Chapter 5 Quantum Field Theory on Curved Backgrounds

Romeo Brunetti and Klaus Fredenhagen

5.1 Introduction

Quantum field theory is an extremely successful piece of theoretical physics. Based on few general principles, it describes with an incredibly good precision large parts of particle physics. But also in other fields, in particular in solid state physics, it yields important applications. At present, the only problem which seems to go beyond the general framework of quantum field theory is the incorporation of gravity. Quantum field theory on curved backgrounds aims at a step toward solving this problem by neglecting the back reaction of the quantum fields on the spacetime metric.

Quantum field theory has a rich and rather complex structure. It appears in different versions that are known to be essentially equivalent. Unfortunately, large parts of the theory are available only at the level of formal perturbation theory, and a comparison of the theory with experiments requires a truncation of the series which is done with a certain arbitrariness.

Due to its rich structure, quantum field theory is intimately related to various fields of mathematics and has often challenged the developments of new mathematical concepts.

In this chapter we will give an introduction to quantum field theory in a formulation which admits a construction on generic spacetimes. Such a construction is possible in the so-called algebraic approach to quantum field theory [1, 2]. The more standard formulation as one may find it in typical text books (see, e.g., [3]) relies heavily on concepts like vacuum, particles, energy, and makes strong use of the connection to statistical mechanics via the so-called Wick rotation. But these concepts lose their meaning on generic Lorentzian spacetimes and are therefore

R. Brunetti (🖂)

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Dipartimento di Matematica, Università di Trento, Via Sommarive 14, I-38050 Povo (TN) e-mail: brunetti@science.unitn.it; romeo.brunetti@gmail.com

K. Fredenhagen (⊠)

II. Institut für Theoretische Physik, Universität Hamburg, Luruper Chaussee 149,

D-22761 Hamburg, Germany

e-mail: klaus.fredenhagen@desy.de

restricted to a few examples with high symmetry. It was a major progress of recent years that local versions of most of these concepts have been found. Their formulation requires the algebraic framework of quantum physics and, on the more technical side, the replacement of momentum space techniques by techniques from microlocal analysis.

The plan of the chapter is as follows. After a general discussion of fundamental physical concepts like states, observables, and subsystems we will describe a general framework that can be used to define both classical and quantum field theories. It is based on the locally covariant approach to quantum field theory [4] which uses the language of categories to incorporate the principle of general covariance.

The first example of the general framework is the canonical formalism of classical field theory based on the so-called Peierls bracket by which the algebra of functionals of classical field configurations is endowed with a Poisson structure.

We then present as a simple example in quantum field theory the free scalar quantum field.

A less simple example is the algebra of Wick polynomials of the free field. Here, for the first time, techniques from microlocal analysis enter. The construction relies on a groundbreaking observation of Radzikowski [5]. Radzikowski found that the so-called Hadamard condition on the two-point correlation function is equivalent to a positivity condition on the wave front set, whose range of application was extended and named "microlocal spectrum condition" few years later [6]. This insight not only, for the first time, permitted the construction of nonlinear fields on generic spacetimes but also paved the way for a purely algebraic construction, which before was also unknown on Minkowski space.

Based on these results, one now can construct also interacting quantum field theories in the sense of formal power series. The construction can be reduced to the definition of time-ordered products of prospective Lagrangians. By the principle of causality, the time-ordered products of *n* factors are determined by products (in the sense of the algebra of Wick polynomials) of time-ordered products of less than *n* factors outside of the thin diagonal $\Delta_n \subset \mathcal{M}^n$ (considered as algebra-valued distributions). The removal of ultraviolet divergences amounts in this framework to the extension of distributions on $\mathcal{M}^n \setminus \Delta_n$ to \mathcal{M}^n . The possible extensions can be discussed in terms of the so-called microlocal scaling degree which measures the singularity of the distribution transversal to the submanifold Δ_n .

5.2 Systems and Subsystems

5.2.1 Observables and States

Experiments on a physical system may be schematically described as maps

experiment : (state, observable)
$$\mapsto$$
 result. (5.1)

Here a state is understood as a prescription for the preparation of the system, and the observable is an operation on the prepared system which yields a definite result. In

classical physics, one assumes that an optimally prepared system (pure state) yields for a given (ideal) observable always the same result (which may be recorded as a real number). Thus observables can be identified with real-valued functions on the set of pure states. The set of observables so gets the structure of an associative, commutative algebra over \mathbb{R} , and the pure states are reobtained as characters of the algebra, i.e., homomorphisms into \mathbb{R} .

In classical statistical mechanics one considers also incomplete preparation prescriptions, e.g., one puts a number of particles into a box with a definite total energy, but without fixing positions and momenta of the individual particles. Such a state corresponds to a probability measure μ on the set of pure states, or, equivalently, to a linear functional on the algebra of observables which is positive on positive functions and assumes the value 1 on the unit observable. For the observable f the state yields the probability distribution

$$(\mu, f) \mapsto f_{\star}\mu, \ f_{\star}\mu(I) = \mu(f^{-1}(I))$$
 (5.2)

on \mathbb{R} . Pure states are the Dirac measures.

In quantum mechanics, the measurement results fluctuate even in optimally prepared states. Pure states are represented by one-dimensional subspaces \mathfrak{L} of some complex Hilbert space, and observables are identified with self-adjoint operators A. The probability distribution of measured values is given by

$$\mu_{A,\mathfrak{L}}(I) = (\Psi, E_A(I)\Psi), \tag{5.3}$$

where Ψ is any unit vector in \mathfrak{L} and $E_A(I)$ is the spectral projection of A corresponding to the interval I.

In quantum statistics, one admits a larger class of states, corresponding to incomplete preparation, which can be described by a density matrix, i.e., a positive trace class operator ρ with trace 1; the probability distribution is given by

$$\mu_{A,\rho}(I) = \operatorname{Tr}\rho E_A(I), \tag{5.4}$$

where the pure states correspond to the rank 1 density matrices.

In spite of the apparently rather different structures one can arrive at a unified description. The set of observables is a real vector space with two products:

1. a commutative, but in general nonassociative product (the Jordan product),

$$A \circ B = \frac{1}{4} \left((A+B)^2 - (A-B)^2 \right), \tag{5.5}$$

arising from the freedom of relabeling measurement results;

2. an antisymmetric product

$$\{A, B\},\tag{5.6}$$

which is known as the Poisson bracket in classical mechanics and is given by $\frac{i}{\hbar}$ times the commutator $[\cdot, \cdot]$ in quantum mechanics. This product originates from the fact that every observable *H* can induce a transformation of the system by Hamilton's (or Heisenberg's) equation

$$\frac{d}{dt}A(t) = \{H, A(t)\}.$$
(5.7)

The two products satisfy the following conditions:

- 1. $A \mapsto \{B, A\}$ is a derivation with respect to both products.
- 2. The associators of both products are related by

$$(A \circ B) \circ C - A \circ (B \circ C) = \frac{\hbar^2}{4} \left(\{ \{A, B\}, C\} - \{A, \{B, C\}\} \right).$$
(5.8)

While the first condition is motivated by the interpretation of Hamilton's equation as an infinitesimal symmetry, there seems to be no physical motivation for the second condition. But mathematically, it has a strong impact: in classical physics $\hbar = 0$, hence the Jordan product is associative; in quantum physics, the condition implies that

$$AB := A \circ B + \frac{\hbar}{2i} \{A, B\}$$
(5.9)

is an associative product on the complexification $\mathfrak{A} = \mathfrak{A}_{\mathbb{R}} \otimes \mathbb{C}$, where the information on the real subspace is encoded in the \star -operation

$$(A \otimes z)^* = A \otimes \overline{z}. \tag{5.10}$$

States are defined as linear functionals on the algebra which assume positive values on positive observables and are 1 on the unit observable. A priori, in the case $\hbar \neq 0$ the positivity condition on the subspace $\mathfrak{A}_{\mathbb{R}}$ of self-adjoint elements could be weaker than the positivity requirement on the complexification \mathfrak{A} . Namely, on the real subspace we call positive every square of a self-adjoint element, whereas on the full algebra positive elements are absolute squares of the form

$$(A - iB)(A + iB) = A^2 + B^2 + \hbar \{A, B\}, A, B \text{ self-adjoint}.$$
 (5.11)

But under suitable completeness assumptions, in particular when \mathfrak{A} is a *C**-algebra, operators as above admit a self-adjoint square root; thus the positivity conditions coincide in these cases. If one is in a more general situation, one has to require that states satisfy the stronger positivity condition, in order to ensure the existence of the GNS representation.

5.2.2 Subsystems

A system may be identified with a unital C^* -algebra \mathfrak{A} . Subsystems correspond to sub- C^* -algebras \mathfrak{B} with the same unit. A state of a system then induces a state on the subsystem by restricting the linear functional ω on \mathfrak{A} to the subalgebra \mathfrak{B} . The induced state may be mixed even if the original state was pure, see Remark 13 on page 23.

One may also ask whether every state on the subalgebra \mathfrak{B} arises as a restriction of a state on \mathfrak{A} . This is actually true, namely let ω be a state on \mathfrak{B} . According to the Hahn–Banach theorem, ω has an extension to a linear functional $\tilde{\omega}$ on \mathfrak{A} with $\|\tilde{\omega}\| = \|\omega\|$. But $\tilde{\omega}(1) = \omega(1) = \|\omega\| = 1$, hence $\tilde{\omega}$ is a state.

Two subsystems \mathfrak{B}_1 and \mathfrak{B}_2 may be called independent whenever the algebras \mathfrak{B}_1 and \mathfrak{B}_2 commute and

$$B_1 \otimes B_2 \mapsto B_1 B_2 \tag{5.12}$$

defines an isomorphism from the tensor product $\mathfrak{B}_1 \otimes \mathfrak{B}_2$ to the algebra generated by \mathfrak{B}_1 and \mathfrak{B}_2 .

Given states ω_i on \mathfrak{B}_i , i = 1, 2, one may define a product state on $\mathfrak{B}_1 \otimes \mathfrak{B}_2$ by

$$(\omega_1 \otimes \omega_2)(B_1 \otimes B_2) = \omega_1(B_1)\omega(B_2), \tag{5.13}$$

see Section 5.5 on page 23 for a thorough discussion. Convex combinations of product states are called separable. As was first observed by Bell, there exist nonseparable states if both algebras contain subalgebras isomorphic to $M_2(\mathbb{C})$. This is the famous phenomenon of entanglement which shows that states in quantum physics may exhibit correlations between independent systems which cannot be described in terms of states of the individual systems. This is the reason, why the notion of locality is much more evident on the level of observables than on the level of states.

5.2.3 Algebras of Unbounded Operators

In applications often the algebra of observables cannot be equipped with a norm. The CCR algebra is a prominent example. In these cases one usually still has a unital *-algebra, and states can be defined as positive normalized functionals. The GNS construction remains possible, but does not lead to a representation by bounded Hilbert space operators. In particular it is not guaranteed that self-adjoint elements of the algebra are represented by self-adjoint Hilbert space operators. There is no general theory available which yields a satisfactory physical interpretation in this situation. One therefore should understand it as an intermediary step toward a formulation in terms of C^* -algebras.

5.3 Locally Covariant Theories

5.3.1 Axioms of Locally Covariant Theories

Before constructing examples of classical and quantum field theories we want to describe the minimal requirements that such theories should satisfy the follow-ing [4]:

- 1. To each globally hyperbolic time-oriented spacetime \mathcal{M} we associate a unital *-algebra $\mathfrak{A}(\mathcal{M})$.
- 2. Let $\chi : \mathcal{M} \to \mathcal{N}$ be an isometric embedding which preserves causal relations in the sense that whenever $\chi(x) \in J^{\mathcal{N}}_+(\chi(y))$ for some points $x, y \in \mathcal{M}$ then $x \in J^{\mathcal{M}}_+(y)$. Then there is an injective homomorphism

$$\alpha_{\chi}: \mathfrak{A}(\mathcal{M}) \to \mathfrak{A}(\mathcal{N}). \tag{5.14}$$

3. Let $\chi:\mathcal{M}\to\mathcal{N}$ and $\chi':\mathcal{N}\to\mathcal{L}$ be causality-preserving isometric embeddings. Then

$$\alpha_{\chi' \circ \chi} = \alpha_{\chi'} \alpha_{\chi}. \tag{5.15}$$

These axioms characterize a quantum field theory as a covariant functor \mathfrak{A} from the category $\mathfrak{M}\mathfrak{a}\mathfrak{n}$ of globally hyperbolic time-oriented Lorentzian manifolds with isometric causality-preserving mappings as morphisms to the category of unital *-algebras \mathfrak{Alg} with injective homomorphisms as morphisms, where \mathfrak{A} acts on morphisms by $\mathfrak{A}\chi = \alpha_{\chi}$.

In addition we require

- 4. Let $\chi_i : \mathcal{M}_i \to \mathcal{N}, i = 1, 2$, be morphisms with causally disjoint images. Then the images of $\mathfrak{A}(\mathcal{M}_1)$ and $\mathfrak{A}(\mathcal{M}_2)$ represent independent subsystems of $\mathfrak{A}(\mathcal{N})$ in the sense of Sect. 5.2.2 (Einstein causality).
- 5. Let $\chi : \mathcal{M} \to \mathcal{N}$ be a morphism such that its image contains a Cauchy surface of \mathcal{N} . Then α_{χ} is an isomorphism (Time slice axiom).

Axiom 4 means that causally separated subsystems do not influence each other. It is equivalent to a tensor structure of the functor \mathfrak{A} , namely $\mathfrak{M}\mathfrak{a}\mathfrak{n}$ is a tensor category by the disjoint union, with the empty set as a unit object, \mathfrak{Alg} has the tensor product of algebras as a tensor structure, with the set of complex numbers as a unit object. We set $\mathfrak{A}(\emptyset) = \mathbb{C}$ and $\mathfrak{A}(\mathcal{N} \otimes \mathcal{M}) = \mathfrak{A}(\mathcal{N}) \otimes \mathfrak{A}(\mathcal{M})$. If ι_i denotes the natural embedding of spacetime \mathcal{N}_i into the disjoint union $\mathcal{N}_1 \otimes \mathcal{N}_2$, then

$$\alpha_{\iota_1}(A_1) = A_1 \otimes 1 , \ \alpha_{\iota_2}(A_2) = 1 \otimes A_2 , \ A_i \in \mathfrak{A}(\mathcal{N}_i) , \ i = 1, 2.$$
(5.16)

The crucial observation is now that a causality-preserving embedding χ of a disjoint union $\mathcal{N}_1 \otimes \mathcal{N}_2$ maps the components $\mathcal{N}_1, \mathcal{N}_2$ into causally disjoint subregions $\chi \circ \iota_1(\mathcal{N}_1), \chi \circ \iota_2(\mathcal{N}_2)$. Hence we obtain the following theorem

Theorem 1. Let \mathfrak{A} be a tensor functor, i.e., for morphisms $\chi_i : \mathcal{N}_i \to \mathcal{M}_i$, i = 1, 2 we have

$$\alpha_{\chi_1 \otimes \chi_2} = \alpha_{\chi_1} \otimes \alpha_{\chi_2}. \tag{5.17}$$

Then \mathfrak{A} satisfies Einstein causality. On the other hand, let \mathfrak{A} be defined only on connected spacetimes and assume that it satisfies Einstein causality. Then it can be uniquely extended to a tensor functor on spacetimes with finitely many connected components.

Axiom 5 may be understood as a consequence of the existence of a dynamical law which has the features of a hyperbolic differential equation with a well-posed Cauchy problem. It relates to cobordisms of Lorentzian manifolds. Namely, we may associate with a Cauchy surface $\Sigma \subset \mathcal{M}$ the inverse limit of algebras $\mathfrak{A}(\mathcal{N}), \Sigma \subset \mathcal{N} \subset \mathcal{M}$. The inverse limit is constructed in the following way. We consider families $(A_{\mathcal{N}})$, indexed by spacetimes \mathcal{N} with $\Sigma \subset \mathcal{N} \subset \mathcal{M}$, which satisfy the condition

$$\alpha_{\mathcal{N}_1\mathcal{N}_2}(A_{\mathcal{N}_2}) = A_{\mathcal{N}_1}.\tag{5.18}$$

where $\mathcal{N}_1 \mathcal{N}_2$ denotes the embedding $\mathcal{N}_2 \subset \mathcal{N}_1$. Two such families are called equivalent if they coincide for sufficiently small spacetimes. The algebra $\mathfrak{A}(\Sigma)$ is now defined as the algebra generated by these equivalence classes. By $\alpha_{\mathcal{M}\Sigma}(A) = \alpha_{\mathcal{M}\mathcal{N}}(A_N)$ one defines a homomorphism from $\mathfrak{A}(\Sigma)$ into $\mathfrak{A}(\mathfrak{M})$. The construction described above can be done for every submanifold. We now use the time slice axiom. Due to this axiom, the homomorphisms $\alpha_{\mathcal{N}_1\mathcal{N}_2}$ are invertible. As a consequence, $\alpha_{\mathcal{M}\Sigma}$ is an isomorphism. Therefore, one obtains a time evolution as a propagation between Cauchy surfaces, namely the propagation from Σ to another Cauchy surface Σ' is described by the isomorphism

$$\alpha_{\Sigma'\Sigma} = \alpha_{\mathcal{M}\Sigma'}^{-1} \alpha_{\mathcal{M}\Sigma}.$$
(5.19)

This solves a longstanding problem dating back to ideas of Schwinger who postulated a generally covariant form of the Schrödinger equation. In its original form, as a unitary map between Hilbert spaces it cannot be realized even for free fields on Minkowski space. But in the sense of algebraic isomorphisms it always holds, provided the time slice axiom is satisfied.

In perturbation theory one wants to change the dynamical law. During the construction of the theory it turns out to be fruitful to relax the conditions so that the time slice axiom does not hold (off-shell formalism). The new dynamical law then defines an ideal of the algebra, such that the quotient again satisfies the time slice axiom.

In algebraic quantum field theory, one considers a net of subalgebras labeled by subregions of a given spacetime and requires that the net satisfies certain axioms, the Haag–Kastler, axioms. The formalism above is a proper generalization in the following sense. If we restrict our functor to the globally hyperbolic subregions \mathcal{N} of a given globally hyperbolic spacetime \mathcal{M} , we obtain a net of subalgebras $(\alpha_{\mathcal{M}\mathcal{N}}(\mathfrak{A}(\mathcal{N})))$ with the proper inclusions. Moreover, isometries of \mathcal{M} immediately induce further embeddings, such that the functoriality of \mathfrak{A} implies covariance under symmetries. Clearly Axioms 4 and 5 correspond to the locality and the primitive causality axioms of the Haag–Kastler framework.

5.3.2 Fields as Natural Transformations

In quantum field theory fields are defined as distributions with values in the algebra of observables. They are required to transform covariantly under isometries of spacetime. On a first sight, it seems that the latter requirement becomes empty on generic spacetimes. Moreover, it seems to be difficult to compare fields which are defined on different spacetimes. But it turns out that the locally covariant framework offers the possibility for a new concept of fields. The idea is that fields have to be defined simultaneously on all spacetimes in a coherent way, namely fields may be defined as natural transformations between a functor, say \mathcal{D} , that associates with each spacetime \mathcal{M} a space of test functions $\mathcal{D}(\mathcal{M})$ and the previous functor of a specific locally covariant theory. Here $\mathcal{D}\chi$ for an embedding $\chi : \mathcal{N} \to \mathcal{M}$ is the pushforward χ_* which is defined on functions with compact support by

$$\chi_* f(x) = \begin{cases} f(\chi^{-1}(x)) , \ x \in \chi(\mathcal{N}) \\ 0 , \ \text{else} \end{cases},$$
(5.20)

thus \mathcal{D} is a covariant functor. A natural transformation Φ from \mathcal{D} to \mathfrak{A} is a family $(\Phi_{\mathcal{M}})_{\mathcal{M}\in\mathfrak{Man}}$ of linear maps $\Phi_{\mathcal{M}}: \mathcal{D}(\mathcal{M}) \to \mathfrak{A}(\mathcal{M})$ which satisfy the following commutative diagram:

$$\begin{array}{ccc} \mathcal{D}(\mathcal{M}) & \stackrel{\varPhi_{\mathcal{M}}}{\longrightarrow} \mathfrak{A}(\mathcal{M}) \\ \\ \chi_* & & & \downarrow^{\alpha_{\chi}} \\ \mathcal{D}(\mathcal{N}) & \stackrel{\varPhi_{\mathcal{N}}}{\longrightarrow} \mathfrak{A}(\mathcal{N}) \end{array}$$

The commutativity of the diagram means that the field $\Phi \equiv (\Phi_M)_{M \in \mathfrak{Man}}$ has the covariance property

$$\alpha_{\chi} \circ \Phi_{\mathcal{M}} = \Phi_{\mathcal{N}} \circ \chi_{*}.$$

In case χ is an isometry of a given spacetime, this reduces to the standard covariance condition for quantum fields.

The covariance condition immediately implies that the field, restricted to a small neighborhood of a given point, can depend only on the metric within the same neighborhood. Together with some more technical conditions, this was used in [7] to prove that fields can be uniquely fixed on all spacetimes by finitely many parameters. This allows a comparison of states on different spacetimes in terms of expectation values of locally covariant fields.

Also other structures in quantum field theory can be understood in terms of natural transformations. In particular one can relax the linearity condition. The naturality requirement turns out to be the crucial condition which restricts the ambiguity of the renormalization procedure.

5.4 Classical Field Theory

Before entering the somewhat involved problems of quantum field theory, we want to demonstrate that many of the general structures are already present in classical field theory. As discussed in Sect. 5.2, this amounts to the replacement of associative complex algebras by real Poisson algebras.

5.4.1 Classical Observables

Let φ be a scalar field on a globally hyperbolic spacetime \mathcal{M} . The space of smooth field configurations is denoted by $\mathfrak{C}(\mathcal{M}) := \mathcal{C}^{\infty}(\mathcal{M})$. \mathfrak{C} may be considered as a contravariant functor by identifying $\mathfrak{C}\chi$ for an embedding χ with the pullback $\chi^* h = h \circ \chi$. The basic observables are the evaluation functionals

$$\varphi(x)(h) = h(x), \ h \in \mathfrak{C}(\mathcal{M}).$$
(5.21)

More generally, we consider spaces of maps $F : \mathfrak{C}(\mathcal{M}) \to \mathbb{C}$ which transform covariantly under embeddings, $\chi_*F(\varphi) = F(\varphi \circ \chi)$. We associate with each map $F : \mathfrak{C}(\mathcal{M}) \to \mathbb{C}$ a closed set $\operatorname{supp}(F)$ in analogy to the convention for distributions by

$$supp(F) = \{x \in \mathcal{M} | \forall neighborhoods \ U \text{ of } x \exists \varphi, h \in \mathfrak{C}(\mathcal{M}), supph \subset U \\ such that F(\varphi + h) \neq F(\varphi) \}.$$
(5.22)

We require that these maps have compact support and are differentiable in the sense that for every φ , $h \in \mathfrak{C}(\mathcal{M})$ the function $\lambda \mapsto F(\varphi + \lambda h)$ is infinitely often differentiable and the *n*th derivative at $\lambda = 0$ is for every φ a symmetric distribution $F^{(n)}(\varphi)$ on \mathcal{M}^n , such that

$$\frac{d^n}{d\lambda^n} F(\varphi + \lambda h)|_{\lambda=0} = \langle F^{(n)}(\varphi), h^{\otimes n} \rangle.$$
(5.23)

Note that these distributions automatically have compact support with

$$\operatorname{supp} F^{(n)}(\varphi) \subset (\operatorname{supp} F)^n.$$
(5.24)

Moreover, $F^{(n)}$, as a map on $\mathfrak{C}(\mathcal{M}) \times \mathcal{C}^{\infty}(\mathcal{M}^n)$, is required to be continuous (see [8] for an introduction to these mathematical notions).

In addition we have to impose conditions on the wave front sets of the functional derivatives (see page 98 for the definition of wave front sets). Here we use different options:

 $\mathcal{F}_0(\mathcal{M}) = \{ F \text{ differentiable with compact support }, WF(F^{(n)}(\varphi)) = \emptyset \}.$ (5.25)

An example for such an observable is

$$F(\varphi) = \frac{1}{n!} \int d\operatorname{vol}_n f(x_1, \dots, x_n) \varphi(x_1) \cdots \varphi(x_n),$$

with a symmetric test function $f \in \mathcal{D}(\mathcal{M}^n)$, with the functional derivatives

$$\langle F^{(k)}(\varphi), h^{\otimes k} \rangle = \frac{1}{k!} \int d\operatorname{vol}_n f(x_1, \dots, x_n) h(x_1) \cdots h(x_k) \varphi(x_{k+1}) \cdots \varphi(x_n).$$
(5.26)

This class unfortunately does not contain the most interesting observables, namely the nonlinear local ones. We call a map *F* local, if it satisfies the following additivity relation for $\varphi, \psi, \chi \in \mathfrak{C}(\mathcal{M})$ with supp $\varphi \cap$ supp $\chi = \emptyset$:

$$F(\varphi + \psi + \chi) = F(\varphi + \psi) - F(\psi) + F(\psi + \chi)). \tag{5.27}$$

For differentiable maps *F* this condition immediately implies that all functional derivatives $F^{(n)}(\varphi)$ have support on the thin diagonal

$$\Delta_n := \{ (x_1, \dots, x_n) \in \mathcal{M}^n, x_1 = \dots = x_n \}.$$
(5.28)

In particular the wave front sets for $n \ge 2$ cannot be empty for $F^{(n)} \ne 0$. The best we can require is that their wave front sets are orthogonal to the tangent bundle of the thin diagonal, considered as a subset of the tangent bundle of \mathcal{M}^n . A simple example is $F = \frac{1}{2} \int dvol f(x)\varphi(x)^2$ with a test function $f \in \mathcal{D}(\mathcal{M})$ where the second functional derivative at the origin is

$$\langle F^{(2)}(0), h \rangle = \int d\operatorname{vol} f(x)h(x, x).$$
(5.29)

The set of local functionals which are compactly supported, infinitely differentiable, and have wave front sets orthogonal to the tangent bundle of the thin diagonal is denoted by $\mathcal{F}_{loc}(\mathcal{M})$. The set of local functionals contains in particular the possible interactions.

Examples for local functionals can be given in terms of functions on the jet bundle,

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$$F(\varphi) = \int d\text{vol} f(j_x(\varphi)), \qquad (5.30)$$

where $j_x(\varphi) = (x, \varphi(x), \nabla \varphi(x), \dots)$. Actually, every $F \in \mathcal{F}_{loc}$ is of this form [9]

Theorem 2. Let $F \in \mathcal{F}_{loc}$. Then there exists a function f on the jet bundle such that (5.30) holds.

Proof. By the fundamental theorem of calculus we have

$$F(\varphi) = F(0) + \int d\lambda \langle F^{(1)}(\lambda\varphi), \varphi \rangle.$$
(5.31)

By the assumption on the wave front set of F, the first derivative is a test function $x \mapsto F^{(1)}(\lambda \varphi)(x)$ with compact support. We have to prove that the value of this function at any point x depends only on the jet of φ at the point x. Let h be a test function with vanishing derivatives at x. Again from the fundamental theorem of calculus we get

$$F^{(1)}(\lambda(\varphi+h))(x) - F^{(1)}(\lambda\varphi)(x) = \int d\mu \langle F^{(2)}(\lambda(\varphi+\mu h))(x), \lambda h \rangle.$$
 (5.32)

But $F^{(2)}(\lambda(\varphi + \mu h))$ is a distribution with support on the diagonal with wave front set orthogonal to the tangent bundle of the diagonal, thus in a chart near *x* it is a finite derivative of a δ distribution in the difference variables with smooth coefficients. Hence the right-hand side of (5.32) vanishes.

The space $\mathcal{F}_{loc}(\mathcal{M})$ is not closed under products. We therefore have to introduce a larger set. We choose a set which will turn out to be closed not only under the classical (pointwise) product but also under the other products we want to introduce, namely the Poisson bracket and the associative product of quantum physics. Moreover it will contain the (renormalized) time-ordered products of local functionals which are needed for the perturbative construction of interactions. These products are defined in terms of functional derivatives multiplied by Green's functions of normal hyperbolic differential operators. One therefore has to choose functionals whose derivatives have wave front sets which allow the multiplication by Green's functions. A convenient condition on the wave front sets is that they contain no covector $(x_1, \ldots, x_n; k_1, \ldots, k_n)$ where all k_i are elements of the closed forward light cone $\overline{V}_+(x_i)$ over the base point $x_i \in \mathcal{M}$ or all of them belong to the respective past light cones. Let $\overline{V}_{\pm} = \{(x, k) \in T^*(\mathcal{M}) | k \in \overline{V}_{\pm}(x)\}$. We then set

$$\mathcal{F}(\mathcal{M}) = \{ F \text{ differentiable with compact support,} \\ WF(F^{(n)}(\varphi)) \cap ((\overline{V}_{+}^{n} \cup \overline{V}_{-}^{n})) = \emptyset \}.$$
(5.33)

This set contains in particular the local functionals. The condition on the wave front sets will turn out to be crucial in quantum field theory.

5.4.2 Classical Dynamics

The dynamics of a classical field theory is usually given in terms of an action, e.g., $S_0(\varphi) = \int d\text{vol } \mathcal{L} \circ j_x(\varphi)$, with

$$\mathcal{L} = \frac{1}{2}g(d\varphi, d\varphi) - V(\varphi), \qquad (5.34)$$

where *V* is a smooth real function. But S_0 is, for noncompact spacetimes \mathcal{M} , not defined for all $\varphi \in \mathfrak{C}(\mathcal{M})$; we therefore multiply \mathcal{L} by a test function $f \in \mathcal{D}(\mathcal{M})$ which is identical to 1 in a given relatively compact open region \mathcal{N} and obtain an element $\mathcal{L}(f) = \int d \operatorname{vol} f(x) \mathcal{L} \circ j_x(\varphi) \in \mathcal{F}_{\operatorname{loc}}(\mathcal{M})$. We then take the functional derivative of the modified action $\mathcal{L}(f)$, restrict it to \mathcal{N} , and obtain the field equation (Euler–Lagrange equation), (which is independent of the choice of f)

$$0 = \mathcal{L}^{(1)}(\varphi) = \frac{\partial \mathcal{L}}{\partial \varphi} - \nabla_{\mu} \frac{\partial \mathcal{L}}{\partial \nabla_{\mu} \varphi} = -\Box \varphi - V'(\varphi).$$
(5.35)

Since \mathcal{N} was arbitrary the field equation has the same form everywhere within \mathcal{M} .

The field equation may be linearized around an arbitrary field configuration φ . This amounts to the computation of the second derivative of the action. Again we restrict ourselves to a relatively compact open subregion \mathcal{N} and determine the second derivative of $\mathcal{L}(f)$, $f \equiv 1$ on \mathcal{N} . The second derivative then may be understood as a differential operator which in the example above takes the form

$$\mathcal{L}^{(2)}(\varphi)h(x) = (-\Box - V''(\varphi(x)))h(x).$$
(5.36)

We will only consider classical actions *S* such that the second derivative is a normal hyperbolic differential operator and thus according to Theorem 4 on page 78 possesses unique retarded and advanced Green's functions $\Delta_S^{R,A}$.

5.4.3 Classical Møller Operators

If the action is a quadratic function, the field equation is linear and may be solved in terms of the Green functions. We now want to interpolate between different actions S which differ by an element in $\mathcal{F}(\mathcal{M})$, in analogy to quantum mechanical scattering theory where isometries (the famous Møller operators) are constructed which intertwine the interacting Hamiltonian, restricted to the scattering states, with the free Hamiltonian. We interpret $S^{(1)}$ as a map from $\mathfrak{C}(\mathcal{M})$ to $\mathcal{E}'(\mathcal{M})$. We want to construct maps $r_{S_1S_2}$ (the retarded Møller operators) from $\mathfrak{C}(\mathcal{M})$ to itself with the properties

$$S_1^{(1)} \circ r_{S_1 S_2} = S_2^{(1)} ; (5.37)$$

$$r_{S_1S_2}(\varphi)(x) = \varphi(x), \ x \notin J_+(\operatorname{supp}(S_1 - S_2)).$$
 (5.38)

We set $S_1 = S + \lambda F$, $S_2 = S$, and differentiate (5.37) with respect to λ . Let $\varphi_{\lambda} = r_{S+\lambda F,S}(\varphi)$. We obtain

$$\langle (S+\lambda F)^{(2)}(\varphi_{\lambda}), \frac{d}{d\lambda}\varphi_{\lambda}\otimes h\rangle + \langle F^{(1)}(\varphi_{\lambda}), h\rangle = 0.$$
(5.39)

Together with condition (5.38) this implies that the Møller operators satisfy the differential equation

$$\frac{d}{d\lambda}\varphi_{\lambda} = -\Delta^{R}_{S+\lambda F}(\varphi_{\lambda})F^{(1)}(\varphi_{\lambda}).$$
(5.40)

This equation has a unique solution in terms of a formal power series in λ . Moreover, by the Nash–Moser theorem, one can show that solutions exist for small λ ([9], to appear).

5.4.4 Peierls Bracket

The Møller operators can be used to endow the algebra of functionals with a Poisson bracket. This was first proposed by Peierls [10], a complete proof was given much later by Marolf [11] (see also [12]). One first defines the retarded product of two functionals F and G by

$$R_{S}(F,G) = \frac{d}{d\lambda}G \circ r_{S+\lambda F,G}|_{\lambda=0}.$$
(5.41)

From (5.40) we obtain the explicit formula in terms of the retarded Green function

$$R_{S}(F,G) = -\langle G^{(1)}, \Delta_{S}^{R} F^{(1)} \rangle.$$
(5.42)

The Peierls bracket is then a measure for the mutual influence of two possible interactions

$$\{F, G\}_{S} = R_{S}(F, G) - R_{S}(G, F) = \langle F^{(1)}, \Delta_{S} G^{(1)} \rangle,$$
(5.43)

with the commutator function $\Delta_S = \Delta_S^R - \Delta_S^A$.

In Peierls original formulation the functionals were restricted to solutions of the Euler–Lagrange equations for *S*. It is then difficult to prove the Jacobi identity. Peierls does not give a general proof and shows instead that his bracket coincides in typical cases with the Poisson bracket in a Hamiltonian formulation.

In the off-shell formalism presented above the proof of the Jacobi identity is straightforward. It relies on the formula for the functional derivative of the retarded propagator

$$\langle\langle f, \Delta_S^R g \rangle^{(1)}, h \rangle = -\langle S^{(3)}, \Delta_S^A f \otimes \Delta_S^R g \otimes h \rangle,$$
(5.44)

which holds since the retarded propagator is an inverse of the operator associated with $S^{(2)}$, the corresponding formula for the advanced propagator and the symmetry of the third derivative of *S* as a trilinear functional.

In our off-shell formalism the Peierls bracket has the form

$$\{F, G\}_S = \langle F^{(1)}, \Delta_S G^{(1)} \rangle,$$
 (5.45)

with the commutator function $\Delta_S = \Delta_S^R - \Delta_S^A$.

The triple $(\mathcal{F}(\mathcal{M}), S, \{\cdot, \cdot\}_S)$ is termed Poisson algebra over *S*.

Let now $J_S(\mathcal{M})$ be the ideal (with respect to the pointwise product) in $\mathcal{F}(\mathcal{M})$ which vanishes on solutions of the field equation,

$$J_{\mathcal{S}}(\mathcal{M}) = \{ F \in \mathcal{F}(\mathcal{M}) | F(\varphi) = 0 \text{ whenever } S^{(1)}(\varphi) \equiv 0 \}.$$
(5.46)

We want to prove that $J_S(\mathcal{M})$ is also an ideal for the Poisson bracket.

Theorem 3. Let $F \in J_S(\mathcal{M})$ and $G \in \mathcal{F}(\mathcal{M})$. Then $\{F, G\}_S \in J_S(\mathcal{M})$.

Proof. Let $\varphi \in \mathfrak{C}(\mathcal{M})$ be a solution of the field equation, i.e., $S^{(1)}(\varphi)(x) = 0 \ \forall x \in \mathcal{M}$. We want to construct a one-parameter family of solutions $\varphi_t \in \varphi_t \in \mathfrak{C}(\mathcal{M})$, $t \in \mathbb{R}$ which satisfy the initial condition $\varphi_0 = \varphi$, and the differential equation

$$\frac{d}{dt}\varphi_t = \Delta_S(\varphi_t)G^{(1)}(\varphi).$$
(5.47)

Provided such a solution exists, φ_t is a solution of the field equation since $S^{(1)}(\varphi_0) = S^{(1)}(\varphi) = 0$ and

$$\frac{d}{dt}S^{(1)}(\varphi_t) = S^{(2)}(\varphi_t)\frac{d}{dt}\varphi_t$$
(5.48)

as $\frac{d}{dt}\varphi_t$ is by construction a solution of the linearized field equation at φ_t . Then $F(\varphi_t) = 0 \ \forall t$ and $0 = \frac{d}{dt}F(\varphi_t)|_{t=0} = \{F, G\}_S(\varphi)$. It remains to show that the differential equation (5.47) has a solution. This follows in the same way as the proof of existence of local solutions for the Møller operators in (5.40).

The theorem allows to define the on-shell Poisson algebra by

$$\mathcal{F}_{\mathcal{S}}(\mathcal{M}) = \mathcal{F}(\mathcal{M})/J_{\mathcal{S}}(\mathcal{M}). \tag{5.49}$$

5.4.5 Local Covariance for Classical Field Theory

We want to show that classical field theory is locally covariant provided the action *S* is induced by a locally covariant field.

Let \mathcal{F} denote the functor which associates with every $\mathcal{M} \in \mathfrak{Man}$ the commutative algebra of functionals $\mathcal{F}(\mathcal{M})$ defined before and to every morphism $\chi : \mathcal{M} \to \mathcal{N}$ the transformation

$$\mathcal{F}\chi(F)(\varphi) = F(\varphi \circ \chi). \tag{5.50}$$

Since χ preserves the metric and the time orientation, forward and backward light cones in the cotangent bundles transform properly. Together with the covariance of the wave front sets this implies that $\mathcal{F}\chi$ maps $\mathcal{F}(\mathcal{M})$ into $\mathcal{F}(\mathcal{N})$.

Let now \mathcal{L} be a natural transformation from \mathcal{D} to \mathcal{F} , i.e., for every $\mathcal{M} \in \mathfrak{Man}$ we have a linear map $\mathcal{L}_{\mathcal{M}} : \mathcal{D}(\mathcal{M}) \to \mathcal{F}(\mathcal{M})$ which satisfies

$$\mathcal{L}_{\mathcal{M}}(f)(\varphi \circ \chi) = \mathcal{L}_{\mathcal{N}}(\chi_* f)(\varphi).$$
(5.51)

Typical examples are given in terms of smooth functions *L* of two real variables by $\mathcal{L}_{\mathcal{M}}(f)(\varphi) = \int d\mathrm{vol}_{\mathcal{M}} f(x) L(\varphi(x), g_{\mathcal{M}}(d\varphi(x), d\varphi(x))).$

Theorem 4. $\mathcal{L}_{\mathcal{M}}(f)$ is local, i.e., satisfies the additivity condition (5.27).

Proof. We first show that $\operatorname{supp} \mathcal{L}_{\mathcal{N}}(f) \subset \operatorname{supp} f$. Let $\operatorname{supp} f \cap \operatorname{supp} f = \emptyset$ and let $\operatorname{supp} f \subset \mathcal{N}$ with $\mathcal{N} \cap \operatorname{supp} h = \emptyset$. Then from (5.51) we have

$$\mathcal{L}_{\mathcal{M}}(f)(\varphi+h) = \mathcal{L}_{\mathcal{N}}(f)((\varphi+h)|_{\mathcal{N}}) = \mathcal{L}_{\mathcal{N}}(f)(\varphi|_{\mathcal{N}}), \tag{5.52}$$

which proves the claim on the support of $\mathcal{L}_{\mathcal{M}}(f)$. Let now $\varphi, \psi, \chi \in \mathfrak{C}(\mathcal{M})$ with $\operatorname{supp} \varphi \cap \operatorname{supp} \chi = \emptyset$. Due to linearity in f we may decompose $\mathcal{L}_{\mathcal{M}}(f)$ into a sum of terms, each of which has disjoint support either with φ or with χ . In both cases the additivity is an immediate consequence of the support properties.

The functional derivatives of $\mathcal{L}_{\mathcal{M}}$ are defined as distributions on \mathcal{M}^n which coincide on \mathcal{N}^n for relatively compact open subregions \mathcal{N} with the functional derivatives of $\mathcal{L}_{\mathcal{M}}(f)$ for test functions f which are identical to 1 on the subregion \mathcal{N} . As before, the first derivative defines the field equation $\mathcal{L}^{(1)}$ and the second functional derivative is supposed to be a normal hyperbolic differential operator. We then can equip $\mathcal{F}(\mathcal{M})$ with the Peierls bracket (5.45) and obtain a functor $\mathcal{F}_{\mathcal{L}}$ from \mathfrak{M} an to the category \mathfrak{Poi} of Poisson algebras which satisfies Axioms 1–4 of locally covariant quantum field theory, where the Poisson bracket on a tensor product is defined by

$$\{F_1 \otimes F_2, G_1 \otimes G_2\} = \{F_1, G_1\} \otimes F_2 G_2 + F_1 G_1 \otimes \{F_2, G_2\}.$$
(5.53)

The field equation defines Poisson ideals $J_{\mathcal{L}}(\mathcal{M}) \subset \mathcal{F}_{\mathcal{L}}(\mathcal{M})$ which transform under embeddings as

$$\mathcal{F}_{\mathcal{L}}\chi J_{\mathcal{L}}(\mathcal{M}) \subset J_{\mathcal{L}}(\mathcal{N}), \tag{5.54}$$

since solutions φ on \mathcal{N} always induce solutions $\varphi \circ \chi$ on \mathcal{M} . For nonlinear field equation there may be, however, also solutions on \mathcal{M} which are not of this form.

We thus obtain another functor $(\mathcal{F}/J)_{\mathcal{L}}$ which describes the on-shell theory where the field equation is satisfied. In this functor, however, the morphisms of the category of Poisson algebras are homomorphisms which are not, in general, injective.

It would be interesting to check whether this theory satisfies the time slice axiom where, in view of the possible noninjectivity of homomorphisms, isomorphy is replaced by surjectivity.

5.5 Quantum Field Theory

5.5.1 Interpretation of Locally Covariant QFT

We now turn to quantum field theory. A model of quantum field theory here is understood as a functor from the category Man of globally hyperbolic spacetimes to the category of unital *-algebras which satisfies the axioms of Sect. 5.3. Our formalism differs from the formalism which may be found in standard text books for quantum field theory in Minkowski space which is either based on a representation of fields by operator-valued distribution on Fock space (canonical formulation) or on the path integral. These formulations suffer from several unsolved mathematical problems; the main reason, however, for our preference of the algebraic formulation of quantum field theory is that the concepts on which the standard approach is based lose their distinguished meaning on generic globally hyperbolic spacetimes. This can be made mathematically precise in the language of category theory by the absence of corresponding natural transformations. On a first sight, the path integral seems to be better behaved since its naive formulation involves only the classical action and the Lebesgue integral over the configuration space. The nonexistence of the Lebesgue integral on infinite-dimensional vector spaces, however, requires a choice of the Feynman propagator which is in conflict with the principle of local covariance.

On Minkowski space, the standard interpretation of the theory is based on the notion of a vacuum state and of associated excitations which are interpreted as particle states. Once a ground state is known, the interpretation of the theory in terms of cross sections is completely fixed. This was shown long ago by Araki and Haag [2] and is the basis for modern approaches to the infrared problem [13, 14]. A crucial ingredient in this analysis is the possibility to compare observables at different positions by the use of translation symmetry.

One of the main concerns for the interpretation of the theory on curved spacetimes is the absence of natural states. Here a natural state is defined as a family of states ω_M on $\mathfrak{A}(\mathcal{M})$, $\mathcal{M} \in \mathfrak{Man}$ such that

$$\omega_{\mathcal{N}} \circ \alpha_{\chi} = \omega_{\mathcal{M}} , \ \chi : \mathcal{M} \to \mathcal{N}.$$
(5.55)

A natural state could be understood as an appropriate generalization of the concept of a vacuum state. But one can show that such a state does not exist in typical cases. This marks the most dramatic point of departure from the traditional framework of quantum field theory.

The best one can do is to associate with each spacetime \mathcal{M} a natural folium of states $S_0(\mathcal{M}) \subset S(\mathfrak{A}(\mathcal{M}))$. A folium of states on a unital *-algebra is a convex set of states which is closed under the operations $\omega \mapsto \omega_A$, $\omega_A(B) = \omega(A^*BA)/\omega(A^*A)$ for elements A, B of the algebra with $\omega(A^*A) \neq 0$. A natural folium of states is a contravariant functor S_0 such that

$$S_0\chi(\omega) = \omega \circ \alpha_{\chi} , \ \chi : \mathcal{M} \to \mathcal{N} , \ \omega \in S_0(\mathcal{N}).$$
 (5.56)

This structure allows to endow our algebras with a suitable topology, but it does not suffice for an interpretation, since it does not allow to select single states within one folium. But there is another structure which makes possible an interpretation of the theory. These are the locally covariant fields, introduced before as natural transformations. By definition they are defined on all spacetimes simultaneously, in a coherent way. Hence states on different spacetimes can be compared in terms of their values on locally covariant fields. This can be used, for instance, for a thermal interpretation of states on spacetimes without a timelike Killing vector [15].

5.5.2 Free Scalar Field

The classical free scalar field satisfies the Klein-Gordon equation

$$(\Box + m^2 + \xi R)\varphi = 0, \tag{5.57}$$

which is the Euler-Lagrange equation for the Lagrangian

$$\mathcal{L} = \frac{1}{2} (g(d\varphi, d\varphi) - (m^2 + \xi R)\varphi^2).$$
(5.58)

Here *R* is the Ricci scalar and $m^2, \xi \in \mathbb{R}$. The Klein–Gordon operator $K = \Box + m^2 + \xi R$ possesses unique retarded and advanced propagators $\Delta^{R,A}$, since we are on globally hyperbolic spacetimes (see Theorem 4 on page 78).

The corresponding functor defining the quantum theory is constructed in the following way. For each \mathcal{M} we consider the *-algebra generated by a family of elements $W_{\mathcal{M}}(f), f \in \mathcal{D}_{\mathbb{R}}(\mathcal{M})$ with the relations

$$W_{\mathcal{M}}(f)^* = W_{\mathcal{M}}(-f),$$
 (5.59)

$$W_{\mathcal{M}}(f)W_{\mathcal{M}}(g) = e^{-\frac{i\hbar}{2}\langle f, \Delta g \rangle} W_{\mathcal{M}}(f+g), \qquad (5.60)$$

$$W_{\mathcal{M}}(Kf) = W_{\mathcal{M}}(0). \tag{5.61}$$

This algebra has a unit $W_{\mathcal{M}}(0) \equiv 1$ and a unique C*-norm, and its completion is the Weyl algebra over the symplectic space $\mathcal{D}(\mathcal{M})/\mathrm{im}K$ with the symplectic form $\langle f, \Delta g \rangle$. With $\alpha_{\chi}(W_{\mathcal{M}}(f)) = W_{\mathcal{N}}(\chi_* f)$ one obtains a functor satisfying also the Axioms 4 and 5. Moreover, $W = (W_{\mathcal{M}})$ is a (nonlinear) locally covariant field. It is, however, difficult to find other locally covariant fields for this functor.

The free field itself is thought to be related to the Weyl algebra by the formula

$$W_{\mathcal{M}}(f) = e^{i\varphi_{\mathcal{M}}(f)}.$$
(5.62)

This relation can be established in the so-called regular representations of the Weyl algebra, in which the one-parameter groups $W_{\mathcal{M}}(\lambda f)$ are strongly continuous. But one can also directly construct an algebra generated by the field itself. It is the unital *-algebra generated by the elements $\varphi_{\mathcal{M}}(f)$, $f \in \mathcal{D}(\mathcal{M})$ by the relations

$$f \mapsto \varphi_M(f)$$
 is linear, (5.63)

$$\varphi_M(f)^* = \varphi_M(\bar{f}), \tag{5.64}$$

$$[\varphi_M(f), \varphi_M(g)] = i\hbar \langle f, \Delta g \rangle, \qquad (5.65)$$

$$\varphi_{\mathcal{M}}(Kf) = 0. \tag{5.66}$$

Again one obtains a functor which satisfies Axioms 1–5. If we omit the condition (5.66) (then the time slice axiom is no longer valid and one is on the off-shell formalism), the algebra may be identified with the space of functionals on the space of field configurations $\mathfrak{C}(\mathcal{M})$,

$$F(\varphi) = \sum_{\text{finite}} \int d\operatorname{vol}_n f_n(x_1, \dots, x_n) \varphi(x_1) \cdots \varphi(x_n),$$
(5.67)

where f_n is a finite sum of products of test functions in one variable and where the product is given by

$$(F \star G)(\varphi) = \sum_{n} \frac{i^{n} \hbar^{n}}{2^{n} n!} \langle F^{(n)}(\varphi), \Delta^{\otimes n} G^{(n)}(\varphi) \rangle.$$
(5.68)

Hence, as a vector space, it may be considered as a subspace of the space $\mathcal{F}_0(\mathcal{M})$ known from classical field theory. Moreover, the involution $A \mapsto A^*$ coincides with complex conjugation. As a formal power series in \hbar , the product can be extended to all of $\mathcal{F}_0(\mathcal{M})$, thus providing $\mathcal{F}_0(\mathcal{M})[[\hbar]]$ with the structure of a unital *-algebra.

The Poisson ideal of the classical theory which is generated by the field equation turns out to coincide with the ideal with respect to the \star -product.

Theorem 5. Let $J_0(\mathcal{M})$ be the set of all $F \in \mathcal{F}_0(\mathcal{M})[[\hbar]]$ with $F(\varphi) = 0$ whenever $K\varphi = 0$. Then $J_0(\mathcal{M})$ is a \star -ideal.

Proof. Let $F \in J_0(\mathcal{M})$, $G \in \mathcal{F}_0(\mathcal{M})$, and $K\varphi = 0$. By the definition of the functional derivative, the distribution $F^{(n)}(\varphi)$ vanishes on *n*-fold tensor products of solutions, hence on $\Delta^{\otimes n} G^{(n)}(\phi)$. Thus $F \star G \in J_0(\mathcal{M})$. This shows that $J_0(\mathcal{M})$ is a right

ideal. But $J_0(\mathcal{M})$ is invariant under complex conjugation, so $(G \star F)^* = F^* \star G^*$, and it is also a left ideal.

5.5.3 The Algebra of Wick Polynomials

In order to include pointwise products of fields, or more generally, local functionals in the sense of Sect. 5.4.1 into the formalism we have to admit more singular coefficients in the expansion (5.67). But then the product may become ill-defined. As an example consider the functionals

$$F(\varphi) = \int d\text{vol } f(x)\varphi(x)^2, \qquad (5.69)$$

$$G(\varphi) = \int d\operatorname{vol} g(x)\varphi(x)^2, \qquad (5.70)$$

with test functions f and g. Insertion into the formula for the product yields

$$(F * G)(\varphi)$$

$$= \int d\operatorname{vol}_2 f(x)g(y) \left(\varphi^2(x)\varphi^2(y) + 4i\hbar\Delta(x, y)\varphi(x)\varphi(y) - 2\hbar^2\Delta(x, y)^2\right)$$
(5.71)

The problematic term is the square of the distribution Δ . Here the methods of microlocal analysis enter, namely the wave front set of Δ is (Strohmaier, Theorem 16)

WF(
$$\Delta$$
) = {($x, y; k, k'$), x and y are connected by a null geodesic γ ,
 $k || g(\dot{\gamma}, \cdot), U_{\gamma}k + k' = 0, U_{\gamma}$ parallel transport along γ }. (5.72)

The product of Δ cannot be defined in terms of Hörmander's criterion for the multiplication of distribution, since the sum of two vectors in the wave front set can yield zero. The crucial fact is now that Δ can be split in the form

$$\Delta = \frac{1}{2}\Delta + iH + \frac{1}{2}\Delta - iH, \qquad (5.73)$$

where the "Hadamard function" *H* is symmetric and the wave front set of $\frac{1}{2}\Delta + iH$ contains only the positive frequency part (Strohmaier, Definition 10)

$$WF\left(\frac{1}{2}\Delta + iH\right) = \{(x, y; k, k') \in WF(\Delta), k \in \overline{V_+}\}.$$
(5.74)

On Minkowski space, Δ depends only on the difference x - y, and one may find H in terms of the Fourier transform of Δ

$$\frac{1}{2}\Delta + iH = \Delta_+, \, \tilde{\Delta}_+(k) = \begin{cases} \tilde{\Delta}(k) \, , \, k \in \overline{V_+} \\ 0 \, , \, \text{else} \end{cases} .$$
(5.75)

On a generic spacetime, the split (5.73) represents a microlocal version of the decomposition into positive and negative energies (microlocal spectrum condition [5]) which is fundamental for quantum field theory on Minkowski space.

If we replace in the definition of the product (5.68) Δ by $\Delta + 2iH$, we obtain a new product \star_H . On $\mathcal{F}_0(\mathcal{M})[[\hbar]]$ this product is equivalent to \star , namely

$$F \star_H G = \alpha_H(\alpha_H^{-1}(F) \star \alpha_H^{-1}(G)), \qquad (5.76)$$

where

$$\alpha_H(F) = \sum \frac{\hbar^n}{n!} \langle H^{\otimes n}, F^{(2n)} \rangle$$
(5.77)

is a linear isomorphism of $\mathcal{F}_0(\mathcal{M})[[\hbar]]$ with inverse $\alpha_H^{-1} = \alpha_{-H}$.

This product now yields well-defined expressions in (5.71); actually, it is well defined on $\mathcal{F}(\mathcal{M})[[\hbar]]$. This is a consequence of Hörmander's criterion for the multiplicability of distributions, namely by the microlocal spectrum condition (5.74) the wave front set of $(\Delta + 2iH)^{\otimes n}$ is contained in $\overline{V}_{+}^{n} \times \overline{V}_{-}^{n}$. Hence by the condition on the wave front set of the *n*th derivatives of $F, G \in \mathcal{F}(\mathcal{M})$ the pointwise product of the distribution $F^{(n)} \otimes G^{(n)}$ with $(\Delta + 2iH)^{\otimes n}$ exists and is a distribution with compact support. Therefore the terms in the formal power series defining the *-product are well defined. Moreover, they are again elements of $\mathcal{F}(\mathcal{M})$. This follows from the fact that the derivatives of $\langle F^{(n)}, (\Delta + 2iH)^{\otimes n}G^{(n)} \rangle$ arise from contractions of the pointwise products $F^{(n+k)} \otimes G^{(n+l)}$ with $(\Delta + 2iH)^{\otimes n}$ in the joint variables.

If we restrict ourselves to polynomial functionals, i.e., those for which the functional derivatives of sufficiently high orders vanish, we may set $\hbar = 1$. Up to taking the quotient by the ideal $J_0(\mathcal{M})$ of the field equation we obtain, on Minkowski space, the algebra of Wick polynomials. We thus succeeded to define on generic spacetimes an algebra containing all local field polynomials.

The annoying feature, however, is that the product depends on the choice of H. Fortunately, the difference w between two Hadamard functions H and H' is smooth.

Theorem 6. Let H, H' be symmetric distributions in two variables satisfying condition (5.74). Then w = H - H' is smooth.

Proof. Since $w = (H - \frac{i}{2}\Delta) - (H' - \frac{i}{2}\Delta)$, the wave front set of w satisfies also condition (5.74). Thus $(x, y; k, k') \in WF(w)$ implies $k \in \overline{V_+}(x)$. But w is symmetric, hence then also $k' \in \overline{V_+}(y)$. But -k' is the parallel transport of k along a null geodesic from x to y. Since \mathcal{M} is time oriented, this implies k = k' = 0. Since by definition, the zero covectors are not in the wave front set, the wave front set of w is empty, hence w is smooth.

The smoothness of w implies that the products $*_H$ and $*_{H'}$ are equivalent

$$F *_{H'} G = \alpha_w(\alpha_w^{-1}(F) *_H \alpha_w^{-1}(G)),$$
(5.78)

where α_w is defined in analogy to (5.77), but is now, due to the smoothness of w, a well-defined linear isomorphism of $\mathcal{F}(\mathcal{M})[[\hbar]]$.

In order to eliminate the influence of H we replace our functionals by families $F = (F_H)$, labeled by Hadamard functions H and satisfying the coherence condition $\alpha_w(F_H) = F_{H+w}$. The product of two such families is defined by

$$(F \star G)_H = F_H \star_H G_H. \tag{5.79}$$

We call this algebra the algebra of quantum observables and denote it by $\mathcal{A}(\mathcal{M})$. The subspace of local elements $A \in \mathcal{A}_{loc}(\mathcal{M})$ is formed by families $A = (A_H)$ with $A_H \in \mathcal{F}_{loc}(\mathcal{M})$. Since α_w leaves $\mathcal{F}_{loc}(\mathcal{M})$ invariant, $A \in \mathcal{A}_{loc}(\mathcal{M})$ if $A_H \in \mathcal{F}_{loc}(\mathcal{M})$ for some Hadamard function H.

 $\mathcal{F}_0(\mathcal{M})$ [[\hbar]] equipped with the product (5.68) is embedded into $\mathcal{A}(\mathcal{M})$ by

$$F \mapsto (F_H)$$
 with $F_H = \alpha_H(F)$. (5.80)

One may equip $\mathcal{F}(\mathcal{M})$ with a suitable topology such that α_w is a homeomorphism and such that $\mathcal{F}_0(\mathcal{M})[[\hbar]]$ is sequentially dense in $\mathcal{A}(\mathcal{M})$ [16].

5.5.4 Interacting Models

In order to treat interactions we introduce a new product \cdot_T on $\mathcal{F}_0(\mathcal{M})[[\hbar]]$, the timeordered product. It is a commutative product which coincides with the *-product if the factors are time ordered:

$$F \cdot_T G = F \star G \text{ if } \operatorname{supp}(F) \gtrsim \operatorname{supp}(G),$$
 (5.81)

where \gtrsim means that there is a Cauchy surface such that the left-hand side and the right-hand side are in the future and past of the surface, respectively. For the free field, we find

$$\varphi(f) \cdot_T \varphi(g) = \varphi(f)\varphi(g) + i\hbar\langle f, \Delta^D g \rangle, \qquad (5.82)$$

with the "Dirac propagator" (see [17])

$$\Delta^D = \frac{1}{2} (\Delta^R + \Delta^A). \tag{5.83}$$

The time-ordered product may be extended to all of $\mathcal{F}_0(\mathcal{M})[[\hbar]]$ by

$$(F \cdot_T G)(\varphi) = \sum_n \frac{i^n \hbar^n}{n!} \langle F^{(n)}, (\Delta^D)^{\otimes n} G^{(n)} \rangle.$$
(5.84)

In text books on quantum field theory, the time-ordered product is usually defined for fields in the Fock space representation. But the Dirac propagator is not a solution of the homogeneous Klein–Gordon equation. Hence $J_0(\mathcal{M})$ is not an ideal with respect to the time-ordered product. Instead from $\Delta_D K =$ id one finds the relation

$$\varphi(Kf) \cdot_T F = \varphi(Kf)F + i\hbar \langle F^{(1)}, \Delta_D Kf \rangle = \varphi(Kf)F + i\hbar \langle F^{(1)}, f \rangle.$$
(5.85)

This relation is the prototype of the so-called Schwinger–Dyson equation by which the field equation of interacting quantum fields can be formulated in terms of expectation values of time-ordered products. Since the ideal generated by the field equation vanishes in the Fock space representation, time ordering on Fock space is not well defined as a product of operators. On $\mathcal{F}_0(\mathcal{M})[[\hbar]]$, however, it is well defined and is even equivalent to the pointwise (classical) product, namely we introduce the "time-ordering operator"

$$TF(\varphi) = \sum_{n} \frac{i^{n} \hbar^{n}}{n!} \langle (\Delta^{D})^{\otimes n}, F^{(2n)}(\varphi) \rangle.$$
(5.86)

T is a linear isomorphism, with the inverse obtained by complex conjugation, and

$$F \cdot_T G = T(T^{-1}(F) \cdot T^{-1}(G)).$$
(5.87)

In terms of T, explicit formulae for interacting fields can be given by the use of the formal *S*-matrix which is just the exponential function computed via the time-ordered product

$$S(F) = T \exp(T^{-1}(F)).$$
 (5.88)

In terms of S we can write down the analog of the Møller operators for quantum field theory, via Bogoliubov's formula

$$R_V(F) \doteq \frac{d}{d\lambda} S(V)^{-1} \star S(V + \lambda F) \bigg|_{\lambda=0} = S(V)^{-1} \star (S(V) \cdot_T F), \qquad (5.89)$$

where the inverse is built with respect to the *-product. R_V is a linear map from $\mathcal{F}_0(\mathcal{M})[[\hbar]]$ to itself and describes the transition from the free action to the action with additional interaction term V. It satisfies two important conditions, retardation and equation of motion. As far as the retardation property is concerned, one observes that if $\operatorname{supp}(V) \gtrsim \operatorname{supp}(F)$, the time-ordered product and the *-product coincide, hence by associativity of the *-product $R_V(F) = F$, so the observable F is not influenced by an interaction which takes place in the future. We now show that the interacting field $f \mapsto R_V(\varphi(Kf))$ satisfies the off-shell field equation

$$R_V(\varphi(Kf)) = \varphi(Kf) + i\hbar R_V(\langle V^{(1)}, f \rangle), \qquad (5.90)$$

where $f \in \mathcal{D}(M)$ and K is the Klein–Gordon operator. (In a more suggestive notation, the field equation above reads

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$$K\varphi_V(x) = K\varphi(x) + i\left(\frac{\delta V}{\delta\varphi(x)}\right)_V,$$
(5.91)

with the free field φ , the interacting field φ_V , and the interacting current $i\left(\frac{\delta V}{\delta \varphi}\right)_V$.) *Proof. S* is the time-ordered exponential, hence by the chain rule we obtain $\langle S(V)^{(1)}, g \rangle = S(V) \cdot_T \langle V^{(1)}, g \rangle$. From (5.85)

$$R_V(\varphi(Kf)) = S(V)^{-1} \star (S(V) \cdot_T \varphi(Kf))$$

= $S(V)^{-1} \star \left(S(V) \cdot \varphi(Kf) + i\hbar S(V) \cdot_T \langle V^{(1)}, f \rangle\right).$

But $S(V) \cdot \varphi(Kf) = S(V) * \varphi(Kf)$ since the higher order terms in \hbar of the *-product vanish due to $\Delta K = 0$. The statement now follows from associativity of the *-product.

5.5.5 Renormalization

The remaining problem is the extension of the time-ordered product to local functionals. Here the problem can only partially be solved by the transition to an equivalent product

$$F \cdot_{T_H} G = \alpha_H(\alpha_H^{-1}(F) \cdot_T \alpha_H^{-1}(G)).$$
(5.92)

This transformation amounts to replacing the Dirac propagator by the Feynman-like propagator $\Delta^D + iH$. Since $\Delta^D + iH$ coincides on the complement of the support of the advanced propagator Δ^A with $\frac{1}{2}\Delta + iH$ and on the complement of the support of the retarded propagator Δ^R with $-\frac{1}{2}\Delta + iH$, its wave front set is

$$WF(\Delta^D + iH) = \{(x, y, k, k') \in WF(\Delta), k \in \overline{V_{\pm}} \text{ if } x \in J_{\pm}(y)\} \cup \{(x, x, k, -k), k \neq 0\}.$$

Thus contrary to the Dirac propagator, pointwise products of these propagators exist outside of the diagonal. The problem which remains to be solved in renormalization is therefore to extend a distribution which is defined on the complement of some submanifold (the thin diagonal in our case) to the full manifold [18].

The construction can be much simplified by the fact that the time-ordered product coincides with the product \star for time-ordered supports. For local functionals the time-ordered product is therefore defined whenever the localizations are different, namely let \mathcal{L}_i , $i = 1, \ldots, n$ be Lagrangians, i.e., natural transformations in the sense of Sect. 5.4.5. Then the time-ordered product $(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_T$ can be defined in terms of an $\mathfrak{A}(\mathcal{M})$ -valued distribution on $\mathcal{M}^n \setminus D$ where D is the subset where at least two variables coincide. Indeed, on tensor products of test functions $f_1 \otimes \cdots \otimes f_n$ with $\sup f_i \gtrsim \sup f_{i+1}$, $i = 1, \ldots, n-1$ the time-ordered product is given by

$$(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_T^{\mathcal{M}}(f_1 \otimes \cdots \otimes f_n) = \mathcal{L}_1^{\mathcal{M}}(f_1) \star \cdots \star \mathcal{L}_n^{\mathcal{M}}(f_n).$$
(5.93)

Moreover, the time-ordered product is required to be symmetric, hence it is well defined on $\mathcal{M}^n \setminus D$.

One now proceeds by induction. The time-ordered product with one factor is the Lagrangian itself. Now assume that time-ordered products of less than *n* factors have been constructed in the sense of $\mathfrak{A}(\mathcal{M})$ -valued distributions $(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_k)_T^{\mathcal{M}}$ on \mathcal{M}^k such that $(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_k)_T$ is a natural transformation from $\mathcal{D}^{\otimes k}$ to \mathfrak{A} which in particular satisfies the causality condition

$$(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_k)_T^{\mathcal{M}}(f \otimes g) = (\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_l)_T^{\mathcal{M}}(f) \star (\mathcal{L}_{l+1} \otimes \cdots \otimes \mathcal{L}_k)_T^{\mathcal{M}}(g)$$
(5.94)

provided supp $(f) \subset \mathcal{M}_1^l$, supp $(g) \subset \mathcal{M}_2^{k-l}$, and $\mathcal{M}_1, \mathcal{M}_2$ are subregions of \mathcal{M} with $\mathcal{M}_1 \gtrsim \mathcal{M}_2$.

We may now, on $\mathcal{M}^n \setminus \Delta_n$, use a decomposition of unity $(\chi_I)_I$, indexed by the nonempty proper subsets of $\{1, \ldots, n\}$, with supports $\operatorname{supp} \chi_I \subset U_I = \{(x_1, \ldots, x_n) \in \mathcal{M}^n | \{x_i, i \in I\} \gtrsim \{x_j, j \notin I\}\}$. Then we define

$$(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_T^{\mathcal{M}} = \sum_I \chi_I (\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_{T,I}^{\mathcal{M}},$$
(5.95)

where $(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_{T,I}^{\mathcal{M}}$ is determined on U_I by

$$(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_{T,I}^{\mathcal{M}}(f_1 \otimes \cdots \otimes f_n) = (\bigotimes_{i \in I} \mathcal{L}_i)_T^{\mathcal{M}}(\bigotimes_{i \in I} f_i) * (\bigotimes_{j \notin I} \mathcal{L}_j)_T^{\mathcal{M}}(\bigotimes_{j \notin I} f_i).$$
(5.96)

This definition does not depend on the choice of the decomposition of unity. This follows from the fact that on intersections $U_I \cap U_J$ the distributions $(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_{T,I}^{\mathcal{M}}$ and $(\mathcal{L}_1 \otimes \cdots \otimes \mathcal{L}_n)_{T,I}^{\mathcal{M}}$ coincide.

The crucial step now is the extension of these distributions to the full space \mathcal{M}^n such that the causality condition (5.94) is satisfied. This can be done [18], but the process is, in general, not unique.

As a result we obtain a renormalized S-matrix S as a generating functional for time-ordered products

$$S(\underline{\mathcal{L}}^{\mathcal{M}}(\underline{f})) = \sum \frac{1}{n!} (\mathcal{L}_{i_1} \otimes \cdots \otimes \mathcal{L}_{i_n})_T^{\mathcal{M}} (f_{i_1} \otimes \cdots \otimes f_{i_n}), \qquad (5.97)$$

with

$$\underline{\mathcal{L}}^{\mathcal{M}}(\underline{f}) = \sum \mathcal{L}_i(f_i).$$
(5.98)

The crucial conditions that restrict the ambiguities in the extension process is now that *S* satisfies the causality condition

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$$S(\underline{\mathcal{L}}^{\mathcal{M}}(\underline{f} + \underline{g})) = S(\underline{\mathcal{L}}^{\mathcal{M}}(\underline{f})) \star S(\underline{\mathcal{L}}^{\mathcal{M}}(\underline{g}))$$
(5.99)

as a consequence of (5.94) and the naturality condition

$$\alpha_{\chi} S(\underline{\mathcal{L}}^{\mathcal{M}}(\underline{f})) = S(\underline{\mathcal{L}}^{\mathcal{N}}(\underline{\chi_* f}))$$
(5.100)

as a consequence of the naturality conditions on the time-ordered products of Lagrangians. These conditions imply the *Main Theorem of Renormalization*:

Theorem 7. Let S_i be two extensions of the formal S-matrix to \mathcal{A}_{loc} fulfilling the causality and naturality conditions. Then there exists a uniquely determined natural equivalence $Z : \mathcal{A}_{loc}[[\hbar]] \to \mathcal{A}_{loc}[[\hbar]]$ (a formal diffeomorphism on the space of interactions) with $Z^{(1)} = \text{id such that}$

$$S_2 = S_1 \circ Z.$$
 (5.101)

The natural equivalences Z occurring in the theorem form a group, the renormalization group in the sense of Stückelberg and Petermann. Typically, additional conditions on S induce cocycles on the renormalization group and the cohomology classes of these cocycles are the famous anomalies of quantum field theory.

We conclude that a Lagrangian alone does not specify a quantum field theoretical model completely. One has in addition to fix a point of the orbit of the interaction under the renormalization group. This amounts to a choice of suitable renormalization conditions. An important class of interactions are the *renormalizable* interactions. They have the property that the orbit under the renormalization group (after imposing suitable conditions) is finite dimensional, such that the theory can be fixed in terms of finitely many parameters.

The method of renormalization described above is termed causal perturbation theory and was first rigorously performed by Epstein and Glaser on Minkowski space [19], based on previous work of Stückelberg and Bogoliubov. Its extension to curved spacetimes was undertaken by Brunetti and Fredenhagen [18], and the implementation of the principle of local covariance and the reduction to finitely many free parameters is due to Hollands and Wald [7, 20]. The extension of the method to gauge theories was performed on Minkowski space by Dütsch, Scharf et al. [21] and generalized to curved spacetimes by Hollands [22].

On Minkowski space, there exist other methods of renormalization, which are known to be equivalent. One of these is the Bogoliubov–Parasiuk–Hepp–Zimmermann method whose involved structure was recently made transparent in terms of the Connes–Kreimer Hopf algebra [23]. Another one is the Wilson–Polchinski method of renormalization group flow equations [16], where the time-ordered product is regularized. The dependence of the theory under a variation of the regularization delivers the so-called flow equation. In the sense of formal power series, the flow equation can always be solved, and the removal of the regularization amounts to asymptotic stability properties of the solutions. The attractive feature of this method is that the concepts do not depend on the perturbative formulation. It

is usually defined in terms of the path integral which seems to make a formulation on curved spacetime difficult. But if interpreted not as an integral but as an integral operator, it can actually be identified with the formal *S*-matrix of causal perturbation theory.

Namely let T_A be a regularized version of the time-ordering operator T obtained by replacing the Feynman propagator $\Delta_D + iH$ by a sufficiently regular distribution $G_A + iH$. Then $S_A = T_A \circ \exp \circ T_A^{-1}$ is a well-defined generating functional for regularized time-ordered products on A. Different regularizations may be compared in terms of the *effective action* $S_{A_1}^{-1} \circ S_{A_2}$ which yields after application to $V \in \mathcal{A}(\mathcal{M})$ a modified interaction $V_{A_1A_2}$ which is interpreted as the "interaction at scale A_1 after integrating out the degrees of freedom beyond A_2 ." This interpretation refers to a regularization by a momentum cutoff and has no immediate generalization to the generic situation on curved space time. But in any case we know from causal perturbation theory [16] that given S there exist renormalization group transformations Z_A such that

$$S = \lim S_A \circ Z_A, \tag{5.102}$$

if $G_A + iH$ converges to $\Delta_D + iH$ in the appropriate sense (Hörmander's topology for distributions with prescribed wave front set). The renormalization transformation Z_A is the operation which adds the necessary counter terms to the interaction. If Acan be identified with a complex variable such that S_A is meromorphic and A = 0corresponds to the removal of the regularization, one can choose Z_A such that it removes the pole at A = 0 and obtains a distinguished choice for S. For instance, in the case of dimensional regularization this defines the so-called minimal renormalization. But such a choice of S is not necessarily appropriate from the point of view of physics. In particular it depends on the choice of the regularization. It can, however, be used to fix a specific point on the orbit of interactions under the renormalization group and thus allow an explicit formulation of renormalization conditions.

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