are such that the sets $\chi_1(M_1)$ and $\chi_2(M_2)$ are spacelike separated in (M, g),

$$\left[\alpha_{\chi_1}(\mathscr{A}(M_1, g_1)), \alpha_{\chi_2}(\mathscr{A}(M_2, g_2))\right] = \{0\}$$

in the sense that all elements in the two considered algebras are mutually commuting.

Finally, one says that a locally covariant quantum field theory fulfils the *time-slice axiom*, if the situation that $\chi \in \hom_{\mathfrak{Man}}((M_1, g_1), (M_2, g_2))$ is such that $\chi(M_1, g_1)$ contains a Cauchy surface of (M_2, g_2) entails

$$\alpha_\chi\left(\mathscr{A}(M_1, g_1)\right) = \mathscr{A}(M_2, g_2)\,.$$

The authors of [21] also give the definition of a state space of a locally covariant quantum field theory and this turns out to be dual to a functor, by the duality relation between states and algebras. One therefore chooses the notation of *covariant functor* for a functor in the strict sense, and calls such a mentioned dual object a *contravariant functor*. We stress once more that the term 'local' refers to the size of spacetime regions. A locally covariant quantum field theory is such that it can be constructed on arbitrarily small (causally convex) spacetime regions without having any information on the remainder of the spacetime. In more detail, this means that the algebraic relations of observables in such small region are already fully determined by the information on this region alone. This follows by application of the above definition to the special case that (M_1, g_1) is a causally convex subset of (M_2, g_2).

As shown in [21], the quantum field theory given by assigning the Borchers-Uhlmann algebra $\mathscr{A}(M)$ of the free Klein-Gordon field to a spacetime (M, g) is a locally covariant quantum field theory fulfilling causality and the time-slice axiom. This follows from the fact that the construction of $\mathscr{A}(M)$ only employs compactly supported test functions and the causal propagator E. The latter is uniquely given on any globally hyperbolic spacetime, particularly, the causal propagator on a causally convex subset (M_1, g_1) of a globally hyperbolic spacetime (M_2, g_2) coincides with the restriction of the same propagator on (M_2, g_2) to (M_1, g_1). Finally, causality follows by the causal support properties of the causal propagator, and the time-slice axiom follows by Lemma 2.3.

Let us now discuss the notion of a *locally covariant quantum field*. These fields are particular observables in a locally covariant quantum field theory which transform covariantly, i.e. loosely speaking, as a tensor and are in addition constructed only out of local geometric data. In categorical terms, this means that they are *natural transformations* between the functors $\mathscr{D}$ and $\mathscr{A}$. We refer to [87] for the notion of a natural transformation, however, its meaning in our context should be clear from the following definition.

Definition 2.15 A *locally covariant quantum field* Φ is a natural transformation between the functors $\mathscr{D}$ and $\mathscr{A}$. Namely, for every object (M, g) in $\mathfrak{Man}$ there exists a morphism $\Phi_{(M,g)} : \Gamma_0(M, g) \to \mathscr{A}(M, g)$ in $\mathfrak{Top}$ such that, for each morphism $\chi \in \hom_{\mathfrak{Man}}((M_1, g_1), (M_1, g_1))$, the following diagram commutes.

$$\begin{array}{ccc} \Gamma_0(M_1,g_1) & \xrightarrow{\Phi_{(M_1,g_1)}} & \mathscr{A}(M_1,g_1) \\ \chi_* \big\downarrow & & \big\downarrow \alpha_\chi \\ \Gamma_0(M_2,g_2) & \xrightarrow[\Phi_{(M_2,g_2)}]{} & \mathscr{A}(M_2,g_2) \end{array}$$

Particularly, this entails that

$$\alpha_\chi \circ \Phi_{(M_1,g_1)} = \Phi_{(M_2,g_2)} \circ \chi_* \,.$$

It is easy to see that the Klein-Gordon field $\phi(f)$ is locally covariant. Namely, the remarks on the local covariance of the quantum field theory given by $\mathscr{A}(M)$ after Definition 2.14 entail that an isometric embedding $\chi : (M_1, g_1) \hookrightarrow (M_2, g_2)$ transforms $\phi(f)$ as

$$\alpha_\chi\,(\phi(f)) = \phi(\chi_* f)\,,$$

or, formally,

$$\alpha_\chi\,(\phi(x)) = \phi\,(\chi(x))\;.$$

Hence, local covariance of the Klein-Gordon field entails that it transforms as a 'scalar'. While the locality and covariance of the Klein-Gordon field itself are somehow automatic, one has to take care that all extended quantities, like Wick powers and time-ordered products thereof, maintain these good properties. The prevalent paradigm in algebraic quantum field theory is that *all* pointlike observables should be theoretically modelled by locally covariant quantum fields.

A comprehensive review of further aspects and results of locally covariant quantum field theory may be found in [46].

2.6 The Quantum Stress-Energy Tensor and the Semiclassical Einstein Equation

The aim of this section is to discuss the semiclassical Einstein equation and the quantum-stress-energy tensor $:T_{\mu\nu}:$ which is the observable whose expectation value enters this equation. As argued in the previous section, all pointlike observables such as the quantum stress-energy tensor should be locally covariant fields in the sense of Definition 2.15. Rather than discussing local covariance for non-linear pointlike observables only at the example of $:T_{\mu\nu}:$, it is instructive to review the construction of general local and covariant Wick polynomials.

2.6.1 Local and Covariant Wick Polynomials

The first construction of local and covariant general Wick polynomials was given in [70] based on ideas already implemented for the stress-energy tensor in [123]. Here we would like to review a variant of the construction of [70] in the spirit of the functional approach to perturbative QFT on curved spacetimes, termed *perturbative algebraic quantum field theory*, cf. [17, 51, 52]. Essentially, this point of view on local Wick polynomials was already taken in [72]. We review here only the case of the neutral Klein-Gordon field, however, the functional approach is applicable to general field theories [51, 52, 105].

In the functional approach to algebraic QFT on curved spacetimes, one considers observables as functionals on the classical field configurations. Upon quantization, these functionals are endowed with a particular non-commutative product which encodes the commutation relations of quantum observables. We have already taken this point of view in the discussion of the Borchers-Uhlmann algebra $\mathscr{A}(M)$ as the result of quantizing a classical symplectic space constructed in Sect. 2.2. In particular, the smeared quantum scalar field $\phi(f)$ was considered as the quantization of the linear functional $F_f : \Gamma(M) \to \mathbb{C}$, $F_f(\phi) = \langle f, \phi \rangle$ with $f \in \Gamma_0^{\mathbb{C}}(M)$. The new aspect in the approach we shall review now is to consider a much larger class of functionals on $\Gamma(M)$. To this avail, we view $\Gamma(M)$ as the space of off-shell configurations of the scalar field, whereas $\mathrm{Sol} \subset \Gamma(M)$ is the space of on-shell configurations. For the purpose of perturbation theory it is more convenient to perform all constructions off-shell first and to go on-shell only in the end, and we shall follow this route as well, even though perturbative constructions are not dealt with in this monograph.

To this end, we call a functional $F : \Gamma(M) \to \mathbb{C}$ smooth if the nth functional derivatives

$$\left\langle F^{(n)}(\phi), \psi_1 \otimes \cdots \otimes \psi_n \right\rangle \doteq \frac{d^n}{d\lambda_1 \dots d\lambda_n} F\left(\phi + \sum_{j=1}^{n} \lambda_j \psi_j\right)\Bigg|_{\lambda_1 = \cdots = \lambda_n = 0} \tag{2.16}$$

exist for all n and all $\psi_1, \dots, \psi_n \in \Gamma_0(M)$ and if $F^{(n)}(\phi) \in \Gamma'(M^n)$, i.e. $F^{(n)}(\phi)$ is a distribution. By definition $F^{(n)}(\phi)$ is symmetric and we consider only polynomial functionals, i.e. $F^{(n)}(\phi)$ vanishes for $n > N$ and some N. We define the support of a functional as

$$\begin{aligned} \mathrm{supp}\, F \doteq \{x \in M \,|\, \forall \text{ neighbourhoods } U \text{ of } x\ \exists \phi, \psi \in \Gamma(M),\ \mathrm{supp}\ \psi \subset U, \\ \text{such that } F(\phi + \psi) \neq F(\phi)\}\,. \end{aligned} \tag{2.17}$$

which coincides with the union of the supports of $F^{(1)}(\phi)$ over all $\phi \in \Gamma(M)$. The relevant space of functionals which encompasses all observables of the free neutral scalar field is the space of *microcausal functionals*

$$\mathscr{F}_{\mu c} \doteq \{F : \Gamma(M) \to \mathbb{C} \mid F \text{ smooth, compactly supported,}$$
$$\mathrm{WF}\left(F^{(n)}\right) \cap \left(\overline{V}_+^n \cup \overline{V}_-^n\right) = \emptyset\Big\}\,, \tag{2.18}$$

where $V_{+/-}$ is a subset of the cotangent space formed by the elements whose covectors are contained in the future/past light cones and $\overline{V}_{+/-}$ denotes is closure. $\mathscr{F}_{\mu c}$ contains two subspaces of importance. On the one hand, it contains the space $\mathscr{F}_{\text{loc}}$ of *local functionals* consisting of sums of functionals of the form

$$F(\phi) = \int_M d_g x \; \mathscr{P}[\phi]_{\mu_1 \ldots \mu_n}(x) \; f^{\mu_1 \ldots \mu_n}(x)$$

where $\mathscr{P}[\phi] \in \Gamma(T^* M^n)$ is a tensor such that $\mathscr{P}[\phi](x)$ is a (tensor) product of covariant derivatives of ϕ at the point x with a total order of n and $f \in \Gamma_0(T M^n)$ is a test tensor. The prime example of a local functional is a smeared field monomial

$$F_{k,f}(\phi) \doteq \int_M d_g x \; \phi(x)^k f(x) \simeq \phi^k(f)\,, \qquad f \in \Gamma_0^{\mathbb{C}}(M)\,. \tag{2.19}$$

One the other hand, $\mathscr{F}_{\mu c}$ contains the space $\mathscr{F}_{\text{reg}}$ of *regular functionals*, i.e. all microcausal functionals whose functional derivatives are smooth such that $F^{(n)}(\phi) \in \Gamma_0^{\mathbb{C}}(M^n)$ for all ϕ and all n. A prime example of a regular functional is a functional of the form

$$F(\phi) = \prod_{j=1}^{n} \langle f_j, \phi \rangle\,, \qquad f_1, \ldots, f_n \in \Gamma_0^{\mathbb{C}}(M)\,. \tag{2.20}$$

Linear functionals are the only functionals which are both local and regular.

Given a bidistribution $H \in \Gamma_0'^{\mathbb{C}}(M^2)$ which (a) satisfies the Hadamard condition Definition 2.11, (b) has the antisymmetric part $H(x, y) - H(y, x) = iE(x, y)$ defined by the causal propagator E and a real symmetric part

$$H_{\text{sym}}(x, y) \doteq \frac{1}{2}\left(H(x, y) + H(y, x)\right)\,,$$

and (c) is a bisolution of the Klein-Gordon equation $P_x H(x, y) = P_y H(x, y) = 0$, we define a product indicated by $\star_H$ on $\mathscr{F}_{\mu c}$ via

$$(F \star_H G)(\phi) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \left\langle F^{(n)}(\phi), H^{\otimes n} G^{(n)}(\phi) \right\rangle, \tag{2.21}$$

i.e. by the sum of all possible mutual contractions of F and G by means of H. This is just an elegant way to implement Wick's theorem by an algebraic product as we shall explain in the following and may be understood in terms of *deformation quantization*, cf. [53] for a review of this aspect. Owing to the Hadamard property of H and the microlocal properties of microcausal functionals, the $\star_H$-product is well-defined on $\mathscr{F}_{\mu c}$ by [75, Theorem 8.2.13] and one can show that $F \star_H G \in \mathscr{F}_{\mu c}$ for all $F, G \in \mathscr{F}_{\mu c}$, i.e. $\mathscr{F}_{\mu c}$ is closed under $\star_H$.

It is not necessary to require that H is positive and thus the two-point function ω_2 of a Hadamard state ω on $\mathscr{A}(M)$. However, independent of whether or not we require H to be positive, its real and symmetric part is not uniquely fixed by the conditions we imposed. Given a different H' satisfying these conditions, it follows that $d \doteq H' - H = H'_{\text{sym}} - H_{\text{sym}}$ is real, symmetric and smooth and that the product $\star_{H'}$ is related to $\star_H$ by

$$F \star_{H'} G = \alpha_d \left(\alpha_{-d}(F) \star_H \alpha_{-d}(H)\right) , \tag{2.22}$$

where $\alpha_d : \mathscr{F}_{\mu c} \to \mathscr{F}_{\mu c}$ is the ‘contraction exponential operator’

$$\alpha_d \doteq \exp\left(\int_{M^2} d_g x \; d_g y \; d(x, y) \frac{\delta}{\delta\phi(x)} \frac{\delta}{\delta\phi(y)}\right) . \tag{2.23}$$

The previous discussion implies that, given a H satisfying the above-mentioned conditions, we can define a meaningful off-shell algebra $\mathscr{W}^0_H(M) \doteq (\mathscr{F}_{\mu c}, \star_H)$, and a corresponding on-shell algebra $\mathscr{W}_H(M) \doteq \mathscr{W}^0_H(M)/\mathscr{I}$, where $\mathscr{I}$ is the ideal generated by $\mathscr{F}_{\mu c,\text{sol}} \subset \mathscr{F}_{\mu c}$, the microcausal functionals which vanish on on-shell configurations $\phi \in \text{Sol} \subset \Gamma(M)$. In fact, we have $\mathscr{W}_H(M) = (\mathscr{F}_{\mu c}/\mathscr{F}_{\mu c,\text{sol}}, \star_H)$ and in the following we shall indicate an equivalence class $[F] \in \mathscr{F}_{\mu c}/\mathscr{F}_{\mu c,\text{sol}}$ by F for simplicity.

As a further implication of the previous exposition we have that $\mathscr{W}_H(M)$ and $\mathscr{W}_{H'}(M)$ constructed with a different H of the required type are isomorphic via $\alpha_d : \mathscr{W}_H(M) \to \mathscr{W}_{H'}(M)$ with $d = H' - H$. In this sense, we can consider $\mathscr{W}_H(M)$ as a particular representation of an abstract algebra $\mathscr{W}(M)$ which is independent of H, cf. [17]. $\mathscr{W}_H(M)$ is in fact a $*$-algebra and $\alpha_d : \mathscr{W}_H(M) \to \mathscr{W}_{H'}(M)$ is a $*$-isomorphism if we define the involution ($*$-operation) on $\mathscr{F}_{\mu c}$ via complex conjugation by

$$F^*(\phi) \doteq \overline{F(\phi)}$$

which implies

$$(F \star_H G)^* \doteq G^* \star_H F^*$$

by the conditions imposed on H. $\mathscr{W}_H(M)$ may be endowed with a topology induced by the so-called Hörmander topology [19, 25], and one can show that all continuous states on $\mathscr{W}_H(M)$ are induced by Hadamard states on the Borchers-Uhlmann algebra $\mathscr{A}(M)$, cf. [69] (in combination with [109]). In fact, we shall now explain why $\mathscr{W}_H(M)$ may be considered as the ‘algebra of Wick polynomials’ and in particular as an extension of $\mathscr{A}(M)$.

To this avail, we first consider two linear functionals $\phi(f_i) \doteq F_{1,f_i}(\phi)$, $i = 1, 2$, cf. (2.19), i.e. the classical field smeared with $f_1, f_2 \in \Gamma_0^{\mathbb{C}}(M)$. The definition of the $\star_H$-product (2.21) implies

$$[\phi(f_1), \phi(f_2)]_{\star_H} \doteq \phi(f_1) \star_H \phi(f_2) - \phi(f_2) \star_H \phi(f_1) = iE(f_1, f_2)\,.$$

This indicates that the product $\star_H$ encodes the correct commutation relations among quantum observables. If we consider instead the quadratic local functionals $\phi^2(f_i) \doteq F_{2,f_i}(\phi)$, $i = 1, 2$, cf. (2.19), i.e. the pointwise square of the classical field smeared with $f_1, f_2 \in \Gamma_0^{\mathbb{C}}(M)$, we find

$$\begin{aligned}\phi^2(f_1) \star_H \phi^2(f_2) = \phi^2(f_1)\phi^2(f_2) \\ &+ 4\int_{M^2} d_gx\, d_gy\; d(x, y)\; \phi(x)\phi(y)H(x, y) f_1(x) f_2(y) \\ &+ 2H^2(f_1, f_2)\,,\end{aligned}$$

which we may formally write as

$$\phi^2(x) \star_H \phi^2(y) = \phi^2(x)\phi^2(y) + 4\phi(x)\phi(y)H(x, y) + 2H^2(x, y)\,.$$

This expression may be compared by the expression obtain via Wick's theorem

$$:\phi^2(x):_H:\phi^2(y):_H=:\phi^2(x)\phi^2(y):_H +4\,:\phi(x)\phi(y):_H\; H(x, y) + 2H^2(x, y)\mathbb{I}\,,$$

if we define $:\cdot:_H$ to be the Wick-ordering w.r.t. the symmetric part H_{sym} of H, e.g.

$$:\phi(x)\phi(y):_H\doteq \phi(x)\phi(y) - H_{\text{sym}}(x, y)\mathbb{I}\,, \qquad :\phi^2(x):_H= \lim_{x\to y}\, :\phi(x)\phi(y):_H\;.$$

Consequently, local functionals $F \in \mathscr{F}_{\text{loc}}$ considered as elements of $F \in \mathscr{W}_H(M)$ correspond to Wick polynomials Wick-ordered with respect to H_{sym}, formally one may write $:F:_H= \alpha_{-H_{\text{sym}}}(F)$ with $\alpha_{-H_{\text{sym}}}$ defined as in (2.23). In fact, the algebra $F \in \mathscr{W}_H(M)$ contains also time-ordered products of Wick polynomials [19, 70, 72] and the perturbative construction of QFT based on $\mathscr{W}_H(M)$ implies that 'tadpoles' are already removed.

We have anticipated that $\mathscr{W}_H(M)$ is an extension of the Borchers-Uhlmann algebra $\mathscr{A}(M)$, which contains only products of the quantum field ϕ at *different* points. To see this, we consider the algebra $\mathscr{A}'(M) \doteq \alpha_{-H_{\text{sym}}}\left((\mathscr{F}_{\text{reg}}/\mathscr{F}_{\text{reg,sol}}, \star_H)\right)$, where $\mathscr{F}_{\text{reg,sol}} \doteq \mathscr{F}_{\text{reg}} \cap \mathscr{F}_{\mu\text{c,sol}}$, $(\mathscr{F}_{\text{reg}}/\mathscr{F}_{\text{reg,sol}}, \star_H)$ is a subalgebra of $\mathscr{W}_H(M) = (\mathscr{F}_{\mu\text{c}}/\mathscr{F}_{\mu\text{c,sol}}, \star_H)$ because $\star_H$ closes on regular functionals and we note that $\alpha_{-H_{\text{sym}}}$ is well-defined on $\mathscr{F}_{\text{reg}}$ although H_{sym} is not smooth. One can check that $\mathscr{A}'(M)$ is in fact the algebra $\mathscr{A}'(M) = (\mathscr{F}_{\text{reg}}/\mathscr{F}_{\text{reg,sol}}, \star_E)$ with the product $\star_E$ given by (2.21) with H replaced by $iE/2$, and that $\mathscr{A}'(M)$ is isomorphic to the Borchers-Uhlmann algebra $\mathscr{A}(M)$ defined in Definition 2.8.

We have mentioned that Hadamard states ω on $\mathscr{A}(M)$ induce meaningful states on $\mathscr{W}_H(M)$ and that in fact all reasonable states on $\mathscr{W}_H(M)$ are of this form. To explain this in more detail, we consider a Gaussian Hadamard state on ω on $\mathscr{A}(M)$ with two-point function ω_2 and the algebra $\mathscr{W}_{\omega_2}(M)$ constructed by means of ω_2. Given this, we can define a Gaussian Hadamard state on $\mathscr{W}_{\omega_2}(M)$ by

$$\omega(F) \doteq F(\phi = 0)\,, \qquad \forall\ F \in \mathscr{F}_{\mu c}$$

which corresponds to the fact that Wick polynomials Wick-ordered w.r.t. to ω_2 have vanishing expectation values in the state ω, e.g. $\omega(:\phi^2(x):_{\omega_2}) = 0$. Note that this definition implies in particular that

$$\omega\left(\phi(f_1) \star_{\omega_2} \phi(f_2)\right) = \omega_2(f_1, f_2)\,,$$

i.e. ω_2 is, as required by consistency, the two-point correlation function of ω also in the functional picture. If we prefer to consider the extended algebra $\mathscr{W}_H(M)$ constructed with a different H, then we can define the state ω on $\mathscr{W}_H(M)$ by a pull-back with respect to the isomorphism $\alpha_d : \mathscr{W}_H(M) \to \mathscr{W}_{\omega_2}(M)$ with $d = \omega_2 - H$ and α_d as in (2.23). In other words, $\omega \circ \alpha_d$ defines a state on $\mathscr{W}_H(M)$, and this definition corresponds to e.g.

$$\omega(:\phi^2(x):_H) = \lim_{x \to y}(\omega_2(x, y) - H(x, y))\,,$$

i.e. to a *point-splitting renormalisation* of the expectation value of the observable $\phi^2(x)$.

We recall that observable quantities should be local and covariant fields as discussed in the previous section. However, not all local elements of the algebra $\mathscr{W}_H(M)$ satisfy this property, i.e. not all local functionals $F \in \mathscr{F}_{\text{loc}}$ considered as elements of $\mathscr{W}_H(M)$ correspond to local and covariant Wick polynomials. In particular the functional $\phi^2(f) = F_{2,f}(\phi) \simeq :\phi^2(f):_H$, cf. (2.19), does not correspond to a local and covariant Wick-square because H is by assumption a bisolution of the Klein-Gordon equation and thus $:\phi^2(f):_H$ does not only depend on the geometry, i.e. the metric and its derivatives, in the localisation region of the test function f, but also on the geometry of the spacetime (M, g) outside of the support of f [70]. This is related to the observation that quite generally local and covariant Hadamard states do not exist [44]. Notwithstanding, local and covariant elements of $\mathscr{W}_H(M)$ do exist and, following [70, 72], they can identified by means of a map $W_H : \mathscr{F}_{\text{loc}} \to \mathscr{F}_{\text{loc}} \subset \mathscr{W}_H(M)$ which should satisfy a number of conditions:

1. W_H commutes with functional derivatives, i.e. $(W_H(F))^{(1)} = W_H(F^{(1)})$ and with the involution $W_H(F)^* = W_H(F^*)$.
2. W_H satisfies the Leibniz rule.
3. W_H is local and covariant.
4. W_H scales almost homogeneously with respect to constant rescalings $m \mapsto \lambda m$ and $g \mapsto \lambda^{-2} g$ of the mass m and metric g.

5. W_H depends smoothly or analytically on the metric g, the mass m and the coupling ξ to the scalar curvature present in the Klein-Gordon equation (2.4).

We refer to [72] for a detailed discussion of these conditions, and only sketch their meaning and physical motivation. To this avail, we consider the smeared local polynomials $\phi^k(f) = F_{k,f}(\phi)$ defined in (2.19) and identify $W_H(\phi^k(x))$ by $:\phi^k(x):$ omitting the smearing function for simplicity. The first of the above axioms then imply that $[:\phi^k(x):, \phi(y)] = imE(x, y) :\phi^{m-1}(x):$, i.e. the Wick-ordered fields satisfy standard commutation relations. The Leibniz rule further demands that $\nabla_\mu :\phi^k(x): = :\nabla_\mu(\phi^k(x)):$, i.e. Wick-ordering commutes with covariant derivatives, and the locality and covariance condition demands that $:\phi^k(x):$ is a local and covariant field in the sense of Definition 2.15. Finally, the scaling condition requires that under constant rescalings $m \mapsto \lambda m$ and $g \mapsto \lambda^{-2} g$, $:\phi^k(x):$ scales (in four spacetime dimensions) as $:\phi^k(x): \mapsto \lambda^k :\phi^k(x): + \mathscr{O}(\log \lambda)$, which among other things implies that $:\phi^k(x):$ has the correct 'mass dimension', and the smoothness/analyticity requirement implies that e.g. $:\phi^2(x):$ may not contain a term like e.g. $\exp(\xi^{-1}) m^{-4} R^{-1}(x) (R_{\mu\nu}(x) R^{\mu\nu}(x))^2$ which would be allowed by the previous conditions.

It has been demonstrated in [70, 72] (see also [91]) that a prescription of defining local and covariant Wick polynomials exists, but that this prescription is not unique. In fact, if we consider (in a geodesically convex neighbourhood) a H of the form (2.12) with $w = 0$, i.e. a purely geometric Hadamard parametrix, then Wick-ordering w.r.t. to this H, e.g. $:\phi^k(x): \doteq :\phi^k(x):_H = \alpha_{-H_{\text{sym}}}(\phi^k(x))$ satisfies all conditions reviewed above. However, this prescription is not the only possibility, but one can consider e.g.

$$:\phi^2(x): = :\phi^2(x):_H + \alpha R(x) + \beta m^2$$

with arbitrary real and dimensionless constants α and β which are analytic functions of ξ. These constants parametrise the *renormalisation freedom* of Wick polynomials, or, in the context of perturbation theory, the renormalisation freedom inherent in removing tadpoles. Note that a change of scale λ in (2.12) can be subsumed in this renormalisation freedom as a particular one-parameter family.

The coefficients parametrising the renormalisation freedom of local Wick polynomials may not be fixed within QFT on curved spacetimes, but have to be determined in a more general framework or by comparison with experiments. We will comment further on this point when discussing the renormalisation freedom of the stress-energy tensor in the context of cosmology in the next chapter. Note that, by local covariance, these coefficients are universal and may be fixed once and for all in all globally hyperbolic spacetimes (of the same dimension). Admittedly, in view of the above presentation of locality and general covariance, one might think that this holds only for spacetimes with isometric subregions (or spacetimes with conformally related subregions on account of [98]). However, given two spacetimes (M_1, g_1) and (M_2, g_2) with not necessarily isometric subregions, one can employ the deformation argument of [54] to deform, say, (M_1, g_1) such that it contains a subregion isometric to a subregion of (M_2, g_2). As the renormalisation freedom is parametrised by constants multiplying curvature terms or dimensionful constants which maintain their form under such a deformation, one can require that the mentioned constants are the same on (M_1, g_1) and (M_2, g_2) in a meaningful way.

2.6.2 The Semiclassical Einstein Equation and Wald's Axioms

The central equation in describing the influence of quantum fields on the background spacetime—i.e. their backreaction—is the *semiclassical Einstein equation*. It reads

$$G_{\mu\nu}(x) = 8\pi G\ \omega(:T_{\mu\nu}(x):)\,, \tag{2.24}$$

where the left hand side is given by the standard Einstein tensor $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}$, G denotes Newton's gravitational constant, and we have replaced the stress-energy tensor of classical matter by the expectation value of a suitable Wick polynomial $:T_{\mu\nu}(x):$ representing the quantum stress-energy tensor evaluated in a state ω. Considerable work has been invested in analysing how such equation can be derived via a suitable semiclassical limit from some potential quantum theory of gravity. We refer the reader to [48, Sect. II.B] for a review of several arguments and only briefly mention that a possibility to derive (2.24) is constituted by starting from the sum of the *Einstein-Hilbert action* $S_{\mathrm{EH}}(g)$ and the matter action $S_{\mathrm{matter}}(g, \Phi)$,

$$S(g, \Phi) \doteq S_{\mathrm{EH}}(g) - S_{\mathrm{matter}}(g, \Phi)\,, \tag{2.25}$$

$$S_{\mathrm{EH}}(g) \doteq \frac{1}{16\pi G} \int_M d_g x\ R = \frac{1}{16\pi G} \int_M dx \sqrt{|\det g|}\ R$$

formally expanding a quantum metric and a quantum matter field around a classical (background) vacuum solution of Einstein's equation, and computing the equation of motion for the expected metric while keeping only 'tree-level' ($\hbar^0$) contributions of the quantum metric and 'loop-level' ($\hbar^1$) contributions of the quantum matter field. In this work, we shall not contemplate on whether and in which situation the above mentioned 'partial one-loop approximation' is sensible, but we shall take the following pragmatic point of view: (2.24) seems to be the simplest possibility to couple the background curvature to the stress-energy of a quantum field in a non-trivial way. We shall therefore consider (2.24) as it stands and only discuss for which quantum states and Wick polynomial definitions of $:T_{\mu\nu}(x):$ it is a self-consistent equation. A rigorous proof that solutions of the semiclassical Einstein equation actually exist in the restricted case of cosmological spacetimes has been given in [99, 101].

We first observe that in (2.24) one equates a 'sharp' classical quantity on the left hand side with a 'probabilistic' quantum quantity on the right hand side. The semiclassical Einstein equation can therefore only be sensible if the fluctuations of the stress-energy tensor $:T_{\mu\nu}(x):$ in the considered state ω are small. In this respect, we already know that we should consider ω to be a Hadamard state and $:T_{\mu\nu}(x):$ to be a Wick polynomial Wick-ordered by means of a Hadamard bidistribution. Namely, the discussion in the previous sections tells us that this setup at least assures *finite fluctuations* of $:T_{\mu\nu}(x):$ as the pointwise products appearing in the computation of such fluctuations are well-defined distributions once their Hadamard property is assumed. In fact, this observation has been the main motivation to consider Hadamard states in the first place [120, 123]. However, it seems one can *a priori* not obtain more than these qualitative observations, and that quantitative statements on the actual size of the fluctuations can only be made *a posteriori* once a solution of (2.24) is found. An extended framework where the left hand side of the semiclassical Einstein equation is also interpreted stochastically is discussed in [100].

Having agreed to consider only Hadamard states and Wick polynomials constructed by the procedures outlined in the last section, two questions remain. Which Hadamard state and which Wick polynomial should one choose to compute the right hand side of (2.24)? The first question can ultimately only be answered by actually solving the semiclassical Einstein equation. Observe that this actually poses a non-trivial problem as the formulation of the semiclassical Einstein equation in principle requires to specify a map which assigns to a metric g a Hadamard state ω_g, whereas we know that a covariant assignment of Hadamard states to spacetimes does not exist [44]. This problem can be partially overcome by defining such a map only on a particular subset of globally hyperbolic spacetimes as we shall see in Sect. 3.2.2. The question of which Wick polynomials should be taken as the definition of a quantum stress-energy tensor is also non-trivial, as Wick-ordering turns out to be ambiguous in curved spacetimes, see [70, 72] and the last section. We have already pointed out at several occasions that one should define the Wick polynomial $:T_{\mu\nu}(x):$ in a local, and, hence, state-independent way. In the context of the semiclassical Einstein equation the reason for this is the simple observation that one would like to solve (2.24) without knowing the spacetime which results from this procedure beforehand, but a state solves the equation of motion and, hence, already 'knows' the full spacetime, thus being a highly non-local object. On account of the above considerations, we can therefore answer the question for the correct Wick polynomial representing $:T_{\mu\nu}(x):$ without having to choose a specific Hadamard state ω beforehand. The following review of the quantum stress-energy tensor will be limited to the case of the free neutral Klein-Gordon field. An analysis of the case of Dirac fields from the perspective of algebraic QFT on curved spacetimes may be found in [26], whereas the case of interacting scalar fields in treated in [72].

To this avail, let us consider the stress-energy tensor of classical matter fields. Given a classical action S_{matter}, the related (Hilbert) stress-energy tensor can be computed as [49, 122]

$$T_{\mu\nu} \doteq \frac{2}{\sqrt{|\det g|}} \frac{\delta S_{\text{matter}}}{\delta g^{\mu\nu}} . \tag{2.26}$$

For the Klein-Gordon action $S(g, \phi) = \frac{1}{2} \langle \phi, P\phi \rangle$ we find

$$\begin{aligned} T_{\mu\nu} =& (1-2\xi)\phi_{;\mu}\phi_{;\nu} - 2\xi\phi_{;\mu\nu}\phi + \xi G_{\mu\nu}\phi^2 \\ &+ g_{\mu\nu}\left\{2\xi(\Box\phi)\phi + \left(2\xi - \frac{1}{2}\right)\phi_{;\rho}\phi_{;}^{\ \rho} - \frac{1}{2}m^2\phi^2\right\} . \end{aligned} \tag{2.27}$$

A straightforward computation shows that the classical stress-energy tensor is covariantly conserved on-shell, i.e.

$$\nabla^\mu T_{\mu\nu} = -(\nabla_\nu\phi)P\phi = 0 .$$

Moreover, a computation of its trace yields

$$g^{\mu\nu}T_{\mu\nu} = (6\xi - 1)\left(\phi\Box\phi + \phi_{;\mu}\phi_{;}^{\ \mu}\right) - m^2\phi^2 - \phi P\phi .$$

Particularly, we see that in the conformally invariant situation, that is, $m = 0$ and $\xi = \frac{1}{6}$, the classical stress-energy tensor has vanishing trace on-shell. In fact, one can show that this is a general result, namely, the trace of a classical stress-energy tensor is vanishing on-shell if and only if the respective field is conformally invariant [49, Theorem 5.1].

In view of the discussion of local and covariant Wick polynomials in the previous section, it seems natural to define the quantum stress-energy tensor $:T_{\mu\nu}(x):$ just as the Wick polynomial $:T_{\mu\nu}(x):_H$ Wick-ordered with respect to a purely geometric Hadamard parametrix $H = \frac{h}{8\pi^2}$ of the form (2.12) with $w = 0$. Given a Hadamard state ω whose two-point function is (locally) of the form $\omega_2 = H + \frac{w}{8\pi^2}$, the expectation value of $:T_{\mu\nu}(x):_H$ in this state may be computed as

$$\omega\left(:T_{\mu\nu}(x):_H\right) = \lim_{x\to y} \frac{D^{\text{can}}_{\mu\nu}(x,y)w(x,y)}{8\pi^2} = \frac{\left[D^{\text{can}}_{\mu\nu}w\right]}{8\pi^2} ,$$

where the bidifferential operator $D^{\text{can}}_{\mu\nu}$ may be obtained from the classical stress-energy tensor as

$$\begin{aligned} D^{\text{can}}_{\mu\nu}(x,y) = \frac{1}{2}\frac{\delta^2 T_{\mu\nu}}{\delta\phi(x)\delta\phi(y)} &= (1-2\xi)g_\nu^{\nu'}\nabla_\mu\nabla_{\nu'} - 2\xi\nabla_\mu\nabla_\nu + \xi G_{\mu\nu} \\ &+ g_{\mu\nu}\left\{2\xi\Box_x + \left(2\xi - \frac{1}{2}\right)g_\rho^{\rho'}\nabla^\rho\nabla_{\rho'} - \frac{1}{2}m^2\right\} , \end{aligned}$$

and where we recall the Synge bracket notation for coinciding point limits of bitensors, cf. Sect. 2.4. Here, unprimed indices denote covariant derivatives at x, primed indices denote covariant derivatives at y and $g_\nu^{\nu'}$ is the bitensor of parallel transport, cf. Sect. 2.4. However, as we shall discuss in a bit more detail in the following, this particular definition of a quantum stress-energy tensor is not satisfactory because it does not yield a covariantly conserved quantity which is a necessary condition for the semiclassical Einstein equation to be well-defined.

The first treatment of the quantum stress-energy tensor from an algebraic point of view was the analysis of Wald in [120]. At the time [120] appeared, workers in the field had computed the expectation value of the quantum stress-energy tensor by different renormalisation methods like adiabatic subtraction, dimensional regularisation, ζ-function regularisation and DeWitt-Schwinger point-splitting regularisation (see [13] and also [62, 88]) and differing results had been found. From the rather modern point of view we have reviewed in the previous sections, it is quite natural and unavoidable that renormalisation in curved spacetimes is ambiguous. However, the axioms for the (expectation value of) the quantum stress-energy tensor introduced in [120] helped to clarify the case at that time and to understand that in principle *all* employed renormalisation schemes were correct in physical terms. Consequently, the apparent differences between them could be understood on clear conceptual grounds. These axioms (in the updated form presented in [123]) are:

1. Given two (not necessarily Hadamard) states ω and ω' such that the difference of their two-point functions $\omega_2 - \omega_2'$ is smooth, $\omega(:T_{\mu\nu}(x):) - \omega'(:T_{\mu\nu}(x):)$ is equal to
$$\left[D^{\text{can}}_{\mu\nu}\ \left(\omega_2(x,y) - \omega_2'(x,y)\right)\right].$$
2. $\omega(:T_{\mu\nu}(x):)$ is locally covariant in the following sense: let
$$\chi : (M,g) \hookrightarrow (M',g')$$
be defined as in Sect. 2.5 and let α_χ denote the associated continuous, unit-preserving, injective $*$-morphisms between the relevant enlarged (abstract) algebras $\mathscr{W}(M,g)$ and $\mathscr{W}(M',g')$. If two states ω on $\mathscr{W}(M,g)$ and ω' on $\mathscr{W}(M',g')$ respectively are related via $\omega = \omega' \circ \alpha_\chi$, then
$$\omega'\left(:T_{\mu'\nu'}(x'):\right) = \chi_*\omega\left(:T_{\mu\nu}(x):\right),$$
where χ_* denotes the push-forward of χ in the sense of covariant tensors.
3. Covariant conservation holds, i.e.
$$\nabla^\mu\omega\left(:T_{\mu\nu}(x):\right) = 0.$$
4. In Minkowski spacetime $\mathbb{M}$, and in the relevant Minkowski vacuum state $\omega_\mathbb{M}$
$$\omega_\mathbb{M}\left(:T_{\mu\nu}(x):\right) = 0.$$
5. $\omega(:T_{\mu\nu}(x):)$ does not contain derivatives of the metric of order higher than 2.

Some of these axioms are just special cases of the axioms for local Wick polynomials reviewed in Sect. 2.6.1. In fact, the first of these axioms is just a variant of the requirement that local Wick polynomials have standard commutation relations. In the case of $:T_{\mu\nu}:$ this implies that two valid definitions of this observable can only differ by a term proportional to the identity. The second axiom is just the locality and covariance of Wick polynomials here formulated on the level of expectation values. The condition that the quantum-stress energy tensor has vanishing expectation value on Minkowski spacetime in the corresponding vacuum state is not compatible with the requirement that local Wick polynomials depend smoothly on the mass m, cf. [91, Theorem 2.1(e)] and can be omitted because it is not essential. The last axiom is motivated by the wish to ensure that the solution theory of the semiclassical Einstein equation does not depart 'too much' from the one of the classical Einstein equation. In particular one would like to have that all solutions of the semiclassical Einstein equation behave well in the classical limit $\hbar \to 0$. Wald himself had realised, however, that this axiom could not be satisfied for massless theories without introducing an artificial length scale into the theory; therefore, the axiom has been discarded.

Using these axioms as well as a variant of the scaling requirement for local Wick polynomials, Wald could prove that a uniqueness result for $\omega(:T_{\mu\nu}:)$ (and thus for $:T_{\mu\nu}:$ itself by the first axiom) can be obtained, namely that two valid definitions $:T_{\mu\nu}:$ and $:T_{\mu\nu}:'$ of the quantum stress-energy tensor can only differ by a term of the form

$$:T_{\mu\nu}:' - :T_{\mu\nu}: = \alpha_1 m^4 g_{\mu\nu} + \alpha_2 m^2 G_{\mu\nu} + \alpha_3 I_{\mu\nu} + \alpha_4 J_{\mu\nu} + \varepsilon K_{\mu\nu}\,, \quad (2.28)$$

where α_i are real and dimensionless constants and the last three tensors appearing above are the conserved local curvature tensors

$$\begin{aligned}
I_{\mu\nu} &\doteq \frac{1}{\sqrt{|\det g|}}\frac{\delta}{\delta g^{\mu\nu}}\int_M d_g x \quad R^2 = -g_{\mu\nu}\left(\frac{1}{2}R^2 + 2\Box R\right) + 2R_{;\mu\nu} + 2RR_{\mu\nu}\,,\\
J_{\mu\nu} &\doteq \frac{1}{\sqrt{|\det g|}}\frac{\delta}{\delta g^{\mu\nu}}\int_M d_g x \quad R_{\alpha\beta}R^{\alpha\beta}\\
&= -\frac{1}{2}g_{\mu\nu}(R_{\mu\nu}R^{\mu\nu} + \Box R) + R_{;\mu\nu} - \Box R_{\mu\nu} + 2R_{\alpha\beta}R^{\alpha\ \ \beta}_{\ \mu\ \ \nu}\,, \qquad (2.29)\\
K_{\mu\nu} &\doteq \frac{1}{\sqrt{|\det g|}}\frac{\delta}{\delta g^{\mu\nu}}\int_M d_g x \quad R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}\\
&= -\frac{1}{2}g_{\mu\nu}R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} + 2R_{\alpha\beta\gamma\mu}R^{\alpha\beta\gamma}{}_{\nu} + 4R_{\alpha\beta}R^{\alpha\ \ \beta}_{\ \mu\ \ \nu}\\
&\qquad - 4R_{\alpha\mu}R^{\alpha}{}_{\nu} - 4\Box R_{\mu\nu} + 2R_{;\mu\nu}\,.
\end{aligned}$$

This uniqueness result follows by using the first of Wald's axioms in order to observe that $:T_{\mu\nu}:' - :T_{\mu\nu}:$ is a c-number. From the locality and covariance axiom in combination with conservation it follows that this c-number must be a local and conserved curvature tensor whereas the scaling condition implies that it has the correct mass dimension. As [47] pointed out, these requirements do not fix $:T_{\mu\nu}:' - :T_{\mu\nu}:$ to be of the above form, but demanding in addition that $:T_{\mu\nu}:$ depends in a smooth or analytic way on m and g as in [70, 72] is sufficient to rule out the additional terms mentioned in [47] so that (2.28) indeed classifies the full renormalisation freedom compatible with the axioms of local Wick polynomials introduced in [70, 72] and the conservation of $:T_{\mu\nu}:$.

In fact, we will see in the next section that changing the scale λ in the regularising Hadamard bidistribution amounts to changing $:T_{\mu\nu}:$ exactly by a tensor of this form and, furthermore, the attempt to renormalise perturbative Einstein-Hilbert quantum gravity at one loop order automatically yields a renormalisation freedom in form of such a tensor as well [116].[1] Moreover, using the *Gauss-Bonnet-Chern theorem* in four dimensions, which states that

$$\int_M d_g x \, \left(R_{\mu\nu\rho\tau}R^{\mu\nu\rho\tau} - 4R_{\mu\nu}R^{\mu\nu} + R^2\right)$$

is a topological invariant and, therefore, has a vanishing functional derivative with respect to the metric [3, 116], one can restrict the freedom even further by removing $K_{\mu\nu}$ from the list of allowed local curvature tensors as $K_{\mu\nu} = 4J_{\mu\nu} - I_{\mu\nu}$. Finally, the above tensors all have a trace proportional to $\Box R$ and thus the linear combination $I_{\mu\nu} - 3J_{\mu\nu}$ is traceless.

2.6.3 A Conserved Quantum Stress-Energy Tensor

After some dispute about computational mistakes (see the discussion in [121]) it had soon be realised that the quantum stress-tensor $:T_{\mu\nu}:_H$ defined by Wick-ordering the canonical expression by means of a purely geometric Hadamard bidistribution H is not conserved although it satisfies the other conditions for local Wick polynomials mentioned at the end of Sect. 2.6.1. The reason for this is the fact that, in contrast to the two-point function of a Hadamard state, a purely geometric Hadamard bidistribution fails to satisfy the equation of motion. Consequently $\nabla^\mu :T_{\mu\nu}:_H =: \nabla^\mu T_{\mu\nu}:_H$ is (in four spacetime dimensions) the covariant divergence of a non-vanishing and non-conserved local curvature term $\nabla^\mu :T_{\mu\nu}:_H = \nabla^\mu C_{\mu\nu} \neq 0$. The obvious solution to this problem has been to compute $C_{\mu\nu}$ and then to define a conserved stress-tensor by

$$:T_{\mu\nu}: \doteq :T_{\mu\nu}:_H - C_{\mu\nu}\mathbb{I}\,, \tag{2.30}$$

[1] In fact, at least in the case of scalar fields, the combination of the local curvature tensors appearing as the finite renormalisation freedom in [116] is, up to a term which seems to be an artifact of the dimensional regularisation employed in that paper, the same that one gets via changing the scale in the regularising Hadamard bidistribution.

i.e. by just subtracting this *conservation anomaly*. It was found that this conserved stress tensor still has a *trace anomaly*, i.e. the trace of any stress-energy tensor which satisfies the Wald axioms is non-vanishing in the conformally invariant case $m = 0$, $\xi = \frac{1}{6}$ [121].

Two proposals have been made in order to motivate the ad-hoc subtraction (2.30) on conceptual grounds. In [91] it has been suggested that the Wick-ordering prescription should be kept, but that the classical expression $T_{\mu\nu}$ entering the definition of $:T_{\mu\nu}:_H$ should be modified in such a way that it coincides with the canonical classical stress-energy tensor on-shell but gives a conserved observable upon quantization. In [72] instead it has been argued that the Wick-ordering prescription should be modified without changing the classical expression. This point of view has the advantage that it fits into the general framework of defining local and covariant Wick polynomials introduced in [70, 72]. In particular it is possible to alter uniformly the definition of all local Wick polynomials induced by Wick-ordering with respect to a purely geometric Hadamard parametrix H in such a way that (a) all axioms for local Wick polynomials mentioned at the end of Sect. 2.6.1 are still satisfied and (b) the canonical stress-energy tensor Wick-ordered with respect to this prescription is conserved [72]. In the aforementioned reference it has also been argued that this point of view has the further advantage that it is applicable even to perturbatively constructed interacting models. Notwithstanding, we shall review the approach of [91] in the following for ease of presentation.

To this avail, we modify the classical stress-energy tensor by setting

$$T^c_{\mu\nu} \doteq T^{\mathrm{can}}_{\mu\nu} + c g_{\mu\nu} \phi P \phi \,,$$

where $T^{\mathrm{can}}_{\mu\nu}$ is the canonical expression and c is a suitable constant to be fixed later. We then define $:T_{\mu\nu}:$ by

$$:T_{\mu\nu}: \doteq :T^c_{\mu\nu}:_H \,,$$

where $:\cdot:_H$ indicates Wick-ordering (i.e. point-splitting regularisation) with respect to a purely geometric $H = \frac{h}{8\pi^2}$ of the form (2.12) with $w = 0$. Following the arguments of the previous section, the expectation value of $:T_{\mu\nu}:$ in a Hadamard state ω whose two-point function is (locally) of the form $\omega_2 = H + \frac{w}{8\pi^2}$ may be computed as

$$\omega\left(:T_{\mu\nu}(x):\right) = \frac{\left[D^{\mathrm{c}}_{\mu\nu} w\right]}{8\pi^2} \,, \tag{2.31}$$

where

$$\begin{aligned} D^c_{\mu\nu} &\doteq D^{\mathrm{can}}_{\mu\nu} + c g_{\mu\nu} P_x \\ &= (1-2\xi) g^{\nu'}_{\nu} \nabla_\mu \nabla_{\nu'} - 2\xi \nabla_\mu \nabla_\nu + \xi G_{\mu\nu} \\ &\quad + g_{\mu\nu} \left\{ 2\xi \Box_x + \left(2\xi - \frac{1}{2}\right) g^{\rho'}_{\rho} \nabla^\rho \nabla_{\rho'} - \frac{1}{2} m^2 \right\} + c g_{\mu\nu} P_x \,. \end{aligned} \tag{2.32}$$

The following result can now be shown [91].

Theorem 2.9 *Let $\omega(:T_{\mu\nu}(x):)$ be defined as in (2.31) with $c = \frac{1}{3}$.*

(a) $\omega(:T_{\mu\nu}(x):)$ is covariantly conserved, i.e.

$$\nabla^\mu \omega\left(:T_{\mu\nu}(x):\right) = 0\,.$$

(b) The trace of $\omega(:T_{\mu\nu}(x):)$ equals

$$g^{\mu\nu}\omega\left(:T_{\mu\nu}(x):\right) = \frac{1}{4\pi^2}\,[v_1] - \frac{1}{8\pi^2}\left(3\left(\frac{1}{6}-\xi\right)\Box + m^2\right)[w]$$

$$= \frac{1}{2880\pi^2}\left(\frac{5}{2}\,(6\xi-1)\,R^2 + 6(1-5\xi)\Box R + C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} + R_{\alpha\beta}R^{\alpha\beta} - \frac{R^2}{3}\right)$$

$$+\frac{1}{4\pi^2}\left(\frac{m^4}{8} + \frac{(6\xi-1)\,m^2 R}{24}\right) - \frac{1}{8\pi^2}\left(3\left(\frac{1}{6}-\xi\right)\Box + m^2\right)[w]\,,$$

which, for $m = 0$ and $\xi = \frac{1}{6}$, constitutes the trace anomaly *of the quantum stress-energy tensor.*

(c) The conservation and trace anomaly are independent of the chosen scale λ in the Hadamard parametrix h. Namely, a change

$$\lambda \;\mapsto\; \lambda'$$

results in

$$\omega(:T_{\mu\nu}(x):) \;\mapsto\; \omega(:T_{\mu\nu}(x):)' = \omega(:T_{\mu\nu}(x):) + \delta T_{\mu\nu}\,,$$

where

$$\delta T_{\mu\nu} \doteq \frac{2\log\lambda/\lambda'}{8\pi^2}\left[D^c_{\mu\nu}\;v\right] = \frac{2\log\lambda/\lambda'}{8\pi^2}\left[D^{\text{can}}_{\mu\nu}\;v\right] \tag{2.33}$$

$$= \frac{2\log\lambda/\lambda'}{8\pi^2}\left(\frac{m^2(6\xi-1)G_{\mu\nu}}{12} - \frac{m^4}{8}g_{\mu\nu} + \frac{1}{360}(I_{\mu\nu} - 3J_{\mu\nu}) - \frac{(6\xi-1)^2}{144}I_{\mu\nu}\right)$$

is a conserved tensor which has vanishing trace for $m = 0$ and $\xi = \frac{1}{6}$.

Proof 1. Leaving c undetermined and employing Synge's rule (cf. Lemma 2.4), we compute

$$8\pi^2\nabla^\mu\omega\left(:T_{\mu\nu}(x):\right) = \nabla^\mu\left[D^c_{\mu\nu}\;w\right] = \left[(\nabla^\mu + g^\mu_{\mu'}\nabla^{\mu'})D^c_{\mu\nu}\;w\right]$$

$$= \left[-\left(g_\nu^{\nu'} \nabla_{\nu'} P_x + c(g_\nu^{\nu'} \nabla_{\nu'} P_x + \nabla_\nu P_x) \right) w \right] .$$

Let us now recall that $P_x(h+w)=0$ and, hence, $P_x w = -P_x h$. Inserting this and the identities found in Lemma 2.5, we obtain

$$8\pi^2 \nabla^\mu \omega \left(:T_{\mu\nu}(x): \right) = -\left[\left(-g_\nu^{\nu'} \nabla_{\nu'} P_x + c(g_\nu^{\nu'} \nabla_{\nu'} P_x + \nabla_\nu P_x) \right) h \right]$$

$$= (6c-2)\,[v_1]_{;\nu} \ .$$

This proves the conservation for $c = \frac{1}{3}$.

2. It is instructive to leave c undetermined also in this case. Employing Synge's rule and the results of Lemma 2.5, we find

$$8\pi^2 g^{\mu\nu} \omega \left(:T_{\mu\nu}(x): \right) = 8\pi^2 g^{\mu\nu} \left[D^c_{\mu\nu} \ w \right]$$

$$= (4c-1)[P_x w] - \left(3\left(\frac{1}{6} - \xi \right) \Box + m^2 \right) [w]$$

$$= (4c-1)6[v_1] - \left(3\left(\frac{1}{6} - \xi \right) \Box + m^2 \right) [w] \, .$$

Inserting $c = \frac{1}{3}$ yields the wanted result.

3. The proof ensues without explicitly computing $\delta T_{\mu\nu}$ in terms of the stated conserved tensors from the following observation. Namely, a change of scale as considered transforms w by a adding a term $2\log\lambda/\lambda' v$. Hence, our computations for proving the first two statements entail

$$\frac{8\pi^2}{2\log\lambda/\lambda'} \nabla^\mu \delta T_{\mu\nu} = \left[\left(-g_\nu^{\nu'} \nabla_{\nu'} P_x + c(g_\nu^{\nu'} \nabla_{\nu'} P_x + \nabla_\nu P_x) \right) v \right] ,$$

$$\frac{8\pi^2}{2\log\lambda/\lambda'} g^{\mu\nu} \delta T_{\mu\nu} = -(4c-1)[P_x v] - \left(3\left(\frac{1}{6} - \xi \right) \Box + m^2 \right) [v] \, .$$

The former term vanishes because $P_x v = 0$ as discussed in Sect. 2.4, and the same holds for the latter term if we insert $\xi = \frac{1}{6}$ and $m = 0$.

The proof the second statement clearly shows that there is a possibility to assure vanishing trace in the conformally invariant case, but this possibility is not compatible with conservation. Moreover, we have stated the last result in explicit terms in order to show how a change of scale in the Hadamard parametrix is compatible with the renormalisation freedom of the quantum stress-energy tensor. Finally, we stress that the term added to the canonical stress-energy tensor is compatible with local covariance because the corresponding change of the quantum stress-energy tensor is proportional to $g_{\mu\nu}[v_1]$, i.e. a local curvature tensor.

We would also like to point out that the above explicit form of the trace anomaly has also been known before Hadamard point-splitting had been developed. Particularly, the same result had been obtained by means of so-called *DeWitt-Schwinger point-splitting* in [23]. This renormalisation prescription is a priori not rigorously defined on Lorentzian spacetimes and the Hadamard point-splitting computation in [121] had therefore been the first rigorous derivation of the trace anomaly of the stress-energy tensor. However, DeWitt-Schwinger point-splitting can be reformulated on rigorous grounds, cf. [62].

2.7 Further Reading

The review of algebraic quantum field theory on curved spacetimes in this chapter has covered aspects of this framework which are relevant for the applications discussed in the following chapter. Recent reviews which deal with aspects and constructions not covered in the present chapter, or provide further details, are [52, 73] and [7, 46, 53, 81], which are part of [16]. A historical account of quantum field theory in curved spacetimes may be found in [124].

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