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**Bulk-to-boundary correspondence for massive
and interacting scalar field theories**

Corrispondenza bulk-bordo per teorie di campo scalari massive e
interagenti

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Abstract

Questa tesi è dedicata allo studio di una corrispondenza bulk-bordo per teorie quantistiche di campo scalari su spazitempi asintoticamente piatti nel caso massivo e interagente. Dopo una breve introduzione alle strutture geometriche alla base di questo lavoro, e in particolare la definizione di spazitempi globalmente iperbolici e asintoticamente piatti, introduciamo il formalismo della teoria quantistica dei campi algebrica perturbativa (pAQFT). Gli osservabili interagenti vengono costruiti perturbativamente mediante la mappa di Møller classica e la sua controparte quantistica, la mappa di Bogoliubov. A partire dalla corrispondenza bulk-bordo per un campo scalare libero, privo di massa e con accoppiamento conforme, sviluppiamo un'estensione per il caso massivo e interagente per studiarne il comportamento asintotico. Nel caso massivo, l'osservabile di campo viene rappresentato come una serie formale in m^2 , i cui coefficienti ammettono indipendentemente una proiezione al bordo. Sullo spaziotempo di Minkowski e in presenza di un cutoff infrarosso, dimostriamo la convergenza della serie al bordo mediante stime in energia per il problema di Goursat. Per una teoria auto-interagente con potenziale quartico, estendiamo perturbativamente la costruzione e calcoliamo la correzione al primo ordine nella costante di accoppiamento della proiezione del tensore energia-impulso al bordo.

This thesis is devoted to the analysis of a bulk-to-boundary correspondence for massive and interacting scalar quantum field theories on asymptotically flat spacetimes. After reviewing the geometric structures underlying the construction, in particular globally hyperbolic and asymptotically flat spacetimes, we introduce the framework of perturbative algebraic quantum field theory (pAQFT). Interacting observables are constructed perturbatively by means of the classical Møller map and its quantum counterpart, the Bogoliubov map. Starting from the bulk-to-boundary correspondence for a free, conformally coupled massless scalar field, we develop extensions to massive and interacting theories in order to study the asymptotic behaviour of the theory. In the massive case, the field observable is constructed as a formal power series in m^2 , whose coefficients admit a projection to future null infinity. On Minkowski spacetime, and in the presence of an infrared cut-off, we prove convergence of the resulting boundary series by means of energy estimates for the characteristic Goursat problem. For a quartically self-interacting theory, we extend the construction perturbatively and compute the first-order correction in the coupling constant to the projected stress-energy tensor at the boundary.

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Chapter 1

Introduction

Quantum field theory (QFT) represents the theoretical framework which describes elementary-particle physics and, more generally, quantum systems with an infinite number of degrees of freedom. In the standard formulation on Minkowski spacetime, quantum fields are represented as operator-valued distributions acting on a suitable Hilbert space. For free theories, the latter can be constructed as a Fock space over the corresponding one-particle Hilbert space, thereby encoding the creation and annihilation of particles. The symmetries of Minkowski spacetime allow one to select a distinguished Poincaré-invariant vacuum and, correspondingly, a decomposition of the fields into positive- and negative-frequency modes. This gives rise to annihilation and creation operators which, for Bosonic theories, satisfy the canonical commutation relations [Wei95; PS19].

Within this framework, exact solutions for interacting theories are in general not available, and interactions are therefore typically treated perturbatively. A central rôle is played by scattering theory, which relates the interacting dynamics to asymptotically free particle states. In Minkowski spacetime, one assumes that the interacting field approaches a free theory sufficiently far in the past and future, so that incoming and outgoing states can be defined in terms of the corresponding free Fock spaces. The relation between these asymptotic states is encoded by the S -matrix, whose matrix elements determine scattering amplitudes. Perturbatively, the S -matrix is expanded as a formal power series in the coupling constants, with coefficients given by *time-ordered products* of quantum fields. These time-ordered products encode all the perturbative contributions associated with the interaction. Even though the resulting series are generally formal rather than convergent, they provide highly accurate physical predictions [Dys52; Wei22; Wei95].

Despite its remarkable success, this framework relies heavily on the un-

derlying background being Minkowski spacetime. As a matter of fact, on a generic curved spacetime, there may be neither a preferred time direction nor a set of isometries that allow one to identify uniquely a ground state. Hence, a direct counterpart of the Poincaré vacuum and of the positive- and negative-frequency splitting cannot, in general, be defined canonically. A framework that does not rely on these structures is therefore required to describe phenomena such as Hawking radiation and cosmological applications such as inflation and baryogenesis [Haw75; Wal75; Gut81; RT99].

These difficulties motivate the introduction of a different approach, called *algebraic quantum field theory* (AQFT) [HK64; Haa10; WG65; Ara99]. This framework disentangles the notion of physical state from that of physical observables, treating the latter as the starting point of the theory and introducing the state only at a later stage [KM15]. For a free scalar field on a globally hyperbolic spacetime [Wal84], one constructs a unital $*$ -algebra $\mathcal{A}(\mathcal{M})$ generated by smeared quantum fields, denoted by $\phi(f)$, subject to the equation of motion, hermiticity and canonical commutation relations determined by the causal propagator of the theory [BGP08].

In this approach, states are introduced as linear, normalised and positive functionals ω on $\mathcal{A}(\mathcal{M})$ and they allow to recover a probabilistic interpretation in terms of expectation values proper of a quantum theory. Once a state has been selected, the *Gelfand-Naimark-Segal theorem* [GN43; Seg47] allows one to associate to any pair $(\mathcal{A}(\mathcal{M}), \omega)$ a suitable Hilbert-space representation, recovering the familiar construction typical of Minkowski-space QFT. Among all possible algebraic states, *Hadamard states* play a distinguished rôle: their short-distance singularity structure has the universal form required by quantum field theory on curved spacetime and locally reproduces that of the Minkowski vacuum [RV96; Rad96]. Once a Hadamard state has been selected, it is possible to enlarge the algebra of observables to include powers of quantum fields via a Wick-ordering procedure, allowing to include physically relevant observables, such as the stress-energy tensor [HW01; HW02; Mor03].

However, the axiomatic formulation of AQFT does not give an explicit perturbative construction of interacting observables on curved backgrounds. For this purpose, it is convenient to adopt a perturbative formulation of the algebraic approach called *perturbative algebraic quantum field theory* (pAQFT) [BF00; Rej16]. Within this framework, observables are encoded in a suitably defined algebra of functionals on the space of kinematic field configurations. The quantisation of the theory is achieved by a deformation of the pointwise product of the algebra [Moy49; DF01; HR19], leading to a representation of its elements as formal power series in $\hbar$. Interactions are introduced through the definition of a time-ordered product, implemented

by means of the Feynman propagator [HW01; HW02; Rej16]. The definition of this product leads to the necessity of performing a renormalisation procedure, which in this context is formulated as the problem of extending powers of the Feynman propagator to the diagonal of $\mathcal{M} \times \mathcal{M}$ [Ste71; GE73].

Once a renormalisation procedure has been carried out, the interaction can be implemented perturbatively via the formal S-matrix. Interacting observables are then constructed by means of the Bogoliubov map [Bog+80; GE73], which expresses them as formal power series in both $\hbar$ and the coupling constant λ .

A central application of quantum field theory is the description of scattering processes. In Minkowski spacetime, scattering theory is conventionally formulated in terms of asymptotic ingoing and outgoing fields, assumed to become asymptotically free sufficiently far in the past and the future. On a generic curved background, however, this description is no longer canonical as it is dependent on the choice of a preferred time coordinate.

A particularly favourable setting to study scattering processes while retaining manifest covariance is provided by *asymptotically flat spacetimes*, which describe isolated gravitational systems whose geometry approaches that of Minkowski spacetime, in a suitable sense, along null directions [Wal84; Ash15]. These spacetimes admit a conformal completion of the physical spacetime $(\mathcal{M}, g)$ into an unphysical one $(\widetilde{\mathcal{M}}, \widetilde{g})$, with infinity represented geometrically as a conformal boundary at a finite coordinate distance. Of particular relevance are future and past null infinities, $\mathcal{I}^+$ and $\mathcal{I}^-$, which represent the accumulation sets of outgoing and incoming radiation, respectively. This construction therefore provides the natural arena on which scattering processes can be described without referring to a coordinate-dependent limit, with asymptotic data assigned directly at past and future null infinities [Fri80; BSZ90; Jou12; Nic24].

Null infinities also enjoy a rich symmetry structure. Although one might expect the asymptotic symmetry group to reduce to the Poincaré one, the transformations that preserve the universal structure of $\mathcal{I}^\pm$ form the infinite-dimensional *Bondi-Metzner-Sachs (BMS) group* [Sac62; Pen63; BVM62]. It contains, in a suitable sense, infinitely many distinct Poincaré subgroups related by a new set of transformations included in the BMS-group, called *supertranslations*. The resulting enlarged symmetry structure plays an important rôle in modern studies of gravitational scattering, where BMS symmetries are related to asymptotic charges and the infrared behaviour of the theory [Str14].

Within the framework of pAQFT, this viewpoint can be implemented through a bulk-to-boundary correspondence. For a massless, conformally

coupled scalar theory, one can construct a $*$ -homomorphism from the algebra of observables in the bulk to a suitably defined algebra at null infinity [DMP06; DPP11; DMP17]. The boundary algebra thus retains information about the asymptotic behaviour of bulk observables. Furthermore, under suitable assumptions, one can construct a unique BMS-invariant state on the boundary algebra, whose pullback identifies a distinguished Hadamard state in the bulk [DMP17]. The correspondence between field theories in the bulk and at the boundary motivates the study of quantum field theories defined intrinsically on null infinity, where the degenerate nature of the metric makes the construction substantially different from that of a theory on a Lorentzian background [DMP06; DGH14; FPT26].

The bulk-to-boundary construction is particularly natural for the case of a massless, conformally coupled scalar field, due to the conformal invariance of the associated equation of motion. The introduction of a mass term in the action breaks conformal invariance and it introduces, after the conformal transformation, a singular potential at null infinity, making the extension of the projection map to a massive theory non-trivial.

Thus, the first objective of this thesis is to tackle this problem in order to obtain a well-defined boundary projection for massive field observables in the pAQFT framework. After defining the fundamental algebra structure and a bulk-to-boundary map for the free theory, we employ the *principle of perturbative agreement*, according to which a quadratic contribution such as a mass term may be treated either as part of the free dynamics or perturbatively as an interaction, with equivalent constructions [DHP17]. By adopting the latter viewpoint, the massive field observable is represented as a formal power series in the square of the mass, with coefficients belonging to the massless theory. Therefore, each term in the perturbative series admits an independent projection to null infinity, yielding a corresponding formal boundary series for the massive field at null infinity.

Specialising to Minkowski spacetime, we employ energy estimates for the Goursat problem, an initial value problem with initial data on a null hypersurface, to prove the convergence of the boundary series in the presence of an infrared cutoff. This establishes the well-posedness of the bulk-to-boundary map within this setting for massive scalar fields.

The second objective of the thesis is to investigate the extension of the bulk-to-boundary construction to interacting quantum theories. By composing the Bogoliubov map with the projection defined for the free theory, we obtain a perturbative description of asymptotic observables for the interacting theory. As a concrete model, we consider a $\lambda\phi^4$ theory and compute, at first order in the coupling λ , the projection of the interacting stress-energy tensor to future null infinity.

The structure of the thesis is the following: Chapter 2 is devoted to outlining the mathematical tools necessary for the core of this work. In Section 2.1 we introduce the key geometric elements needed for the description of a quantum field theory in the aforementioned setting. In particular, in Section 2.1.1 basic notions of causality theory and globally hyperbolic spacetimes are introduced, while in Section 2.1.2 we define the notion of asymptotically flat spacetimes and present some of their core properties. Then, in Section 2.2 we present the pAQFT framework. We start by introducing the kinematical field configurations in Section 2.2.1 and we define physical observables as an algebra of functionals thereon, satisfying certain conditions on their singular structure, in Section 2.2.2. The dynamics is then introduced in Section 2.2.3 via the Lagrangian formalism. The equation of motion for the field theory arises as stationary points of the associated action. Section 2.2.4 treats the quantisation of the theory, obtained by a deformation of the pointwise product of the algebra of observables to recover the canonical commutation relations. The notion of algebraic state and the GNS theorem are presented in Section 2.2.5, allowing to recover a Hilbert space description of the theory.

Given our goal to analyse an interacting quantum field theory, in Section 2.2.6 we introduce interactions at the level of the classical theory. The classical Møller map is introduced in order to perturbatively construct classical interacting observables. The quantum case is presented in Section 2.2.7, where we introduce the definition of time-ordered product and the associated renormalisation procedure. Furthermore, we present the Bogoliubov map, which represents the quantisation of the Møller map. Finally, in Section 2.2.8 we introduce the algebra of asymptotic observables constructed at null infinity and we present the construction of a bulk-to-boundary map for the free, massless, conformally coupled scalar theory.

Subsequently, we move to the analysis of the massive case in Chapter 3. Here we implement the principle of perturbative agreement to define the massive theory as a deformation of the massless one and construct perturbatively a projection map for the massive field observable. The resulting boundary series is analysed after a succinct overview of the Goursat problem, and the well-posedness of the projection is established by energy estimates.

In Chapter 4, we introduce an extension of the bulk-to-boundary map to perturbative series of interacting observables. After introducing the stress-energy tensor and its main properties within the pAQFT framework, we explicitly compute its projection to future null infinity at first order in perturbation theory for a quartic interaction potential.

Chapter 2

Mathematical Tools

2.1 Geometric setting

The core of this work is focused on the analysis of a quantum scalar field theory at the lightlike boundary of a distinguished class of spacetime, the asymptotically flat ones. The interest towards the study of these spacetimes stems, for example, from the analysis of quantum field theories in isolated gravitational systems such as the Schwarzschild black hole. The aim of this chapter is to outline the geometric structures underlying the discussion in the following chapters. We present a succinct but self-contained overview of fundamental notions in Lorentzian geometry that shall be employed throughout the work. A preliminary key ingredient in this regard is the identification of a suitable class of backgrounds, enjoying notable properties. Among the plethora of Lorentzian manifolds with boundary, we focus on those which are globally hyperbolic, see Definition 2.6. They represent the arena of algebraic quantum field theory, see Chapter 2, allowing for well-posedness of initial value problems while avoiding physically pathological scenarios.

Subsequently, we introduce *asymptotically flat* spacetimes, which constitute one of the main focuses of our study. These manifolds are characterized by the property of behaving similarly to Minkowski spacetime when approaching infinity along lightlike curves. We conclude by outlining some of their main properties, with particular emphasis on a characterization of the asymptotic symmetries.

For a complete analysis of these topics, we refer the reader to [Wal84, Chapters 8, 11] and [BGP08, Chapter 1].

2.1.1 Global hyperbolicity

We start by establishing some key notions in Lorentzian geometry.

Definition 2.1. We call *spacetime* a smooth, Hausdorff, second-countable, connected, oriented and time-oriented d -dimensional manifold $\mathcal{M}$ equipped with a Lorentzian metric g , whose signature reads $(-, +, \dots, +)$.

Henceforth, we shall confine our attention to four dimensional backgrounds, since these are the one carrying the most physical significance. Moreover, unless otherwise stated, in this section we shall only consider manifolds with empty boundary.

In Lorentzian manifolds we can distinguish between three different classes of vectors:

Definition 2.2. Let (M, g) be a Lorentzian manifold and let $T_p\mathcal{M}$ be the tangent space at $p \in \mathcal{M}$. Moreover, let g_p denote the scalar product induced on $T_p\mathcal{M}$ by the metric g . We say that a vector $v \in T_p\mathcal{M} \setminus \{0\}$ is **timelike**, **lightlike (null)** or **spacelike** if $g_p(v, v) < 0$, $g_p(v, v) = 0$ or $g_p(v, v) > 0$ respectively.

By looking at their tangent vector, we can also define curves that are spacelike, timelike or lightlike:

Definition 2.3. Let $(\mathcal{M}, g)$ be a Lorentzian manifold and let

$$\gamma : I \rightarrow \mathcal{M}, \quad I \subseteq \mathbb{R},$$

be a curve at least $C^1(I; \mathcal{M})$ with nowhere vanishing tangent vector. We say that γ is **timelike**, **lightlike** or **spacelike** if $\dot{\gamma}(\lambda)$ is timelike, lightlike or spacelike as per Definition 2.2 for all $\lambda \in I$. Here $\dot{\gamma}(\lambda)$ denotes the tangent vector to the curve at $\gamma(\lambda)$. We say that γ is a **causal curve** if $\dot{\gamma}(\lambda)$ is either timelike or lightlike for all λ .

This definition allows one to determine whether two regions of a spacetime are causally connected.

Definition 2.4. Let $(\mathcal{M}, g)$ be a spacetime as per Definition 2.1. Let $p \in \mathcal{M}$, we call **chronological future** of p the set

$$I^+(p) \doteq \{q \in \mathcal{M} \mid \exists \gamma : [0, 1] \rightarrow \mathcal{M} \text{ timelike,} \\ \text{future-directed curve, } \gamma(0) = p, \gamma(1) = q\}.$$

Similarly we define the **causal future** of p as

$$J^+(p) \doteq \{q \in \mathcal{M} \mid \exists \gamma : [0, 1] \rightarrow \mathcal{M} \text{ causal,} \\ \text{future-directed curve, } \gamma(0) = p, \gamma(1) = q\}.$$

The chronological and causal pasts, denoted by $I^-(p)$ and $J^-(p)$ respectively, are defined analogously by reversing the time orientation.

Moreover, let $S \subset \mathcal{M}$ be a subset. The **chronological future** of S is the set

$$I^+(S) = \bigcup_{p \in S} I^+(p),$$

whilst the **causal future** of S reads

$$J^+(S) = \bigcup_{p \in S} J^+(p),$$

and analogously for the chronological and causal past of S .

Once these structures have been defined, we can proceed by introducing the notion of globally hyperbolic spacetimes. The reasons for considering this distinguished class of backgrounds are twofold. On the one hand noteworthy is the absence of physically pathological scenarios, such as closed causal curves. On the other hand they possess distinguished hypersurfaces thanks to which a well-defined initial value problem for a hyperbolic differential operator, such as the Klein-Gordon one, can be consistently formulated. To this end, we need some preliminary definitions.

Definition 2.5. Let $(\mathcal{M}, g)$ be a spacetime as per Definition 2.1 and let $\Sigma \subset \mathcal{M}$. We say that Σ is **achronal** if

$$\Sigma \cap I^+(\Sigma) = \emptyset,$$

where $I^+(\Sigma)$ denotes the chronological future of Σ as per Definition 2.4. Moreover, we define the **future domain of dependence** of Σ as

$$D^+(\Sigma) = \{p \in \mathcal{M} \mid \forall \gamma : \mathbb{R} \supseteq J \rightarrow \mathcal{M} \text{ past-inextendible causal curve through } p, \\ \text{Im}(\gamma) \cap \Sigma \neq \emptyset\}.$$

Similarly, we define the **past domain of dependence** $D^-(\Sigma)$ by replacing past-inextendibility with future-inextendibility and the (total) **domain of dependence** by setting $D(\Sigma) \doteq D^+(\Sigma) \cup D^-(\Sigma)$.

Domains of dependence are at the heart of the definition of *Cauchy surfaces*, whose existence completely characterizes globally hyperbolic spacetimes.

Definition 2.6. Let $(\mathcal{M}, g)$ be a spacetime as per Definition 2.1 and let $\Sigma \subset \mathcal{M}$ be a subset of $\mathcal{M}$. We say that Σ is a **Cauchy hypersurface** if and only if it is closed, achronal and $D(\Sigma) = \mathcal{M}$, where $D(\Sigma)$ is the domain of dependence of Σ as per Definition 2.5. We say that $\mathcal{M}$ is a **globally hyperbolic manifold** if and only if it admits a Cauchy hypersurface.

Using Definition 2.6 to establish global hyperbolicity of a generic spacetime is often impractical. For this reason, we give an equivalent characterization.

Theorem 2.1. *Let $(\mathcal{M}, g)$ be a spacetime as per Definition 2.1. Then $\mathcal{M}$ is globally hyperbolic as per Definition 2.6 if and only if it is isometric to $\mathbb{R} \times \Sigma$ equipped with a metric whose line element reads*

$$ds^2 = -\beta dt^2 + d\tilde{s}_t^2, \quad \beta \in C^\infty(\mathbb{R} \times \Sigma),$$

where $d\tilde{s}_t^2$ is the line element of a smooth Riemannian metric h_t on the manifold $\Sigma_t \doteq \{t\} \times \Sigma$ depending smoothly on t . Furthermore, β is a strictly positive, smooth function on $\mathbb{R} \times \Sigma$. Moreover, every Σ_t identifies a smooth spacelike Cauchy surface in $\mathcal{M}$ as per Definition 2.6.

For a proof of this theorem we refer to [BS05, Th. 1.1].

Among the properties of globally hyperbolic spacetimes, we here highlight one that would be helpful in the following. We first introduce the notion of strongly causal spacetime

Definition 2.7. *Let $(\mathcal{M}, g)$ be a spacetime as per Definition 2.1. We say that $\mathcal{M}$ is **strongly causal** if, for all $p \in \mathcal{M}$ and for all open neighborhoods $U \subset \mathcal{M}$, $p \in U$, there is another open subset $V \subseteq U$ which is causally convex, namely, every causal curve whose endpoints lie in V is entirely contained within V .*

Proposition 2.1. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6, then, $\mathcal{M}$ is strongly causal as per Definition 2.7.*

For a proof, we refer to [Wal84, Lemma 8.3.8].

2.1.2 Asymptotically flat spacetimes

While global hyperbolicity ensures the well-posedness of initial value problems for hyperbolic differential operators, in this work we are interested in the analysis of the asymptotic behaviour of physical observables. Therefore, it is necessary to restrict our attention to spacetimes that enjoy suitable asymptotic properties, heuristically they mimic the flat Minkowski spacetime at large distances.

Definition 2.8. *Let $(\mathcal{M}, g)$ be a spacetime as per Definition 2.1. We say that $\mathcal{M}$ is **asymptotically flat at future null and timelike infinity** if there exist another spacetime $(\tilde{\mathcal{M}}, \tilde{g})$, a smooth embedding with open image $\iota : \mathcal{M} \rightarrow \tilde{\mathcal{M}}$, a smooth function $\Omega \in C^\infty(\iota(\mathcal{M}))$ and a preferred point $i^+ \in \tilde{\mathcal{M}}$, such that the following conditions hold:*

1. $\iota(\mathcal{M}) \subseteq \tilde{\mathcal{M}}$ is a manifold with boundary $\partial\mathcal{M}$. Moreover, it holds that $J^-(i^+; \tilde{\mathcal{M}})$ is closed and satisfies

$$J^-(i^+; \tilde{\mathcal{M}}) \setminus \partial J^-(i^+; \tilde{\mathcal{M}}) = \iota(\mathcal{M}).$$

Here $J^-(i^+; \tilde{\mathcal{M}})$ denotes the causal past of i^+ with respect to the causal structure of $\tilde{\mathcal{M}}$. Additionally, $\partial\mathcal{M} = \mathcal{I}^+ \cup \{i^+\}$, where

$$\mathcal{I}^+ = \partial J^-(i^+; \tilde{\mathcal{M}}) \setminus \{i^+\},$$

2. $(\tilde{\mathcal{M}}, \tilde{g})$ is strongly causal in an open neighborhood of $\mathcal{I}^+$ as per Definition 2.7,
3. $\tilde{g}|_{\iota(\mathcal{M})} = \Omega^2 g$ and $\Omega|_{\iota(\mathcal{M})}$ is strictly positive. Moreover, $\Omega|_{\partial\iota(\mathcal{M})} = 0$, $d\Omega \neq 0$ everywhere on $\mathcal{I}^+$ while it vanishes at i^+ , where $d\Omega$ denotes the exterior derivative of Ω . Additionally, it holds that $\tilde{\nabla}_\mu \tilde{\nabla}_\nu \Omega(i^+) = -2\tilde{g}_{\mu\nu}(i^+)$,
4. There exists a smooth function $\omega \in C^\infty(\tilde{\mathcal{M}})$ that is strictly positive on $\mathcal{M} \cup \mathcal{I}^+$ such that, calling n the vector field whose local components read $n^a = \tilde{g}^{ab} \partial_b \Omega$, $\tilde{\nabla}_a(\omega^4 n^a) = 0$. Here $\tilde{\nabla}_a$ are the components of the Levi-Civita connection of $\tilde{\mathcal{M}}$, and the integral curves of the vector field $\omega^{-1}n$ are complete on $\mathcal{I}^+$,
5. The vacuum Einstein equations $R_{\mu\nu} = 0$ are fulfilled in a neighborhood of $\mathcal{I}^+$, where $R_{\mu\nu}$ is the Ricci tensor.

A few remarks are in due order.

Remark 2.1. We can similarly define a spacetime that is **asymptotically flat at past null and timelike infinity** by identifying a preferred point i^- such that the interior of its causal future corresponds to the embedded physical spacetime. In this case we shall denote the boundary as $\partial\iota(\mathcal{M}) = \mathcal{I}^- \cup \{i^-\}$.

Remark 2.2. There also exists another possible notion of infinity, namely the spatial one. However, since our focus shall mainly be towards the null structure, we will not discuss this other scenario and we refer the reader to [Wal84, Section 11.1] for a detailed analysis.

Remark 2.3. The fourth condition in Definition 2.8 entails that $\mathcal{I}^+$ is diffeomorphic to $\mathbb{R} \times \mathbb{S}^2$, regardless of the underlying manifold. Thus, for every asymptotically flat spacetime, it is possible to choose on $\mathcal{I}^+$ a set of coordinates $(u, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^2$, called **Bondi coordinates**. Here the coordinate u in particular can be regarded as the affine parameter of the null geodesic generating $\mathcal{I}^+$, see [Wal84, Section 11.1].

To provide a concrete realization of Definition 2.8, we now outline the conformal completion of standard 4-dimensional Minkowski space $\mathbb{M}^4$.

We start with the line element of the metric η , which, in standard spherical coordinates $(t, r, \theta, \phi) \in \mathbb{R} \times (0, \infty) \times \mathbb{S}^2$, reads

$$ds^2 = -dt^2 + dr^2 + r^2 d\mathbb{S}^2(\theta, \phi), \quad d\mathbb{S}^2(\theta, \phi) = d\theta^2 + \sin^2 \theta d\phi^2. \quad (2.1)$$

We introduce the advanced and retarded null coordinates

$$\begin{cases} u \doteq t - r \\ v \doteq t + r \end{cases}, \quad \begin{cases} t = \frac{u+v}{2} \\ r = \frac{v-u}{2} \end{cases}.$$

Since $r > 0$, it necessarily follows that $v > u$. The line element of η can be rewritten as:

$$ds^2 = -du \, dv + \frac{1}{4}(v - u)^2 d\mathbb{S}^2(\theta, \phi). \quad (2.2)$$

The asymptotic behaviour along null geodesics corresponds to the limits $u \rightarrow -\infty$ (past null infinity $\mathscr{I}^-$) and $v \rightarrow \infty$ (future null infinity $\mathscr{I}^+$). We apply a conformal transformation $\eta \mapsto \Omega^2 \eta$ in order to bring future and past null infinities to a finite coordinate distance. This is achieved by another change of coordinates:

$$\begin{cases} V \doteq \tan^{-1}(v), \\ U \doteq \tan^{-1}(u), \end{cases}$$

where the domain of definition of these new coordinates is

$$(U, V) \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \times \left(-\frac{\pi}{2}, \frac{\pi}{2}\right).$$

The asymptotic boundaries correspond now to $V = \frac{\pi}{2}$ for $\mathscr{I}^+$ and $U = -\frac{\pi}{2}$ for $\mathscr{I}^-$. Due to the monotonicity of the arctangent function, the condition $V > U$ is preserved. The metric transforms as

$$ds^2 = -\frac{1}{\cos^2 U \cos^2 V} dU \, dV + \frac{\sin^2(V - U)}{4 \cos^2 U \cos^2 V} d\mathbb{S}^2(\theta, \phi). \quad (2.3)$$

Note that we cannot safely extend the metric at $U = -\frac{\pi}{2}$ and $V = \frac{\pi}{2}$ due to the singularity in the metric. Hence, we apply a conformal transformation with conformal factor $\Omega(U, V) = 2 \cos U \cos V$ to obtain

$$d\tilde{s}^2 = -4 dU \, dV + \sin^2(V - U) d\mathbb{S}^2(\theta, \phi). \quad (2.4)$$

Finally, it is convenient to introduce the additional coordinate transformation

$$\begin{cases} T \doteq V + U, \\ R \doteq V - U. \end{cases}$$

The final form of the conformally transformed metric is

$$d\tilde{s}^2 = -dT^2 + dR^2 + \sin^2(R) d\mathbb{S}^2(\theta, \phi). \quad (2.5)$$

Observe that Equation (2.5) is nothing but the line element of the Einstein static universe $\mathbb{R} \times \mathbb{S}^3$, which plays the role of the unphysical spacetime $\tilde{\mathcal{M}}$ in Definition 2.8. The smooth embedding $\iota : \mathbb{M}^4 \rightarrow \mathbb{R} \times \mathbb{S}^3$ maps Minkowski spacetime into the open set:

$$\iota(\mathbb{M}^4) = \{(T, R, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^3 \mid -\pi < T \pm R < \pi, R > 0\} \subset \mathbb{R} \times \mathbb{S}^3. \quad (2.6)$$

The boundary of $\iota(\mathbb{M}^4)$ in $\mathbb{R} \times \mathbb{S}^3$ can be decomposed as follows

$$\partial\overline{\iota(\mathbb{M}^4)} = \mathcal{I}^+ \cup \mathcal{I}^- \cup i^+ \cup i^- \cup i_0$$

. We have

- Future null infinity

$$\mathcal{I}^+ = \{(T, R, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^3 \mid T + R = \pi, T \neq 0, R \neq 0\},$$

- Past null infinity

$$\mathcal{I}^- = \{(T, R, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^3 \mid T - R = -\pi, T \neq 0, R \neq 0\},$$

- Future timelike infinity

$$i^+ = \{(T, R, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^3 \mid R = 0, T = \pi\},$$

- Past timelike infinity

$$i^- = \{(T, R, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^3 \mid R = 0, T = -\pi\},$$

- Spatial infinity

$$i_0 = \{(T, R, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^3 \mid R = \pi, T = 0\}.$$

We now focus on the structure associated to future null infinity $\mathcal{I}^+$. The first condition in Definition 2.8 is satisfied since $\mathcal{I}^+$ is the accumulation set of all future-directed null geodesics originating from $\mathbb{M}^4$. Therefore it cannot intersect the causal past of any point inside of it. Moreover, since the Einstein static universe $\mathbb{R} \times \mathbb{S}^3$ is globally hyperbolic, also the second condition is met. By construction, we have that

$$\tilde{g}|_{\iota(\mathbb{M}^4)} = \Omega^2 \eta, \quad \Omega = 2 \cos U \cos V = \cos T + \cos R,$$

where Ω can be extended to the entire Einstein static universe. Moreover, it vanishes whenever $U = \pm \frac{\pi}{2}$ or $V = \pm \frac{\pi}{2}$, and therefore also on $\mathcal{I}^+$. Its exterior derivative reads

$$d\Omega = -2 \sin U \cos V dU - 2 \cos U \sin V dV.$$

On future null infinity, this never vanishes since $\mathcal{I}^+ = \{(U, V) \mid V = \frac{\pi}{2}, U \neq \pm \frac{\pi}{2}\}$ and thus we obtain

$$d\Omega|_{\mathcal{I}^+} = -2 \cos U dV,$$

Hence also the third condition is satisfied. Finally, since the Minkowski spacetime is a solution to the vacuum Einstein equations, also the last condition is met.

An important observation regarding the metric structure induced on the future null boundary is that it is non-unique. As a matter of fact, we can rescale the conformal factor by another scalar, strictly positive smooth function $\omega \in C^\infty(\tilde{\mathcal{M}})$. In this way we obtain the following rescaling

$$\tilde{h} \mapsto \omega^2 \tilde{h}, \quad n \mapsto \omega^{-1} n,$$

where $\tilde{h}$ is the metric induced on $\mathcal{I}^+$ by $\tilde{g}$ and n is the vector field whose integral curves generate $\mathcal{I}^+$. However, the topology of $\mathbb{R} \times \mathbb{S}^2$ is left unchanged. The freedom in the choice of this additional factor ω is a *gauge freedom*, which identifies equivalence classes of metric structures on $\mathcal{I}^+$.

We denote these equivalence classes with the triple $[(\mathcal{I}^+, \tilde{h}, n)]$, where $\tilde{h}$ denotes the metric induced on $\mathcal{I}^+$ by $\tilde{g}$, that of the unphysical spacetime $\tilde{\mathcal{M}}$. Thus, we say that $(\mathcal{I}^+, \tilde{h}_1, n_1) \sim (\mathcal{I}^+, \tilde{h}_2, n_2)$ if there exists a smooth, strictly positive function ω such that $\tilde{h}_1 = \omega^2 \tilde{h}_2$ while $n_1 = \omega^{-1} n_2$.

This important property of asymptotically flat spacetimes is linked to another one, called *universality*, according to which all conformal boundaries $\mathcal{I}^+$ for different spacetimes are diffeomorphic to one another. More precisely, for every pair of asymptotically flat spacetimes $(\mathcal{M}_1, g_1)$, $(\mathcal{M}_2, g_2)$, once two representatives of the equivalence class of metric structures $(\mathcal{I}_1^+, \tilde{h}_1, n_1)$, $(\mathcal{I}_2^+, \tilde{h}_2, n_2)$ are selected, there exists a diffeomorphism $\gamma : \mathcal{I}_1^+ \rightarrow \mathcal{I}_2^+$ such that $\gamma^* \tilde{h}_1 = \tilde{h}_2$ and $\gamma^* n_1 = n_2$. Here γ^* denotes the pullback of the diffeomorphism γ . This property stems from the possibility of choosing Bondi coordinates for every asymptotically flat spacetime, see [Wal84, Section 11.1], see also Remark 2.3.

Given the universal nature of the boundary $\mathcal{I}^+$, one might wonder whether this structure admits a distinguished class of symmetries, which can be regarded as those of our spacetime, asymptotically. This motivates the definition of the BMS group, which plays an important rôle in the study of the properties of asymptotically flat spacetimes.

Definition 2.9. Let $(\mathcal{M}, g)$ be an asymptotically flat spacetime as per Definition 2.8 and let $\mathcal{I}^+$ denote future null infinity. Moreover, let $\tilde{h}$ denote the metric on $\mathcal{I}^+$ induced by that of the unphysical spacetime while n is the vector field whose integral curves form $\mathcal{I}^+$. We call **Bondi-Metzner-Sachs (BMS) group** the group of diffeomorphisms $\gamma : \mathcal{I}^+ \rightarrow \mathcal{I}^+$ such that

$$\gamma(\mathcal{I}^+) = \mathcal{I}^+, \quad \gamma^* \tilde{h} = \omega^2 \tilde{h}, \quad \gamma^* n = \omega^{-1} n, \quad \omega \in C^\infty(\mathcal{I}^+),$$

where ω is a strictly positive, smooth function.

An explicit realization of this group is obtained as follows. We first choose a Bondi frame, whose coordinates read $(u, \theta, \phi) \in \mathbb{R} \times \mathbb{S}^2$ and then we apply the stereographic projection to define the coordinates $(\zeta, \bar{\zeta}) \in \mathbb{C}^2$ via the defining relations

$$\begin{cases} \zeta \doteq e^{i\phi} \cot(\frac{\theta}{2}) \\ \bar{\zeta} \doteq e^{-i\phi} \cot(\frac{\theta}{2}) \end{cases}.$$

It turns out that, in this frame, the BMS group is

$$G_{\text{BMS}} = SO(3, 1)_\uparrow \ltimes C^\infty(\mathbb{S}^2),$$

where $\ltimes$ denotes the semidirect product between the proper orthochronous Lorentz group $SO(3, 1)_\uparrow$ and $C^\infty(\mathbb{S}^2)$. Given an element $(\Lambda, f) \in SO(3, 1)_\uparrow \ltimes C^\infty(\mathbb{S}^2)$ the action on an arbitrary point $p = (u, \zeta, \bar{\zeta}) \in \mathcal{I}^+$ reads

$$\begin{cases} u' \doteq K_\Lambda(\zeta, \bar{\zeta})(u + f(\zeta, \bar{\zeta})) \\ \zeta' \doteq \Lambda \zeta \doteq \frac{a_\Lambda \zeta + b_\Lambda}{c_\Lambda \zeta + d_\Lambda} \\ \bar{\zeta}' \doteq \Lambda \bar{\zeta} \doteq \frac{\bar{a}_\Lambda \bar{\zeta} + \bar{b}_\Lambda}{\bar{c}_\Lambda \bar{\zeta} + \bar{d}_\Lambda} \end{cases}, \quad (2.7)$$

where

$$K_\Lambda(\zeta, \bar{\zeta}) = \frac{1 + \zeta \bar{\zeta}}{(a_\Lambda \zeta + b_\Lambda)(\bar{a}_\Lambda \bar{\zeta} + \bar{b}_\Lambda) + (c_\Lambda \zeta + d_\Lambda)(\bar{c}_\Lambda \bar{\zeta} + \bar{d}_\Lambda)},$$

$$\Pi^{-1}(\Lambda) = \begin{pmatrix} a_\Lambda & b_\Lambda \\ c_\Lambda & d_\Lambda \end{pmatrix}.$$

Here $\Pi : SL(2, \mathbb{C}) \rightarrow SO(3, 1)_\uparrow$ is the surjective covering homomorphism from $SL(2, \mathbb{C})$ to $SO(3, 1)_\uparrow$. Thus, the matrix $\Pi^{-1}(\Lambda)$ is defined up to a global sign that plays no rôle. Moreover, the group structure is given by the product $\odot$, which acts on two elements $(\Lambda', f'), (\Lambda, f) \in SO(3, 1)_\uparrow \ltimes C^\infty(\mathbb{S}^2)$ as

$$(\Lambda', f') \odot (\Lambda, f) = (\Lambda' \Lambda, f + (K_{\Lambda^{-1}} \circ \Lambda) \cdot (f' \circ \Lambda)). \quad (2.8)$$

Here $\circ$ denotes the composition of maps while $\cdot$ denotes the pointwise product of functions.

One might expect the asymptotic symmetry group of an asymptotically flat spacetime to be isomorphic to the Poincaré group. However, the semidirect product with $C^\infty(\mathbb{S}^2)$ reveals a much richer symmetry structure. Within this structure, we can identify a subgroup isomorphic to the Poincaré group by restricting to $\mathcal{P} = SO(3,1)_\uparrow \ltimes T^4$, where T^4 is the four-dimensional subgroup defined as

$$T^4 = \left\{ \alpha \in C^\infty(\mathbb{S}^2) \mid \alpha(\zeta, \bar{\zeta}) = \sum_{l=0}^1 \sum_{m=-l}^l \alpha_{lm} Y_{lm}(\zeta, \bar{\zeta}), \alpha_{lm} \in \mathbb{C} \right\},$$

where the terms Y_{lm} denote the standard spherical harmonics. This subspace T^4 is isomorphic to the group of spacetime translations $\mathbb{R}^4$.

We can thus decompose the space $C^\infty(\mathbb{S}^2)$ as a direct sum of vector spaces $T^4 \oplus \text{ST}$, where ST denotes the complement of T^4 and whose elements are called *pure supertranslations*. An important feature of this decomposition is that, while the Lorentz group acts on T^4 invariantly, the complement ST is not preserved.

If we act on the Poincaré subgroup with a pure supertranslation $g = (\mathbb{I}, f) \in G_{\text{BMS}}$, $f \in \text{ST}$, the conjugated subgroup $g^{-1} \odot \mathcal{P} \odot g$ remains isomorphic to the Poincaré group. Consequently, different choices of supertranslations lead to distinct, non-equivalent embeddings of the Poincaré group within G_{BMS} . In this sense, the BMS group contains infinitely many distinct copies of the Poincaré group related by elements of ST.

The existence of this enlarged asymptotic symmetry group, and the resulting ambiguity in selecting a canonical Poincaré subgroup, plays a fundamental rôle in the study of asymptotically flat spacetimes and is closely related to the definition of asymptotic charges at null infinity. In suitable asymptotically BMS-invariant theories, identifying effects linked to the specific choice of a Poincaré subgroup can yield information on the underlying geometry of the bulk. For a complete analysis of the BMS group we refer to [Sac62].

2.2 Algebraic Quantum Field Theory

In this section we establish a rigorous mathematical framework for a scalar quantum field theory on globally hyperbolic spacetimes without boundary using the perturbative algebraic approach (pAQFT). The exposition proceeds in three stages. The first part formalizes classical free field theory, defining the configuration space, the algebra of observables, and the underlying classical dynamics. In the following we address the quantization of this algebra via deformation quantization, hence encoding the canonical commutation relations (CCR). Finally, the last part of this section focuses on the interacting theory by employing perturbative techniques to construct interacting observables from their free counterparts.

2.2.1 Kinematical configurations

Constructing a field theory requires specifying the admissible kinematical field configurations. Physically, this amounts to specifying the type of field under consideration, such as a scalar or spinorial field. Mathematically, the internal degrees of freedom of these fields are encoded by selecting an appropriate smooth vector bundle over the spacetime manifold.

Definition 2.10. *Let $\mathcal{M}$ be a smooth manifold. A **smooth vector bundle of rank k** is a smooth manifold E equipped with a triple $[\mathcal{M}, \pi, \mathbb{R}^k]$, where $\pi : E \rightarrow \mathcal{M}$ is a surjective, smooth map such that:*

1. *for each $p \in \mathcal{M}$, the set $\pi^{-1}(p) \doteq V_p$ is a real vector space of dimension k ,*
2. *for each $p \in \mathcal{M}$, there exists an open neighborhood U of p and a smooth map $\Psi : \pi^{-1}(U) \rightarrow U \times \mathbb{R}^k$ such that*
 - *$\pi_U \circ \Psi = \pi$, where $\pi_U : U \times \mathbb{R}^k \rightarrow U$ is the projection on the first entry,*
 - *for each $q \in U$, $\Psi|_q : V_q \rightarrow \{q\} \times \mathbb{R}^k$ is a vector space isomorphism.*

*The map Ψ is called **local trivialization** of E . We shall denote a smooth vector bundle E over a manifold $\mathcal{M}$ by $E \xrightarrow{\pi} \mathcal{M}$.*

In order to fully characterise a field theory at a classical level, we need to define the corresponding kinematical configurations. These are naturally identified with the smooth sections of a suitable vector bundle.

Definition 2.11. Let $E \xrightarrow{\pi} \mathcal{M}$ be a smooth vector bundle as per Definition 2.10. We call a **section** of the vector bundle E a smooth map $\sigma : \mathcal{M} \rightarrow E$ such that $\pi \circ \sigma = \text{id}_{\mathcal{M}}$, where π is the bundle projection. We denote the space of smooth sections by $\mathcal{E}(E)$. Denoting by V the typical fibre of E , we also assume that there exists a real pairing $\langle \cdot, \cdot \rangle_E : V \times V \rightarrow \mathbb{R}$.

Remark 2.4. In the context of field theories, the space of smooth sections of a vector bundle $\mathcal{E}(E)$ is often called **space of configurations**.

Example 2.1. For a real scalar field theory, which is the main focus of this work, we consider the trivial line bundle $E \doteq \mathcal{M} \times \mathbb{R}$. Its smooth sections are naturally identified with the space of smooth real-valued functions on the spacetime $C^\infty(\mathcal{M}; \mathbb{R}) \doteq \mathcal{E}(\mathcal{M})$.

The configuration space can be endowed with a Fréchet topology. Here we state the definition of this topology in the case of a scalar field theory. For more details on higher-spin fields we refer to [Rej16, Chapter 3].

Definition 2.12. Let $\Omega \subseteq \mathbb{R}^n$ be an open set. The standard Fréchet topology on $C^\infty(\Omega; \mathbb{R})$ is induced by the family of seminorms

$$p_{K,m}(\phi) = \sup_{\substack{x \in K \\ |\alpha| \leq m}} |\partial^\alpha \phi(x)|, \quad \alpha \in \mathbb{N}_0^n,$$

where $K \subset \Omega$ is compact and $m \in \mathbb{N}_0$. Furthermore, we can endow the configuration space $\mathcal{E}(\mathcal{M})$ as per Definition 2.11 with an analogous Fréchet topology by means of local coordinate charts. Let $\{(U_\beta, \psi_\beta)\}_{\beta \in I}$ be a countable atlas of $\mathcal{M}$, where $\bigcup_{\beta \in I} U_\beta = \mathcal{M}$, and each chart map $\psi_\beta : U_\beta \rightarrow \Omega_\beta \subset \mathbb{R}^n$ is a diffeomorphism. Moreover, let $\{K_\beta\}_{\beta \in I}$ be a countable family of compact subsets of $\mathcal{M}$ such that $K_\beta \subset U_\beta$ for all $\beta \in I$, $\bigcup_{\beta \in I} K_\beta = \mathcal{M}$. Then the topology of $\mathcal{E}(\mathcal{M})$ is defined by the family of seminorms $\{p_m^{(\beta)}\}_{\beta \in I, m \in \mathbb{N}}$ such that

$$p_m^{(\beta)}(f) = p_{\psi_\beta(K_\beta),m}(f \circ \psi_\beta^{-1}), \quad f \in \mathcal{E}(\mathcal{M}),$$

where $p_{\psi_\beta(K_\beta),m}$ denotes the seminorm on $C^\infty(\Omega_\beta; \mathbb{R})$ defined above.

A notable subspace of $\mathcal{E}(\mathcal{M})$ is that of smooth functions with compact support $C_0^\infty(\mathcal{M}) \doteq \mathcal{D}(\mathcal{M})$. We can also endow $\mathcal{D}(\mathcal{M})$ with a topology, which is not Fréchet but is locally convex, since $\mathcal{M}$ cannot be compact.

Definition 2.13. Let $\Omega \subset \mathbb{R}^n$ be an open set and let $\{K_j\}_{j \in \mathbb{N}}$ be an exhausting sequence of compact sets for Ω , namely, $K_j \subset \overset{\circ}{K}_{j+1}$, $\forall j \in \mathbb{N}$, K_j is

compact for any j and $\bigcup_{j \in \mathbb{N}} K_j = \Omega$. Here $\overset{\circ}{K}_j$ denotes the interior of K_j . We set

$$\mathcal{D}_{K_j}(\Omega) = \{f \in \mathcal{E}(\Omega) \mid \text{supp}(f) \subseteq K_j\}.$$

We can endow the space $\mathcal{D}_{K_j}(\Omega)$ with a Fréchet topology induced by the collection of seminorms

$$p_m^{(j)}(f) = \sup_{\substack{x \in K_j \\ |\alpha| \leq m}} |\partial^\alpha f(x)|, \quad f \in \mathcal{D}_{K_j}(\Omega), \quad m \in \mathbb{N}, \quad \alpha \in \mathbb{N}_0^n.$$

Then, denoting the set of compactly supported, smooth functions on Ω by $\mathcal{D}(\Omega)$, it holds that

$$\mathcal{D}(\Omega) = \bigcup_{j \in \mathbb{N}} \mathcal{D}_{K_j}(\Omega).$$

The topology of $\mathcal{D}(\Omega)$ is the final topology with respect to the inclusion maps $\{\iota_j\}_{j \in \mathbb{N}}$, $\iota_j : \mathcal{D}_{K_j}(\Omega) \hookrightarrow \mathcal{D}(\Omega)$.

Moreover, we endow the space of compactly supported smooth functions on a manifold $\mathcal{M}$ with a topology by means of coordinate charts. Let us consider an exhaustion sequence of compact sets $\{K_j\}_{j \in \mathbb{N}}$ for $\mathcal{M}$ defined analogously as above. It holds that

$$\mathcal{D}(\mathcal{M}) = \bigcup_{j \in \mathbb{N}} \mathcal{D}_{K_j}(\mathcal{M}), \quad \mathcal{D}_{K_j}(\mathcal{M}) = \{f \in \mathcal{E}(\mathcal{M}) \mid \text{supp}(f) \subseteq K_j\}.$$

For each $j \in \mathbb{N}$ we endow $\mathcal{D}_{K_j}(\mathcal{M})$ with a Fréchet topology by selecting a finite subcover of coordinate charts $(U_\beta^{(j)}, \psi_\beta^{(j)})_{\beta \in \{1, \dots, N_j\}}$ covering K_j and a collection of compact sets $\{L_\beta^{(j)}\}_{\beta \in \{1, \dots, N_j\}}$ such that $L_\beta^{(j)} \subset U_\beta^{(j)}$ and $\bigcup_{\beta \in \{1, \dots, N_j\}} L_\beta^{(j)} = K_j$. Then the topology of $\mathcal{D}_{K_j}(\mathcal{M})$ is induced by the set of seminorms

$$p_m^{(j)}(f) \doteq \max_{\beta} \sup_{\substack{x \in \psi_\beta^{(j)}(L_\beta^{(j)}) \\ |\alpha| \leq m}} |\partial^\alpha (f \circ (\psi_\beta^{(j)})^{-1})|, \quad f \in \mathcal{D}_{K_j}(\mathcal{M}), \quad \alpha \in \mathbb{N}_0^n.$$

The topology of $\mathcal{D}(\mathcal{M})$ is the final topology with respect to the maps $\iota_j : \mathcal{D}_{K_j}(\mathcal{M}) \hookrightarrow \mathcal{D}(\mathcal{M})$.

2.2.2 Observables on the configuration space

Once the kinematical configurations are established, it is necessary to characterise the physical observables of the system. Since a physical measurement assigns a value to a field configuration, we realise the set of observables as

smooth functionals on the configuration space. Among all smooth functionals, we identify the subclasses of those which are microcausal, regular and local. They will be the objects we need to construct the classical algebra of observables.

Because our ultimate goal is to work with a quantum scalar field theory, from now on we shall specialize to the case of the trivial line bundle $E = \mathcal{M} \times \mathbb{R}$ and work directly with complex-valued functionals. We refer to [Rej16, Ch. 3] for the case of higher spin fields.

Definition 2.14. Let $F : \mathcal{E}(\mathcal{M}) \rightarrow \mathbb{C}$ be a continuous functional on the configuration space with respect to the topology in Definition 2.12 and let $\phi, \eta \in \mathcal{E}(\mathcal{M})$. The **Fréchet derivative** of F at ϕ in the direction η is defined as

$$F^{(1)}(\phi; \eta) = \lim_{s \rightarrow 0} \frac{1}{s} (F(\phi + s\eta) - F(\phi)),$$

whenever the limit exists. We say that F is differentiable at ϕ if the derivative exists for all $\eta \in \mathcal{E}(\mathcal{M})$ and continuously differentiable if it is differentiable and the map $F^{(1)} : \mathcal{E}(\mathcal{M}) \times \mathcal{E}(\mathcal{M}) \rightarrow \mathbb{C}$ is continuous with respect to the product topology of $\mathcal{E}(\mathcal{M}) \times \mathcal{E}(\mathcal{M})$.

Derivatives of higher orders are defined iteratively:

$$F^{(k)}(\phi; \eta_1, \dots, \eta_k) = \frac{\partial^k}{\partial s_1 \dots \partial s_k} F(\phi + s_1 \eta_1 + \dots + s_k \eta_k) \Big|_{s_1=s_2=\dots=s_k=0}, \quad (2.9)$$

where $\eta_1, \dots, \eta_k \in \mathcal{E}(\mathcal{M})$. If $F^{(k)} : \mathcal{E}(\mathcal{M}) \times \mathcal{E}(\mathcal{M})^k \rightarrow \mathbb{C}$ exists and is jointly continuous for all $k \in \mathbb{N}$, then F is said to be (Bastiani) **smooth**.

We denote by $\mathcal{F}(\mathcal{M})$ the space of smooth functionals on the space of configurations. Moreover, we say that $F \in \mathcal{F}(\mathcal{M})$ is a **polynomial functional** if all Fréchet derivatives above a certain order vanish.

Definition 2.15. Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\mathcal{F}(\mathcal{M})$ be the space of smooth functionals as per Definition 2.14. We define the **spacetime support** of $F \in \mathcal{F}(\mathcal{M})$ as

$$\text{supp}(F) = \{p \in \mathcal{M} \mid \text{for every open neighborhood } U \text{ of } p, \exists \phi, \psi \in \mathcal{E}(\mathcal{M}), \\ \text{supp}(\psi) \subset U \text{ s.t. } F(\phi + \psi) \neq F(\phi)\}.$$

The following proposition highlights a property of the Fréchet derivative that will be useful in the construction of the algebra of observables.

Proposition 2.2. Let $F \in \mathcal{F}(\mathcal{M})$ be a smooth functional on the configuration space as per Definition 2.14 and let $F^{(k)}$ denote its k -th order derivative. For every smooth function $\phi \in \mathcal{E}(\mathcal{M})$, the map $F^{(k)}(\phi) : \mathcal{E}(\mathcal{M})^k \rightarrow \mathbb{C}$ is multilinear and continuous with respect to the corresponding topologies.

For a proof, we refer to [Rej16, Prop. 3.1].

We now define a product on a suitable class of functionals, which is needed to promote the set of observables to an algebra. Since the product between generic functionals is, in general, ill-defined, we must restrict our attention to a distinguished subclass. In order to do so, we shall use some tools from the theory of distributions, which will play a pivotal rôle in the following. In particular, we shall identify the higher-order Fréchet derivatives of functionals with compactly supported distributions. The microlocal tools introduced in Appendix A.1 allow us to identify the natural class of functionals for which a product is well defined. On account of Theorem A.4, this class is characterized by a condition on the wavefront sets of the Fréchet derivatives. We refer to these functionals as *microcausal*.

Definition 2.16. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\mathcal{F}(\mathcal{M})$ be the space of smooth functionals as per Definition 2.14. We say that $F \in \mathcal{F}(\mathcal{M})$ is a **microcausal functional** if*

$$\text{WF}(F^{(k)}(\phi)) \subset T^*(\mathcal{M}^k) \setminus \left(\bigcup_{x \in \mathcal{M}} (\overline{V}_x^+)^k \cup \bigcup_{x \in \mathcal{M}} (\overline{V}_x^-)^k \right), \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \forall k \in \mathbb{N}. \quad (2.10)$$

Here $\overline{V}_x^\pm$ denotes the closed future (+)/past (-) lightcone in $T_x^*\mathcal{M}$ while $\text{WF}(F^{(k)}(\phi))$ denotes the wavefront set as per Definition A.4 of the k -th order Fréchet derivative of F as per Definition 2.14. We denote the space of microcausal functionals as $\mathcal{F}_{\mu\text{c}}(\mathcal{M})$.

Remark 2.5. *The set of microcausal functionals is the appropriate functional set only when considering polynomial functionals. As a matter of fact, as we will later show, microcausal functionals can be endowed with a Poisson structure by means of the Peierls brackets. However, for non-polynomial functionals, the Peierls brackets generally fail to preserve the class of microcausal functionals, motivating the introduction of the larger class of equicausal functionals. Since all the observables that we shall consider fall under the polynomial category, we will not address this issue here and we refer to [HRV24] for a detailed analysis.*

Remark 2.6. *Let us point out that, given any microcausal functional $F \in \mathcal{F}_{\mu\text{c},\text{pol}}(\mathcal{M})$ of polynomial type, it is possible to completely characterise its action in terms of linear functionals in the following way*

$$F(\phi) = \sum_{k=0}^N \frac{1}{k!} \langle F_k, \phi^{\otimes k} \rangle, \quad \phi \in \mathcal{E}(\mathcal{M}), N \in \mathbb{N},$$

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where $F_k \in \mathcal{E}'(\mathcal{M}^k)$ is the compactly supported distribution obtained as

$$F_k = F^{(k)}(0).$$

Here $F^{(k)}(0)$ denotes the Fréchet derivative as per Definition 2.14 of F evaluated at the vanishing configuration $0 \in \mathcal{E}(\mathcal{M})$. Additionally, there is no issue regarding convergence of the series since only a finite number of terms are non vanishing, being the functional of polynomial type.

Within the domain of microcausal functionals, two distinct subspaces can be identified: the *local functionals* and the *regular functionals*. Our interest in the first class is due to the fact that all physically relevant observables, such as the stress-energy tensor, are local. Moreover, regular functionals are a useful intermediate tool to introduce structures on the algebra, such as the Peierls brackets, without dealing with the technical difficulties coming from the wavefront set.

Definition 2.17. Let $F \in \mathcal{F}_{\mu c}(\mathcal{M})$ be a microcausal functional as per Definition 2.16. We say that F is a **regular functional** if

$$F^{(k)}(\phi) \in \mathcal{D}(\mathcal{M}^k) \hookrightarrow \mathcal{E}'(\mathcal{M}^k), \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \forall k \in \mathbb{N},$$

where, by a slight abuse of notation, we use the same symbol for the distribution and for the function that generates it. Here $F^{(k)}(\phi)$ denotes the k -th order Fréchet derivative at ϕ as per Definition 2.14. We denote the space of regular functionals by $\mathcal{F}_{\text{reg}}(\mathcal{M})$.

Example 2.2. A notable example of a regular functional is the smeared linear field Φ_f :

$$\Phi_f(\phi) \doteq \int_{\mathcal{M}} d\mu_x f(x) \phi(x), \quad \phi \in \mathcal{E}(\mathcal{M}), f \in \mathcal{D}(\mathcal{M}).$$

Since it is the linear functional generated by a smooth function, its wavefront set is empty on account of Proposition A.1.

Computing the Fréchet derivative yields:

$$\begin{aligned} \Phi_f^{(1)}(\phi; \eta) &= \left. \frac{d}{ds} \right|_{s=0} \int_{\mathcal{M}} d\mu_x f(x) (\phi(x) + s\eta(x)) = \int_{\mathcal{M}} d\mu_x f(x) \eta(x), \\ \Phi_f^{(k)}(\phi; \eta_1, \dots, \eta_k) &= 0, \quad \forall k > 1. \end{aligned}$$

Because $\Phi_f^{(1)}(\phi)$ is generated by the smooth function f and all the higher derivatives vanish, it is a regular functional as per Definition 2.17.

Finally, the physical interactions of a field theory are modelled by local functionals.

Definition 2.18. Let $F \in \mathcal{F}_{\mu c}(\mathcal{M})$ be a microcausal functional as per Definition 2.16. We say that F is a **local functional** if $\text{WF}(F^{(1)}(\phi)) = \emptyset$ for all $\phi \in \mathcal{E}(\mathcal{M})$, where WF denotes the wavefront set of the compactly supported distribution $F^{(1)}(\phi)$ as per Definition A.4, and

$$\text{supp}(F^{(k)}(\phi)) \subset \text{Diag}_k(\mathcal{M}) = \{\underbrace{(x, \dots, x)}_k \in \mathcal{M}^k\}, \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \forall k \in \mathbb{N}.$$

Here $\text{supp}(F^{(k)}(\phi))$ denotes the support of the compactly supported distribution as in Definition A.1.

We denote the space of local functionals by $\mathcal{F}_{\text{loc}}(\mathcal{M})$.

Example 2.3. Consider the quadratic functional representing a mass term or local interaction:

$$\Phi_f^2(\phi) = \int_{\mathcal{M}} d\mu_x f(x) \phi^2(x), \quad f \in \mathcal{D}(\mathcal{M}), \phi \in \mathcal{E}(\mathcal{M}). \quad (2.11)$$

Evaluating the Fréchet derivatives yields:

$$\begin{aligned} (\Phi_f^2)^{(1)}(\phi; \eta) &= \frac{d}{ds} \Phi_f^2(\phi + s\eta) \Big|_{s=0} = \frac{d}{ds} \Big|_{s=0} \int_{\mathcal{M}} d\mu_x f(x) (\phi(x) + s\eta(x))^2 = \\ &= 2 \int_{\mathcal{M}} d\mu f(x) \phi(x) \eta(x). \\ (\Phi_f^2)^{(2)}(\phi; \eta_1, \eta_2) &= \frac{\partial^2}{\partial s_1 \partial s_2} \Big|_{s_1=s_2=0} \int_{\mathcal{M}} d\mu_x f(x) (\phi(x) + s_1\eta_1(x) + s_2\eta_2(x))^2 = \\ &= 2 \int_{\mathcal{M}} d\mu f(x) \eta_1(x) \eta_2(x). \\ (\Phi_f^2)^{(k)}(\phi; \eta_1, \dots, \eta_k) &= 0, \quad \forall k > 2. \end{aligned}$$

The second order Fréchet derivative is supported on the diagonal $\text{Diag}_2(\mathcal{M})$, while higher derivatives vanish. We conclude that $\Phi_f^2 \in \mathcal{F}_{\text{loc}}(\mathcal{M})$.

We are now ready to define the classical algebra of observables for a scalar field theory

Definition 2.19. Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6. We call **classical microcausal algebra** for a scalar field theory the commutative, unital $*$ -algebra, as per Definition B.2, $\mathcal{A}_{\text{cl}}(\mathcal{M}) = (\mathcal{F}_{\mu c, \text{pol}}(\cdot, \cdot), *)$, where:

- $\mathcal{F}_{\mu c, pol}$ is the subspace of microcausal functionals as per Definition 2.16 formed by those of polynomial type as per Definition 2.14,
- The product is defined as

$$\begin{aligned} \cdot : \mathcal{F}_{\mu c, pol}(\mathcal{M}) \times \mathcal{F}_{\mu c, pol}(\mathcal{M}) &\rightarrow \mathcal{F}_{\mu c, pol}(\mathcal{M}), \\ (F, G) &\rightarrow F \cdot G \doteq \iota^*(F \otimes G), \quad \forall F, G \in \mathcal{F}_{\mu c, pol}(\mathcal{M}). \end{aligned}$$

Here ι^* denotes the pullback of the diagonal map

$$\begin{aligned} \iota : \mathcal{E}(\mathcal{M}) &\rightarrow \mathcal{E}(\mathcal{M}) \times \mathcal{E}(\mathcal{M}), \\ \iota(\phi) &= (\phi, \phi) \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \end{aligned}$$

- The involution $*$ is defined via the defining relation $F^*(\phi) = \overline{F(\phi)}$ for all $F \in \mathcal{F}_{\mu c, pol}(\mathcal{M})$ and $\phi \in \mathcal{E}(\mathcal{M})$. Here $\bar{\cdot}$ denotes the complex conjugate in $\mathbb{C}$.

Moreover, we say that an element $F \in \mathcal{F}_{\mu c, pol}(\mathcal{M})$ is an **observable** if $F^* = F$.

2.2.3 Dynamics

Once we have defined the fundamental kinematical structures and the observables of our field theory, we can proceed by codifying the dynamics. We shall follow the Lagrangian approach, introducing a suitable map, namely the Lagrangian, from which the equations of motion are derived. This will allow us to introduce the notion of *on-shell* algebra of observables, as well as that of *Green operator*, which shall play a pivotal rôle in the remainder of our discussion.

Definition 2.20. Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6. We call **generalised Lagrangian** a map $\mathcal{L} : \mathcal{D}(\mathcal{M}) \rightarrow \mathcal{F}_{loc}(\mathcal{M})$ such that:

- $\mathcal{L}(f + \rho + h) = \mathcal{L}(f + \rho) - \mathcal{L}(\rho) + \mathcal{L}(\rho + h)$ for any $f, \rho, h \in \mathcal{D}(\mathcal{M})$ such that f and h have disjoint supports,
- $\text{supp}(\mathcal{L}(f)) \subset \text{supp}(f)$ for all $f \in \mathcal{D}(\mathcal{M})$. Here $\text{supp}(\mathcal{L}(f))$ denotes the spacetime support of the local functional $\mathcal{L}(f)$ as per Definition 2.15,
- For any $\psi \in \text{Iso}(\mathcal{M})$, where $\text{Iso}(\mathcal{M})$ denotes the group of isometries of the spacetime $\mathcal{M}$, it holds that $\mathcal{L}(f)(\psi^*\phi) = \mathcal{L}(\psi_*f)(\phi)$, where ψ^* denotes the pullback of the isometry and $\psi_* = (\psi^{-1})^*$ is the push-forward.

Example 2.4. As an example of generalised Lagrangian, consider that associated to the free, conformally coupled scalar field that will be at the centre of our analysis. Let us consider a globally hyperbolic manifold $(\mathcal{M}, g)$. The generalised Lagrangian associated to a massless, conformally coupled scalar field is the map $\mathcal{L} : \mathcal{D}(\mathcal{M}) \rightarrow \mathcal{F}_{loc}(\mathcal{M})$ such that, for all $f \in \mathcal{D}(\mathcal{M})$ and for all $\phi \in \mathcal{E}(\mathcal{M})$ it holds that:

$$\mathcal{L}(f)(\phi) = -\frac{1}{2} \int_{\mathcal{M}} d\mu_x \left(g^{\mu\nu} \nabla_{\mu} \phi(x) \nabla_{\nu} \phi(x) + \frac{R}{6} \phi^2(x) \right) f(x). \quad (2.12)$$

Here ∇_{μ} denotes the component in some local chart of the Levi-Civita connection on $\mathcal{M}$, while R denotes the scalar curvature. Note that the second term within brackets in Equation (2.12) identifies a local functional as shown in Example 2.3. An analogous computation shows that the kinetic contribution is also local, proving that $\mathcal{L}(f) \in \mathcal{F}_{loc}(\mathcal{M})$.

We can furthermore identify equivalence classes of generalised Lagrangians in order to encode the property that the field dynamics is insensitive to the presence in the Lagrangian density of total divergences. These equivalence classes identify the *action* of our theory.

Definition 2.21. Let $\mathcal{L}_1, \mathcal{L}_2$ be two generalised Lagrangians as per Definition 2.20. We call **action** an equivalence class of Lagrangians, where the equivalence relation is

$$\mathcal{L}_1 \sim \mathcal{L}_2 \iff \text{supp}((\mathcal{L}_1 - \mathcal{L}_2)(f)) \subset \text{supp}(df), \quad f \in \mathcal{D}(\mathcal{M}).$$

Here df denotes the differential of the function f . In the following, we shall denote the action with S rather than $[\mathcal{L}]$ to make contact with standard notation used in the literature.

Once an action has been assigned, we can introduce the *Euler-Lagrange derivative* in order to obtain the equation of motion.

Definition 2.22. Let S be an action as per Definition 2.21 and let $\mathcal{L}$ denote a representative of the equivalence class S . The **Euler-Lagrange derivative** is a map $S' : \mathcal{E}(\mathcal{M}) \rightarrow \mathcal{D}'(\mathcal{M})$ such that

$$S'(\phi)(h) = \mathcal{L}(f)^{(1)}(\phi; h), \quad \phi \in \mathcal{E}(\mathcal{M}), f, h \in \mathcal{D}(\mathcal{M}), f|_{\text{supp}(h)} = 1.$$

Here $\mathcal{L}(f)^{(1)}$ denotes the Fréchet derivative of the functional $\mathcal{L}(f)$ as per Definition 2.14.

Remark 2.7. Note that the functional $\mathcal{L}(f)^{(1)}(\phi; \cdot)$ is a compactly supported distribution and therefore it could be smeared against all smooth functions on $\mathcal{M}$ rather than just the compactly supported ones. However, the restriction to compactly supported test functions in Definition 2.22 is made in order to make the Euler-Lagrange derivative independent of the test function f . This is necessary since f serves only as a cutoff but carries no physical meaning and therefore the dynamical structures of a field theory should be independent of it. Moreover, in order for Definition 2.22 to be well-posed, it must be independent of the choice of representative in the equivalence class. As a matter of fact, let $\mathcal{L}_1 \sim \mathcal{L}_2$ be any two representatives of an action S as per Definition 2.21. It holds that

$$\mathcal{L}_1(f)^{(1)}(\phi; h) = \mathcal{L}_2(f)^{(1)}(\phi; h) + ((\mathcal{L}_1 - \mathcal{L}_2)(f))^{(1)}(\phi; h), \quad \phi \in \mathcal{E}(\mathcal{M}).$$

Since they are in the same equivalence class, $\text{supp}(\mathcal{L}_1 - \mathcal{L}_2)(f) \subset \text{supp}(df)$. Since f is constant on $\text{supp}(h)$, we have $df|_{\text{supp}(h)} = 0$ and thus $\text{supp}(\mathcal{L}_1 - \mathcal{L}_2)(f) \cap \text{supp}(h) = \emptyset$. Therefore, by Definition 2.15, it holds that $(\mathcal{L}_1 - \mathcal{L}_2)(f)(\phi + sh) = (\mathcal{L}_1 - \mathcal{L}_2)(f)(\phi)$ for all $s \in \mathbb{R}$ and the Fréchet derivative vanishes, yielding

$$\mathcal{L}_1(f)^{(1)}(\phi; h) = \mathcal{L}_2(f)^{(1)}(\phi; h),$$

and that the Euler-Lagrange derivative is a property of the action rather than of the generalised Lagrangian.

From the definition of Euler-Lagrange derivative we can derive the equation of motion of our theory.

Definition 2.23. Let S be an action as per Definition 2.21 and let S' denote the Euler-Lagrange derivative of S as per Definition 2.22. The **equation of motion** corresponding to S is

$$S'(\phi)(h) = 0, \quad \forall h \in \mathcal{D}(\mathcal{M}), \quad (2.13)$$

understood as a condition on $\phi \in \mathcal{E}(\mathcal{M})$. We denote the subset of $\mathcal{E}(\mathcal{M})$ of smooth functions that satisfy Equation (2.13) by $\mathcal{E}_S(\mathcal{M})$ and we call it the **solution space** for the dynamics induced by S .

Example 2.5. As an example, let us take a look at the equation of motion linked to the Lagrangian in Example 2.4. Applying Definition 2.23 to

Equation (2.12) yields

$$\begin{aligned}
 \mathcal{L}(f)^{(1)}(\phi; h) &= \frac{d}{ds} \Big|_{s=0} \mathcal{L}(f)(\phi + sh) = \\
 &= -\frac{1}{2} \frac{d}{ds} \Big|_{s=0} \int_{\mathcal{M}} d\mu_x (g^{\mu\nu} \nabla_\mu (\phi + sh)(x) \nabla_\nu (\phi + sh)(x) + \\
 &\quad + \frac{R}{6} (\phi(x) + sh(x))^2) f(x) = \\
 &= -\frac{1}{2} \int_{\mathcal{M}} d\mu_x \left(2g^{\mu\nu} \nabla_\mu \phi(x) \nabla_\nu h(x) + \frac{R}{3} \phi(x) h(x) \right),
 \end{aligned}$$

where we used that $f = 1$ on the support of h and the symmetry of the metric tensor. By integrating the first term by parts we obtain

$$\mathcal{L}(f)^{(1)}(\phi; h) = \int_{\mathcal{M}} d\mu_x \left(\square_g \phi(x) - \frac{R}{6} \phi(x) \right) h(x), \quad \square_g = g^{\mu\nu} \nabla_\mu \nabla_\nu. \quad (2.14)$$

By requiring $S'(\phi) = 0$ for all $h \in \mathcal{D}(\mathcal{M})$, we obtain the **Klein-Gordon equation** for a massless, conformally coupled scalar field

$$\left(\square - \frac{R}{6} \right) \phi(x) = 0. \quad (2.15)$$

Remark 2.8. Let us consider a generalised Lagrangian $\mathcal{L}$ and a smooth, compactly-supported function $f \in \mathcal{D}(\mathcal{M})$. If we compute the second order Fréchet derivative of $\mathcal{L}(f)$ we obtain $\mathcal{L}(f)^{(2)}(\phi) \in \mathcal{E}'(\mathcal{M} \times \mathcal{M})$ for any $\phi \in \mathcal{E}(\mathcal{M})$. By means of the Schwartz kernel theorem A.1 we can identify a map $P_S(\phi) : \mathcal{E}(\mathcal{M}) \rightarrow \mathcal{D}'(\mathcal{M})$ such that

$$\langle P_S(\phi) \eta, h \rangle = \mathcal{L}(f)^{(2)}(\phi; \eta, h). \quad (2.16)$$

Thus, any generalised Lagrangian yields an operator from the configuration space to the space of distributions that generates the linearized equation of motion

$$P_S(\phi) \psi = 0, \quad \psi \in \mathcal{E}(\mathcal{M}).$$

Remark 2.9. If the action S is at most quadratic in ϕ , as it is for the scalar theory we shall consider, we obtain

$$P_S(\phi) \doteq P_0, \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \quad (2.17)$$

meaning that we get a single linear operator independent of the field configuration. In this scenario, the equation of motion reads $P_0 \phi = 0$. Since this is precisely the situation considered here for the generalised Lagrangian of a free, massless, conformally coupled scalar field, from now on we shall focus on this scenario.

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A crucial property of the operator P_0 in Equation (2.17) that we need to require in the context of perturbative algebraic quantum field theory is that it is normally hyperbolic, namely, for local coordinates $\{x^\mu\}_{\mu=0}^3$ we have

$$P_0 = -g^{\mu\nu} \partial_\mu \partial_\nu + A^\mu \partial_\mu + B,$$

where A^μ are the components of a smooth vector field on $\mathcal{M}$ and B is a smooth scalar function. For a detailed analysis of this class of operators we refer to [BGP08]. The reason for such a request lies in the existence, for this specific class of operators, of two distinct maps, namely, the *advanced* and *retarded* Green operators. They will play a pivotal rôle in the following, providing fundamental tools for the analysis of the solution space of the equation of motion.

Definition 2.24. *Let S be an action as per Definition 2.21 which is at most quadratic and let P_0 denote the normally hyperbolic operator associated to S as in Remark 2.8. We call **advanced (A) and retarded (R) Green operator** of P_0 the continuous maps*

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

such that

$$\begin{cases} P_0 \circ \Delta^{A/R} = \text{id}_{\mathcal{D}(\mathcal{M})} \\ \Delta^{A/R} \circ P_0|_{\mathcal{D}(\mathcal{M})} = \text{id}_{\mathcal{D}(\mathcal{M})} \\ \text{supp}(\Delta^{A/R}(f)) \subset J^{-/+}(\text{supp}(f)), \quad \forall f \in \mathcal{D}(\mathcal{M}) \end{cases},$$

where $J^{-/+}$ denotes the causal past and future of the support of f as per Definition 2.4 respectively.

The next proposition guarantees that on globally hyperbolic spacetimes such operators always exist.

Proposition 2.3. *Let $(\mathcal{M}, g)$ be a globally hyperbolic manifold as per Definition 2.6 and let S be an action as per Definition 2.21. Moreover, let P_0 be the normally hyperbolic operator induced by S as in Remark 2.8. Then there exist unique advanced and retarded Green operators as per Definition 2.24.*

For a proof we refer to [BGP08, Th. 3.3.1 and Cor. 3.4.3].

Remark 2.10. *It is possible to further expand the domain of definition of the retarded and advanced Green operators. As a matter of fact, let us consider a past-compactly supported function $f \in \mathcal{E}_{pc}(\mathcal{M})$, namely, a smooth function*

such that $\text{supp}(f) \cap J^-(p)$ is compact for every $p \in \mathcal{M}$. Then, we can define $\Delta^R(f)$ as the smooth, past-compact function such that $\Delta^R(f)(x) \doteq \Delta^R(\chi_x f)(x)$, where χ_x is a compactly supported smooth function such that $\chi_x(y) = 1$ for all $y \in J^+(\text{supp}(f)) \cap J^-(x)$.

We can analogously extend the action of Δ^A to the set of future-compact functions $\mathcal{E}_{fc}(\mathcal{M})$.

Remark 2.11. Let us consider the advanced and retarded Green operators $\Delta^{A/R}$ for the Klein-Gordon operator P_0 in (2.15). Let $\phi \in \mathcal{E}(\mathcal{M})$ be a smooth function and $f \in \mathcal{D}(\mathcal{M})$ a smooth, compactly supported one. Then, integrating by parts, it holds that

$$\langle P_0 \phi, f \rangle = \int_{\mathcal{M}} d\mu_x (P_0 \phi)(x) f(x) = \int_{\mathcal{M}} d\mu_x \phi(x) (P_0 f)(x) = \langle \phi, P_0 f \rangle. \quad (2.18)$$

Moreover, if $h \in \mathcal{D}(\mathcal{M})$ the following chain of equalities holds

$$\langle \Delta^R(f), h \rangle = \langle \Delta^R(f), P_0 \Delta^A(h) \rangle = \langle P_0 \Delta^R(f), \Delta^A(h) \rangle = \langle f, \Delta^A(h) \rangle.$$

Here we used that the operator P_0 is formally self-adjoint with respect to the standard pairing $\langle \cdot, \cdot \rangle : \mathcal{E}(\mathcal{M}) \times \mathcal{D}(\mathcal{M}) \rightarrow \mathbb{R}$. Therefore, we obtain that the formal adjoint of the retarded operator is the advanced operator and vice versa.

Remark 2.12. If we apply the Schwartz Kernel Theorem A.1 to the advanced and retarded propagators, we can identify two distinct bidistributions, which we shall denote by the same symbol, $\Delta^{A/R} \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$, called the **advanced and retarded fundamental solutions**. By means of Remark A.2, we denote the integral kernel by $\Delta^{A/R}(x, y)$. On account of the remark above, it holds that

$$\Delta^A(x, y) = \Delta^R(y, x).$$

The existence of an advanced and of a retarded Green operator allows us to define another object, namely the *causal propagator*, which is of fundamental importance for the solution theory of the equation of motion.

Definition 2.25. Let $\Delta^{A/R}$ denote the advanced and retarded Green operators as per Definition 2.24 for a normally hyperbolic operator P_0 induced by an action S , as per Definition 2.21, via the second Euler-Lagrange derivative as per Definition 2.22. We call **causal propagator** the map

$$\Delta_S \doteq \Delta^R - \Delta^A : \mathcal{D}(\mathcal{M}) \rightarrow \mathcal{E}(\mathcal{M}). \quad (2.19)$$

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Remark 2.13. On account of Remark 2.11, if we compute the formal adjoint of Δ_S with respect to the pairing $\langle \cdot, \cdot \rangle : \mathcal{E}(\mathcal{M}) \times \mathcal{D}(\mathcal{M}) \rightarrow \mathbb{R}$, we obtain, given two compactly supported smooth functions $f, h \in \mathcal{D}(\mathcal{M})$,

$$\langle \Delta_S(f), h \rangle = \langle (\Delta^R - \Delta^A)(f), h \rangle = \langle f, (\Delta^A - \Delta^R)(h) \rangle = -\langle f, \Delta_S h \rangle,$$

which shows that the causal propagator is formally skew-adjoint. At the level of integral kernels, this yields

$$\Delta_S(x, y) = -\Delta_S(y, x).$$

Remark 2.14. Let us take a compactly supported smooth function $f \in \mathcal{D}(\mathcal{M})$ and apply the causal propagator associated to a normally hyperbolic operator P_0 . It holds that

$$P_0 \Delta_S(f) = P_0 \Delta^R(f) - P_0 \Delta^A(f) = f - f = 0. \quad (2.20)$$

Thus, any smooth, real-valued function of the form $\Delta_S(f)$, $f \in \mathcal{D}(\mathcal{M})$ is a solution to the equation $P_0 \phi = 0$.

The definition of the causal propagator allows one to give an explicit characterisation of the solution space for Klein-Gordon equation (2.15). To this end, we first need an ancillary definition

Definition 2.26. Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\phi \in \mathcal{E}(\mathcal{M})$ be a smooth function thereon. We say that ϕ is **spacelike compact** if, for any spacelike Cauchy surface $\Sigma \subset \mathcal{M}$, it holds that $\text{supp}(\phi) \cap \Sigma$ is compact. We denote the space of smooth, spacelike compact functions by $\mathcal{E}_{sc}(\mathcal{M})$.

Proposition 2.4. Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let us consider the conformally coupled Klein-Gordon equation

$$\begin{cases} (\square_g - \frac{R}{6}) \phi = 0 \\ \phi|_{\Sigma} = \phi_0, \quad n^\mu \partial_\mu \phi = \phi_1 \end{cases}.$$

Here $\square_g = g^{\mu\nu} \nabla_\mu \nabla_\nu$ is the d'Alembert operator, $\Sigma \subset \mathcal{M}$ is a spacelike Cauchy hypersurface on which smooth, compactly supported initial data $\phi_0, \phi_1 \in \mathcal{D}(\Sigma)$ are assigned. Moreover, n^μ is the outward-pointing, unit normal vector to Σ . Let Δ_S be the causal propagator associated to the Klein-Gordon operator $P_0 \doteq \square_g - \frac{R}{6}$ as per Definition 2.25. Then, there exists a vector space isomorphism between $\mathcal{E}_{S,sc}(\mathcal{M})$ and the quotient

$$\frac{\mathcal{D}(\mathcal{M})}{P_0(\mathcal{D}(\mathcal{M}))},$$

via the map $\frac{\mathcal{D}(\mathcal{M})}{P_0(\mathcal{D}(\mathcal{M}))} \ni [f] \rightarrow \Delta_S(f) \in \mathcal{E}_{S,sc}(\mathcal{M})$. Here $\mathcal{E}_{sc}(\mathcal{M})$ denotes the space of spacelike compact smooth function as per Definition 2.26.

For a proof, we refer to [DMP17, Proposition 3.1.2].

The reason for the choice of the coupling with the scalar curvature in Equation (2.15) lies in the fact that the associated equation of motion turn out to be conformally invariant. Thus, both the operator P_0 , its Green operators and solutions transform in a distinguished way under the conformal mapping of the spacetime, as highlighted in the following proposition.

Proposition 2.5. *Let $(\mathcal{M}, g)$ be a 4-dimensional globally hyperbolic spacetime as per Definition 2.6 and let $P_0 = \square_g - \frac{R}{6}$ be the Klein-Gordon operator. Moreover, let $\Delta^{A/R}$ denote the advanced and retarded Green operators as per Definition 2.24 and let Δ_S denote the causal Green operator as per Definition 2.25 associated to P_0 . Moreover, let $\Omega \in C^\infty(\mathcal{M}; (0, \infty))$. Then, if we denote by $\widetilde{P}_0$ the Klein-Gordon operator associated to $\tilde{g} = \Omega^2 g$, by $\widetilde{\Delta}^{A/R}$ the advanced and retarded Green operators and by $\widetilde{\Delta}_S$ the causal propagator associated to $\widetilde{P}_0$, it holds that*

$$\begin{cases} \widetilde{P}_0 = \Omega^{-3} P_0 \Omega \\ \widetilde{\Delta}^{A/R} = \Omega^{-1} \Delta^{A/R} \Omega^3, \quad \widetilde{\Delta}_S = \Omega^{-1} \Delta_S \Omega^3 \end{cases} \quad (2.21)$$

Proof. The first equality in Equation (2.21) is a by-product of the definition of the Levi-Civita connection and of the scalar curvature for the metrics g and $\tilde{g}$. Thus the result can be recovered by a direct computation, see [Wal84, Appendix D]. Since $(\mathcal{M}, \tilde{g})$ is still a globally hyperbolic spacetime, Proposition 2.3 entails that the Klein-Gordon operator $\widetilde{P}_0$ admits unique advanced and retarded Green operators as per Definition 2.24. Therefore it suffices to verify that the remaining expressions in Equation (2.21) satisfy the defining properties of Definition 2.24. A direct computation yields

$$\widetilde{P}_0(\Omega^{-1} \Delta^{A/R}(\Omega^3 f)) = \Omega^{-3} P_0 \Omega \Omega^{-1} \Delta^{A/R} \Omega^3 f = f, \quad \forall f \in \mathcal{D}(\mathcal{M}),$$

where we used that $P_0 \Delta^{A/R} = \text{id}_{\mathcal{D}(\mathcal{M})}$. Analogously it can be shown that $(\Omega^{-1} \Delta^{A/R} \Omega^3) \widetilde{P}_0|_{\mathcal{D}(\mathcal{M})} = \text{id}_{\mathcal{D}(\mathcal{M})}$. Lastly, since Ω is nowhere vanishing, it holds that $\text{supp}(\Omega^3 f) = \text{supp}(f)$ for all $f \in \mathcal{D}(\mathcal{M})$. Therefore, $\text{supp}(\Delta^R(\Omega^3 f)) \subset J_g^+(\text{supp}(f))$, where J_g^+ denotes the causal future as per Definition 2.4 with respect to the causal structure induced by g , while $\text{supp}(\Omega^{-1} \Delta^R(\Omega^3 f)) = \text{supp}(\Delta^R(\Omega^3 f))$. Since the causal structure is left unchanged by conformal transformations, even the last of the defining properties in Definition 2.24 is met. Thus, we have shown that $\Omega^{-1} \Delta^R \Omega^3$ is the retarded Green operator of $\widetilde{P}_0$, and an analogous result holds for the advanced one. The transformation of the causal propagator is a direct consequence of its definition. $\square$

Remark 2.15. *Proposition 2.5 entails that any solution ϕ to the conformally coupled Klein-Gordon equation (2.15) transforms under conformal mappings of the metric in a distinguished way. As a matter of fact, let us consider the conformal transformation $g \mapsto \tilde{g} = \Omega^2 g$ with $\Omega \in C^\infty(\mathcal{M})$ a nowhere vanishing smooth function and let $\Phi \doteq \Omega^{-1}\phi$. On account of Proposition 2.5, it holds*

$$\widetilde{P_0}\Phi = \Omega^{-3}P_0\Omega\Phi = \Omega^{-3}P_0\phi = 0.$$

Since the function Ω^{-3} is nowhere vanishing, it holds that ϕ is a solution of $P_0\phi = 0$ if and only if $\Phi = \Omega^{-1}\phi$ is a solution of $\widetilde{P_0}\Phi = 0$.

We can now show how information on the dynamics can be encoded in the algebra of observables.

Definition 2.27. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\mathcal{A}_{cl}(\mathcal{M})$ be the classical microcausal algebra as per Definition 2.19. Let S be an action as per Definition 2.21. Then, we call **ideal of the equation of motion** the ideal, as per Definition B.3,*

$$\mathcal{I}_S(\mathcal{M}) = \{F \in \mathcal{F}_{\mu c, pol}(\mathcal{M}) \mid F(\phi) = 0, \forall \phi \in \mathcal{E}_S(\mathcal{M})\}.$$

*Here $\mathcal{E}_S(\mathcal{M})$ denotes the space of solutions of the equation of motion of S as per Definition 2.23. Moreover, we call the **classical on-shell microcausal algebra** the quotient*

$$\mathcal{A}_{cl}^{on}(\mathcal{M}) \doteq \frac{\mathcal{A}_{cl}(\mathcal{M})}{\mathcal{I}_S}.$$

The causal propagator associated to the equation of motion allows also to endow the classical microcausal algebra with a Poisson structure by means of the *Peierls brackets*. We shall start by giving the definition and we will then show that, for microcausal functionals of polynomial type, they indeed induce a well-defined closed Poisson structure.

Definition 2.28. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\mathcal{A}_{cl}(\mathcal{M})$ be the classical polynomial microcausal algebra for a scalar theory as per Definition 2.19. Moreover, let S be an action as per Definition 2.21 which is at most quadratic and let P_0 be the normally hyperbolic operator associated to S as in Remark 2.8. If Δ_S denotes the causal propagator associated to P_0 , we define the **Peierls brackets** as*

$$\{\cdot, \cdot\}_S : \mathcal{F}_{\mu c, pol}(\mathcal{M}) \times \mathcal{F}_{\mu c, pol}(\mathcal{M}) \rightarrow \mathcal{F}_{\mu c, pol}(\mathcal{M}),$$

such that, for all $\phi \in \mathcal{E}(\mathcal{M})$,

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

Here $F^{(1)}$ denotes the first order Fréchet derivative as per Definition 2.14 and the pairing $\langle \cdot, \cdot \rangle$ is obtained as the smearing of the bidistribution $\Delta_S \cdot (F^{(1)}(\phi) \otimes G^{(1)}(\phi))$ against two compactly supported smooth functions $f, h \in \mathcal{D}(\mathcal{M})$ such that $f|_{\text{supp}(F^{(1)}(\phi))} = 1$ and $h|_{\text{supp}(G^{(1)}(\phi))} = 1$. At the level of integral kernel this reads

$$\int_{\mathcal{M}^2} d\mu_x d\mu_y F^{(1)}(\phi)(x) \Delta_S(x, y) G^{(1)}(\phi)(y).$$

Note that the product $\Delta_S \cdot (F^{(1)}(\phi) \otimes G^{(1)}(\phi))$ in Definition 2.28 is in general ill-defined for a generic functional, as Hörmander's criterion must be checked. The next proposition shows both that the Peierls brackets are well-defined on the whole algebra of microcausal functionals and that they indeed endow the algebra of observables with a Poisson structure.

Proposition 2.6. *Let $\mathcal{A}_{cl}(\mathcal{M})$ be the classical polynomial microcausal algebra of observables for a scalar theory as per Definition 2.19. Let S be an action as per Definition 2.21 while $\{\cdot, \cdot\}_S$ denotes the Peierls brackets as per Definition 2.28. Then, $(\mathcal{A}_{cl}(\mathcal{M}), \{\cdot, \cdot\}_S)$ is a closed Poisson $*$ -algebra.*

For a proof we refer to [BFR19, Th. 4.1.4].

2.2.4 Deformation quantization

We are now ready to introduce the quantization of the classical microcausal algebra for a scalar field theory in Definition 2.19. To this end, we shall apply a procedure known in the literature as *deformation quantization*, which consists in the deformation of the pointwise product of the classical algebra in order to implement the canonical commutation relations (CCR) while leaving the elements of the algebra unchanged. We first introduce the deformed product in a general setting and we shall then discuss which choices of possible deformations produce a physically meaningful quantization.

A key ingredient in the construction of the deformed product is the choice of a distinguished bidistribution $K \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ and a formal deformation parameter $\hbar$. The deformation is achieved by means of the formal product $\star_{\hbar K}$, defined on $F, G \in \mathcal{F}_{\mu c, pol}(\mathcal{M})$ by

$$F \star_{\hbar K} G = \iota^* \circ e^{D_{\hbar K}} [F \otimes G], \quad (2.22)$$

$$D_{\hbar K} = \hbar \langle K, \frac{\delta}{\delta \phi} \otimes \frac{\delta}{\delta \phi'} \rangle. \quad (2.23)$$

Here the exponential in Equation (2.22) is understood as a formal power series in $\hbar$, while ι^* denotes the pullback with respect to the diagonal map

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$\iota : \mathcal{E}(\mathcal{M}) \rightarrow \mathcal{E}(\mathcal{M}) \times \mathcal{E}(\mathcal{M})$ such that $\iota(\phi) = (\phi, \phi)$ for all $\phi \in \mathcal{E}(\mathcal{M})$. Moreover, $\frac{\delta}{\delta\phi}$ denotes the map that associates to any functional its Fréchet derivative at $\phi \in \mathcal{E}(\mathcal{M})$.

Suppose now that $F, G \in \mathcal{F}_{\text{reg}}(\mathcal{M})$ are regular functionals. Then, the product in Equation (2.22) can be expressed as

$$(F \star_{\hbar K} G)(\phi) = \sum_{k=0}^{\infty} \frac{\hbar^k}{k!} \langle F^{(k)}(\phi), K^{\otimes k} G^{(k)}(\phi) \rangle. \quad (2.24)$$

Notice that Equation (2.24) involves products of functional derivatives with the integral kernels $K^{\otimes k}$. On account of Hörmander's criterion such operations are not always well-defined when working with microcausal functionals. In order for Equation (2.22) to be meaningful also in this case, we need to select a distinguished bidistribution K .

Definition 2.29. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $K \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be a bidistribution on $\mathcal{M}$ as per Definition A.1. We say that K satisfies the **microlocal spectrum condition** if*

$$\text{WF}(K) = \{(x, \xi_x; y, -\xi_y) \in \mathring{T}^*(\mathcal{M} \times \mathcal{M}) \mid (x, \xi_x) \sim (y, \xi_y), \xi_x \triangleright 0\}.$$

Here $\text{WF}(K)$ denotes the wavefront set of K as per Definition A.4 while $\mathring{T}^*(\mathcal{M} \times \mathcal{M}) \doteq T^*(\mathcal{M} \times \mathcal{M}) \setminus \{0\}$ denotes the punctured cotangent space. Furthermore, $(x, \xi_x) \sim (y, \xi_y)$ if there exists a null geodesic γ connecting x to y such that ξ_x is tangent to γ at x and future directed while ξ_y is the parallel transport of ξ_x along γ .

The microlocal spectrum condition identifies a distinguished class of bidistributions that generate a well-defined product. The remainder of this section is devoted to identifying a family of bidistributions in order to encode in our theory the canonical commutation relations and the properties of covariance and locality expected from a quantum field theory. From now on, we shall refer to the case of a scalar field theory whose dynamics is generated by an action which is at most quadratic and that yields the equation of motion in terms of a normally hyperbolic operator P_0 .

A natural first candidate for the deforming bidistribution in Equation (2.24) is $\frac{i}{2}\Delta_S$, where Δ_S denotes the causal propagator for a scalar field. This choice automatically encodes in the algebraic structure information about the dynamics of the underlying theory. Additionally, it translates the idea that in order to quantize a theory one should replace the classical bracket, namely, the Peierls bracket, with $-\frac{i}{\hbar}$ times the commutator of the observables. As

a matter of fact, a direct computation shows that, for $F, G \in \mathcal{F}_{\text{reg}}(\mathcal{M})$ and $\phi \in \mathcal{E}(\mathcal{M})$,

$$\left(F \star_{\hbar \frac{i}{2} \Delta_S} G - G \star_{\hbar \frac{i}{2} \Delta_S} F \right) (\phi) = i\hbar \langle F^{(1)}(\phi), \Delta_S G^{(1)}(\phi) \rangle + \mathcal{O}(\hbar^2).$$

Note that the coefficient of $i\hbar$ in the left-hand side is precisely the Peierls bracket as per Definition 2.28. Thus the star product provides a deformation quantization of the classical Poisson algebra. However, for observables with non-vanishing second-order Fréchet derivative, Hörmander's criterion for the product of distributions might fail and thus the product cannot, in general, be extended to the whole $\mathcal{F}_{\mu c, \text{pol}}(\mathcal{M})$. The problem lies in the form of the wavefront set of the causal propagator Δ_S which, as shown in [DH72] and [RV96], is of the form

$$\text{WF}(\Delta_S) = \{(x, \xi_x; y, -\xi_y) \in T^*(\mathcal{M} \times \mathcal{M}) \mid (x, \xi_x) \sim (y, \xi_y)\}. \quad (2.25)$$

Here $(x, \xi_x) \sim (y, \xi_y)$ if there exists a null geodesic γ connecting x and y such that ξ_x is tangent to γ at x while ξ_y is the parallel transport of ξ_x along γ . Therefore, it does not satisfy the microlocal spectrum condition.

To circumvent this problem, we start by observing that only the anti-symmetric part of the distribution contributes to the commutator. We can thus choose a bidistribution $\Delta_+ \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ that satisfies the microlocal spectrum condition as per Definition 2.29 and whose antisymmetric part coincides with $\frac{i}{2}\Delta_S$.

Definition 2.30. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let S be an action, at most quadratic, as per Definition 2.21 which induces a dynamics by means of a normally hyperbolic operator P_0 . Moreover, let $\Delta_S \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be the integral kernel of the causal propagator as per Definition 2.25 and let Δ_+ be a bidistribution such that*

- Δ_+ satisfies the microlocal spectrum condition as per Definition 2.29,
- The antisymmetric part of Δ_+ coincides with $\frac{i}{2}\Delta_S$.

We define the **quantum microcausal algebra** as the unital $*$ -algebra, as per Definition B.2,

$$\mathcal{A}_{\Delta_+}(\mathcal{M}) = (\mathcal{F}_{\mu c, \text{pol}}(\mathcal{M}), \star_{\hbar \Delta_+}, *).$$

Here $\mathcal{F}_{\mu c, \text{pol}}(\mathcal{M})$ is the space of microcausal functionals as per Definition 2.16 of polynomial type, $\star_{\hbar \Delta_+}$ is the deformed product as per Equation (2.22) and $*$ is the involution defined via $F^*(\phi) = \overline{F(\phi)}$ for all $\phi \in \mathcal{E}(\mathcal{M})$ and for all $F \in \mathcal{F}_{\mu c, \text{pol}}(\mathcal{M})$. Furthermore $\bar{\cdot}$ denotes the complex conjugate in $\mathbb{C}$.

Remark 2.16. *Let us show that this choice for the deformed product naturally encodes the classical commutation relations for the field observables. Let us consider two linear smeared fields $\Phi_f, \Phi_{f'} \in \mathcal{A}_{\Delta_+}(\mathcal{M})$, where $f, f' \in \mathcal{D}(\mathcal{M})$ are compactly supported smooth functions. Computing the commutator yields*

$$\begin{aligned} [\Phi_f, \Phi_{f'}](\phi) &= \Phi_f \star_{\hbar\Delta_+} \Phi_{f'}(\phi) - \Phi_{f'} \star_{\hbar\Delta_+} \Phi_f(\phi) = \\ &= i\hbar \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) f'(y) \Delta_S(x, y), \quad \forall \phi \in \mathcal{E}(\mathcal{M}) \end{aligned}$$

where $\Delta_S(x, y)$ denotes the integral kernel of the causal propagator.

Example 2.6. *Let us compute the product for the squared fields $\Phi_f^2, \Phi_{f'}^2 \in \mathcal{A}_{\Delta_+}(\mathcal{M})$ as in Example 2.3, with $f, f' \in \mathcal{D}(\mathcal{M})$.*

$$\begin{aligned} (\Phi_f^2 \star_{\hbar\Delta_+} \Phi_{f'}^2)(\phi) &= \Phi_f^2(\phi) \Phi_{f'}^2(\phi) + \hbar \langle (\Phi_f^2)^{(1)}(\phi), \Delta_+(\Phi_{f'}^2)^{(1)}(\phi) \rangle \\ &\quad + \frac{\hbar^2}{2} \langle (\Phi_f^2)^{(2)}(\phi), \Delta_+^{\otimes 2}(\Phi_{f'}^2)^{(2)}(\phi) \rangle. \end{aligned}$$

In terms of integral kernel this expression reads

$$\begin{aligned} (\Phi_f^2 \star_{\hbar\Delta_+} \Phi_{f'}^2)(\phi) &= \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) \phi^2(x) f'(y) \phi^2(y) \\ &\quad + 4\hbar \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) \phi(x) \Delta_+(x, y) f'(y) \phi(y) \quad (2.26) \\ &\quad + 2\hbar^2 \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) \Delta_+^2(x, y) f'(y). \end{aligned}$$

Notice that the term Δ_+^2 is a well-defined distribution on account of Definition 2.29 and Theorem A.4.

Note that in Definition 2.30 the antisymmetric part of the bidistribution is fixed, while its symmetric part remains arbitrary, provided that the bidistribution satisfies the microlocal spectrum condition. Consequently, there exist infinitely many possible choices for Δ_+ that define a deformed product and consequently a quantum algebra.

To remove this ambiguity, one singles out a distinguished class of bidistributions, known as *Hadamard parametrices*. Their singular behaviour is completely determined by the local geometry and the dynamics. This naturally encodes the locality and covariance properties we expect in a quantum field theory on curved backgrounds.

Definition 2.31. *Let $(\mathcal{M}, g)$ be a 4-dimensional globally hyperbolic spacetime as per Definition 2.6. We say that a bidistribution $H \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ is a*

Hadamard parametrix if, for any $x \in \mathcal{M}$ and for all geodesically convex neighborhood $\mathcal{O} \subset \mathcal{M}$ of x , there exist $U, V, W \in \mathcal{E}(\mathcal{O} \times \mathcal{O})$ and a collection $\{V_n\}_{n \in \mathbb{N}} \subset \mathcal{E}(\mathcal{O} \times \mathcal{O})$, such that, denoting by $H(x, y)$ the integral kernel of H , it holds, for all $y \in \mathcal{O}$,

$$H(x, y) = \lim_{\varepsilon \rightarrow 0} \left(\frac{U(x, y)}{4\pi^2 \sigma_\varepsilon(x, y)} + V(x, y) \ln \frac{\sigma_\varepsilon(x, y)}{\lambda^2} \right) + W(x, y), \quad (2.27)$$

$$V(x, y) = \sum_{n=0}^{\infty} \sigma^n(x, y) V_n(x, y). \quad (2.28)$$

Here the limit is taken in the topology of $\mathcal{D}'(\mathcal{O} \times \mathcal{O})$, $\lambda > 0$ is a real constant and the functions U, V are uniquely defined by the geometry of the spacetime and the dynamics. Moreover, $\sigma_\varepsilon(x, y) = \sigma(x, y) + 2i\varepsilon(T(x) - T(y)) + \varepsilon^2$, where $\sigma(x, y)$ is the halved squared geodesic distance and $T : \mathcal{O} \rightarrow \mathbb{R}$ is a local time function increasing towards the future.

Remark 2.17. Note that any Hadamard distribution as per Definition 2.31 satisfies the microlocal spectrum condition as per Definition 2.29. This is a consequence of Radzikowski's theorem, see [Rad96, Th. 5.1]. This result also guarantees that the antisymmetric part of H coincides with $\frac{i}{2}\Delta_S$. Therefore, H satisfies the conditions in Definition 2.30 and thus generates a well-defined deformed product for the algebra of observables.

Remark 2.18. The functions $U(x, y)$ and $V_n(x, y)$ in Definition 2.31 are obtained by imposing that the bidistribution H is such that $P_0^{(x)}H$ and $P_0^{(y)}H$ are smooth functions, where P_0 is the normally hyperbolic operator derived from the action and the subscripts (x) and (y) denote the variable with respect to which the derivatives are taken.

This requirement reduces to a set of recursive transport equations that U and V_n must satisfy. It is furthermore necessary to assign, in order to solve the transport equations, initial conditions for U and V_n . For the function U , we impose that, in the coinciding point limit, it must hold that

$$[U] \doteq \lim_{y \rightarrow x} U(x, y) = 1.$$

This condition is imposed in order to make sure that the short-distance behaviour of our theory mimics that of Minkowski spacetime, where it holds that $U(x, y) = 1$ for all $x, y \in \mathbb{M}^4$. For any term V_n , we can recursively recover initial conditions for the coinciding point limit in terms of the initial

data of U and $V_0, \dots, V_{n-1}$. The transport equations for these functions read

$$\begin{cases} 2(\nabla^\mu \sigma) \nabla_\mu U + (\square_g^{(x)} \sigma - 4)U = 0 \\ P_0^{(x)} U + 2(\nabla^\mu \sigma) \nabla_\mu V_0 + (\square_g^{(x)} \sigma - 2)V_0 = 0 \\ P_0^{(x)} V_n + 2(n+1)(\nabla^\mu \sigma) \nabla_\mu V_{n+1} + (n+1)(\square_g^{(x)} \sigma + 2n)V_{n+1} = 0 \quad \forall n \geq 0 \\ [U] = 1, \quad [V_0] = -\frac{1}{2}[P_0^{(x)} U], \quad [V_{n+1}] = -\frac{1}{2(n+1)(n+2)}[P_0^{(x)} V_n] \quad \forall n \geq 0 \end{cases} \quad (2.29)$$

And the same holds by replacing x by y .

Note that we did not state any hypothesis regarding the convergence of the series in Equation (2.28). As a matter of fact, if $\{V_n\}_{n \in \mathbb{N}}$ are the solutions to Equation (2.29), the convergence of the series is in general not guaranteed and it has to be interpreted as an asymptotic expansion. We now state a Theorem regarding sufficient conditions for the convergence to hold, referring to [Fri75, Th. 4.3.1 and Lemma 4.3.2] for the proof.

Theorem 2.2. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let P_0 be a normally hyperbolic operator. Moreover, let $\{V_n\}_{n \in \mathbb{N}}$ be the solutions to Equation (2.29). Then:*

1. *If every coefficient of the differential operator P_0 is analytic, then, $\forall x \in \mathcal{M}$ there exists an open geodesically convex neighborhood $\mathcal{O} \subset \mathcal{M}$ where $V \doteq \sum_{n=0}^{\infty} V_n \sigma^n$ is an analytic function,*
2. *If $\rho : \mathbb{R} \rightarrow [0, 1]$ is a compactly supported smooth function such that $\rho(s) = 1$ for all $s \in [-\frac{1}{2}, \frac{1}{2}]$ and $\rho(s) = 0$ for all $s \in \mathbb{R}, |s| \geq 1$, then, for all $x \in \mathcal{M}$, there exists an open geodesically convex neighborhood $\mathcal{O} \subset \mathcal{M}$ and a sequence $\{k_n\}_{n \in \mathbb{N}}$ of positive and strictly increasing real numbers reaching infinity as $n \rightarrow \infty$ such that the series*

$$\sum_{n=0}^{\infty} V_n(x, y) \sigma^n(x, y) \rho(k_n \sigma(x, y)),$$

converges uniformly, together with its derivatives, to a smooth function V in $\mathcal{O} \times \mathcal{O}$.

Having introduced the Hadamard parametrix, we can now define the *locally covariant* algebra of observables, which will be the final form of the algebra of the theory.

Definition 2.32. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $H \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be a Hadamard parametrix as per*

Definition 2.31. We call **locally covariant algebra of microcausal, polynomial functionals** the unital $*$ -algebra, as per Definition B.2 $\mathcal{A}_{loc}(\mathcal{M}) = (\overline{\mathcal{F}_{loc,pol}(\mathcal{M})}, \star_{\hbar H}, *)$, where $\overline{\mathcal{F}_{loc,pol}(\mathcal{M})}$ is the algebraic closure, with respect to the algebra product, of the subalgebra $\mathcal{F}_{loc,pol}(\mathcal{M}) \subset \mathcal{F}_{\mu c,pol}(\mathcal{M})$ of local functionals of polynomial type. Moreover, $*$ is the involution defined analogously to Definition 2.19 and $\star_{\hbar H}$ is the product defined in Equation (2.24).

Remark 2.19. Note that the deformed product in Definition 2.32 is not uniquely defined. As a matter of fact, in the definition of a Hadamard parametrix, we have the freedom of choosing the smooth remainder W in Equation (2.27). Therefore, two different Hadamard parametrices H_1 and H_2 yield different algebras $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$. However, these algebras are $*$ -isomorphic via the map

$$\begin{aligned} \alpha_{H_2-H_1} : \mathcal{A}_{loc}^{(1)}(\mathcal{M}) &\rightarrow \mathcal{A}_{loc}^{(2)}(\mathcal{M}), \\ F &\mapsto \alpha_{H_2-H_1} F = e^{\frac{1}{2}\langle \hbar(H_2-H_1), \frac{\delta^2}{\delta\phi^2} \rangle} F. \end{aligned} \quad (2.30)$$

Here the exponential has to be interpreted as a formal power series in $\hbar$, while $\frac{\delta^2}{\delta\phi^2}$ denotes the map that associates F to its second-order Fréchet derivative at ϕ .

Remark 2.20. The elements of the locally covariant algebra in Definition 2.32 can be understood as Wick polynomials. To give a representation in terms of the usual normal-ordered way, let us consider a bidistribution H of Hadamard form as per Definition 2.31 and let us denote its singular part by H_{0+} . For any element $F \in \mathcal{A}_{loc}(\mathcal{M})$ we first introduce the abstract Wick ordering:

$$: F :_{H_{0+}} \doteq \alpha_{-H_{0+}}(F). \quad (2.31)$$

Here $\alpha_{-H_{0+}}$ is defined analogously to Equation (2.30). Then, we introduce the **operator ordering map**

$$\alpha_H : \mathcal{A}_{loc}(\mathcal{M}) \rightarrow \mathcal{A}_H(\mathcal{M}),$$

which is a $*$ -isomorphism between the locally covariant algebra of microcausal functionals and the quantum microcausal algebra with product deformed by means of H .

Then, α_H gives a concrete representation of the abstract Wick-ordered polynomial $: F :$. As an example, if we consider the squared field functional $\Phi_f^2 \in \mathcal{A}_{loc}(\mathcal{M})$ and its abstract normal-ordered version $: \Phi_f^2 :$, the application of the operator ordering map yields

$$\alpha_H(: \Phi_f^2 :)(\phi) = \alpha_{H-H_{0+}}(\Phi_f^2)(\phi) = \Phi_f^2(\phi) + \hbar \int_{\mathcal{M}} d\mu_x W(x, x) f(x) \quad \phi \in \mathcal{E}(\mathcal{M}). \quad (2.32)$$

Here $W \doteq H - H_{0+}$ is the smooth part of the Hadamard parametrix. By evaluating this functional against the configuration $\phi = 0$ we obtain the usual expression for the expectation value of Wick ordered squared scalar field. Additionally, referencing Example 2.6, we can interpret the result as the implementation of Wick's theorem for the product of Wick-ordered squared fields. To make contact with the standard representation regarding the contraction of fields, we implement the following notation

$$\Phi_f^2(\phi) \star_{hH} \Phi_{f'}^2(\phi) = \Phi_f^2(\phi) \Phi_{f'}^2(\phi) + 4\hbar \overbrace{\Phi_f^2(\phi) \Phi_{f'}^2(\phi)} + 2\hbar^2 \overbrace{\Phi_f(\phi) \Phi_f(\phi) \Phi_{f'}(\phi) \Phi_{f'}(\phi)}, \quad (2.33)$$

where each contraction is achieved by means of the Hadamard bidistribution H .

2.2.5 Algebraic states

While in the previous sections we constructed the algebra of observables of the theory, in order to recover observable quantities, such as expectation values of field observables, it is necessary to define a notion of physical state. Within the algebraic approach, this is represented as a linear functional on the algebra of observables satisfying suitable properties.

Definition 2.33. Let $(\mathcal{A}, \cdot, *)$ be a unital $*$ -algebra as per Definition B.2. An **algebraic state** ω on $\mathcal{A}$ is a map

$$\omega : \mathcal{A} \rightarrow \mathbb{C},$$

such that:

1. ω is $\mathbb{C}$ -linear,
2. ω is normalised, i.e., if $\mathbf{1} \in \mathcal{A}$ denotes the unit of the algebra, then

$$\omega(\mathbf{1}) = 1,$$

3. ω is positive, namely, for all $a \in \mathcal{A}$,

$$\omega(a^* \cdot a) \geq 0.$$

Here $*$ denotes the involution while $\cdot$ is the product of the algebra.

Unlike the standard formulation of quantum field theories, the algebraic approach does not start by defining a Hilbert-space representation. Instead, we first construct the algebra of observables and define the notion of physical

state only at a later stage. This viewpoint is especially advantageous on generic curved spacetimes, where, in general, no distinguished vacuum state analogous to the Poincaré-invariant one on Minkowski spacetime can be defined. However, once an algebraic state has been selected, we can recover a Hilbert-space representation through the *Gelfand–Naimark–Segal* construction.

Theorem 2.3. *Let $\mathcal{A}$ be a unital $*$ -algebra as per Definition B.2 and let ω be an algebraic state as per Definition 2.33. Then there exists a dense subset of a complex Hilbert space $\mathcal{D}_\omega \subset \mathcal{H}_\omega$, a $*$ -representation of $\mathcal{A}$ as per Definition B.5,*

$$\pi_\omega : \mathcal{A} \rightarrow \mathcal{L}(\mathcal{D}_\omega),$$

and a unit vector $\Omega_\omega \in \mathcal{D}_\omega$ such that

$$\omega(a) = (\Omega_\omega, \pi_\omega(a)\Omega_\omega), \quad \forall a \in \mathcal{A},$$

and

$$\mathcal{D}_\omega = \{\pi_\omega(a)\Omega_\omega, a \in \mathcal{A}\}.$$

Moreover, the GNS triple $(\mathcal{D}_\omega, \pi_\omega, \Omega_\omega)$ is uniquely defined up to unitary equivalences.

For a proof we refer to [BFR19, Th. 1].

Remark 2.21. *By means of algebraic states we can endow the abstract algebra of observables with a probabilistic interpretation. Indeed, given an observable $a \in \mathcal{A}$, we interpret $\omega(a)$ as its expectation value in the state ω . In particular, since observables enjoy the property $a^* = a$, then the compatibility of the involution with the GNS representation implies that $\omega(a)$ is real, as expected for a measurable physical quantity.*

2.2.6 Interacting classical field theory

In the previous, we have introduced the algebraic structures needed for the description of a free quantum field theory in the AQFT framework. Goal of the present section is to encode into the algebraic framework also interactions, which are fundamental for the description of any physical model. In general, interacting models, such as the $\lambda\phi^4$ model for scalar fields, yield non-homogeneous equations of motion. Finding explicit solutions to these equations of motion is often not possible. For this reason, the perturbative approach proves to be particularly useful as it allows to construct solutions as formal power series in a parameter which plays the rôle of the coupling

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constant of the theory. In the following, we shall mainly follow [Rej16], introducing first the *Møller map* for a classical theory and then, in the next section, its quantum counterpart, the *Bogoliubov map*. These maps are the fundamental tools that allow us to express interacting observables as formal power series of their free counterparts.

For any interacting field theory, the starting point is the specification of an action, as per Definition 2.21, which is split into a free part and an interacting potential. We shall adopt the following notation

$$S_{\lambda V}(\phi) = S_0(\phi) + \lambda V(\phi), \quad V \in \mathcal{F}_{\text{loc}}(\mathcal{M}), \quad (2.34)$$

where $\lambda \in \mathbb{R}$ is the coupling constant of the interaction, which will subsequently be used as a formal perturbative parameter. Additionally, as already discussed in Section 2.2.3, the equation of motion for the free theory is

$$S'_0(\phi) = 0,$$

while, for the interacting theory, it reads

$$S'_{\lambda V}(\phi) = 0 \iff S'_0(\phi) = -\lambda V'(\phi).$$

Here, the prime denotes the Euler-Lagrange derivative of the action as per Definition 2.22. In the following, we shall denote the sets of field configurations that satisfy the equation of motion by $\mathcal{E}_{S_0}(\mathcal{M})$ and $\mathcal{E}_{\lambda V}(\mathcal{M})$ for the free and interacting theory, respectively. These solution spaces turn out to be submanifolds of the configuration space $\mathcal{E}(\mathcal{M})$. Additionally, if the interacting potential is at most quadratic in the configuration, the resulting equations of motion are linear in the field and thus $\mathcal{E}_{\lambda V}(\mathcal{M})$ turns out to be an affine subspace of $\mathcal{E}(\mathcal{M})$. For a complete overview we refer to [Rej16, Ch. 4].

The Møller map, which we shall now define, is the unique map that allows us to intertwine the free and the interacting theory. We first characterize its action on the configuration space and then extend its action to the space of functionals.

Definition 2.34. *Let $(\mathcal{M}, g)$ be a globally hyperbolic manifold as per Definition 2.6 and let S_0 be an action as per Definition 2.21. Moreover, let us define a second action:*

$$S_{\lambda V} = S_0 + \lambda V, \quad V \in \mathcal{F}_{\text{loc}}(\mathcal{M}), \lambda \in \mathbb{R}.$$

*We call the **retarded Møller map** the map $r_{\lambda V} : \mathcal{E}(\mathcal{M}) \rightarrow \mathcal{E}(\mathcal{M})$ such that*

$$S'_{\lambda V} \circ r_{\lambda V} = S'_0, \quad r_{\lambda V}(\phi)|_{\mathcal{M} \setminus J^+(\text{supp}(V))} = \phi|_{\mathcal{M} \setminus J^+(\text{supp}(V))}.$$

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Here, S'_0 denotes the Euler-Lagrange derivative of S_0 as per Definition 2.22. Similarly, we define the **advanced Møller map** as the map $a_{\lambda V} : \mathcal{E}(\mathcal{M}) \rightarrow \mathcal{E}(\mathcal{M})$ such that

$$S'_{\lambda V} \circ a_{\lambda V} = S'_0, \quad a_{\lambda V}(\phi)|_{\mathcal{M} \setminus J^-(\text{supp}(V))} = \phi|_{\mathcal{M} \setminus J^-(\text{supp}(V))}.$$

Remark 2.22. It follows from Definition 2.34 that, if we consider three different actions S_1, S_2, S_3 , we can introduce the retarded Møller maps $r_{(1,2)}$, $r_{(2,3)}$, $r_{(1,3)}$, where $r_{(ij)}$ denotes the Møller map that associates the theory described by S_i with the theory described by $S_j = S_i + (S_j - S_i)$. Then, it holds that

$$r_{(2,3)} \circ r_{(1,2)} = r_{(1,3)},$$

and analogously for the advanced Møller maps $a_{(i,j)}$.

Remark 2.23. Let us consider an interacting action

$$S_{\lambda V} = S_0 + \lambda V,$$

as in Definition 2.34 and let us denote by $\mathcal{E}_{S_0}(\mathcal{M})$ the solution space for the free theory and $\mathcal{E}_{\lambda V}(\mathcal{M})$ the solution space for the interacting one. Then, for any $\phi \in \mathcal{E}_{S_0}(\mathcal{M})$, the retarded Møller map satisfies $r_{\lambda V}(\phi) \in \mathcal{E}_{\lambda V}(\mathcal{M})$. As a matter of fact, a direct computation yields

$$S'_{\lambda V}(r_{\lambda V}(\phi)) = S'_0(\phi) = 0.$$

Thus, the retarded Møller map intertwines the free and interacting solution spaces.

An explicit form for the retarded Møller map can be obtained when the free action is quadratic. For the quadratic Klein–Gordon action considered here, the Euler–Lagrange derivative of the free action S_0 is $S'_0(\phi) = P_0\phi$, while for the interacting action we obtain $S'_0(\phi) + \lambda V^{(1)}(\phi) = P_0\phi + \lambda V^{(1)}(\phi)$. Thus, it must hold that

$$P_0\phi = P_0(r_{\lambda V}\phi) + \lambda V^{(1)}(r_{\lambda V}\phi), \quad \forall \phi \in \mathcal{E}(\mathcal{M}).$$

Since P_0 is a linear operator, we obtain

$$P_0(r_{\lambda V}\phi - \phi) = -\lambda V^{(1)}(r_{\lambda V}\phi).$$

Given the support constraints in Definition 2.34, the function $r_{\lambda V}\phi - \phi$ is supported only in the causal future of $\text{supp}(V)$. Since V has compact support, this difference has past-compact support. Therefore, we can apply the

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extension to past-compact functions of the retarded Green operator $\Delta_{S_0}^R$ associated to P_0 to both terms to obtain the Yang–Feldman equation for the retarded Møller map:

$$r_{\lambda V}(\phi) = \phi - \lambda \Delta_{S_0}^R(V^{(1)}(r_{\lambda V}\phi)). \quad (2.35)$$

We can then solve the equation order by order in λ to recover a perturbative expression for the interacting configuration $r_{\lambda V}\phi$.

In the rest of this work, particular attention will be devoted to the analysis of a quadratic interacting term. For this reason, we shall outline here some properties of the Møller map for this type of interaction. For an in-depth analysis, we refer to [DHP17].

Proposition 2.7. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6. Additionally, let S_0 be the action, as per Definition 2.21, associated to the Klein-Gordon Lagrangian as per Equation (2.12) and let $S_{\lambda V}$ be the following action:*

$$\begin{aligned} S_{\lambda V}(\phi) &= S_0(\phi) + \lambda V(\phi) = \\ &= -\frac{1}{2} \int_{\mathcal{M}} d\mu_x f(x) \left(g^{\mu\nu} \nabla_\mu \phi(x) \nabla_\nu \phi(x) + \frac{R}{6} \phi^2(x) + \lambda \chi(x) \phi^2(x) \right). \end{aligned}$$

Here $\phi \in \mathcal{E}(\mathcal{M})$, while $\chi \in \mathcal{D}(\mathcal{M})$ is an infrared cutoff and $f \in \mathcal{D}(\mathcal{M})$ is the same compactly supported function that appears in Equation (2.12), which additionally satisfies $f|_{\text{supp } \chi} \equiv 1$. Moreover, $\lambda \in \mathbb{R}$ is the coupling constant. Then the classical retarded Møller map $r_{\lambda V}$ as per Definition 2.34 has the form

$$r_{\lambda V} = \text{id} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)}.$$

Here $\Delta_{S_{\lambda V}}^R$ denotes the retarded Green operator as per Definition 2.24 associated to the normally hyperbolic operator induced by $S_{\lambda V}$ as per Remark A.2, while $V^{(1)}$ denotes the linear map on $\mathcal{E}(\mathcal{M})$ induced by the Fréchet derivative of V as per Definition 2.14. Moreover, it holds that

$$r_{\lambda V} \circ (\text{id} + \lambda \Delta_{S_0}^R \circ V^{(1)}) = \text{id}.$$

Proof. Let us start by observing that $V^{(1)}$ induces a linear map on $\mathcal{E}(\mathcal{M})$ whose action on any configuration $\phi \in \mathcal{E}(\mathcal{M})$ reads $V^{(1)}(\phi)(x) = -\chi(x)\phi(x)$. Additionally, the equation of motion associated to S_0 and $S_{\lambda V}$ are governed by the operators $P_0 = \square_g - \frac{R}{6}$ and $P_{\lambda V} = \square_g - \lambda\chi - \frac{R}{6}$ respectively. Since ϕ is a smooth function and χ is smooth with compact support, $V^{(1)}$ maps smooth functions to smooth functions with compact support and therefore we can safely compose it with the retarded Green operator $\Delta_{S_{\lambda V}}^R$ associated to $P_{\lambda V}$,

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which exists on account of Proposition 2.3. Additionally, for any $h \in \mathcal{D}(\mathcal{M})$ the function $\Delta_{S_{\lambda V}}^R(h)$ satisfies

$$\text{supp}(\Delta_{S_{\lambda V}}^R(h)) \subseteq J^+(\text{supp}(h)),$$

and thus has past-compact support. Hence, for any $\phi \in \mathcal{E}(\mathcal{M})$, it holds that $(\phi - \lambda \Delta_{S_{\lambda V}}^R(V^{(1)}\phi))|_{\mathcal{M} \setminus J^+(\text{supp}(V))} = \phi$. By direct computation it holds that

$$\begin{aligned} P_{\lambda V}((\text{id} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)})\phi) &= P_{\lambda V}\phi - P_{\lambda V} \circ \Delta_{S_{\lambda V}}^R(\lambda V^{(1)}(\phi)) = \\ &= P_{\lambda V}\phi - \lambda V^{(1)}(\phi) = \square_g \phi - \lambda \chi \phi - \frac{R}{6}\phi + \lambda \chi \phi = P_0\phi. \end{aligned}$$

This proves that $\text{id} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)}$ satisfies the defining properties in Definition 2.34. Furthermore, uniqueness of $r_{\lambda V}$ follows from uniqueness of the solution to the corresponding Cauchy problem

$$\begin{cases} P_{\lambda V}(\psi) = P_0\phi \\ \psi|_{\mathcal{M} \setminus J^+(\text{supp}(V))} = \phi|_{\mathcal{M} \setminus J^+(\text{supp}(V))} \end{cases}, \quad \phi \in \mathcal{E}(\mathcal{M}),$$

see [Gin09, Cor. 5].

Finally, to determine the inverse of $r_{\lambda V}$, a direct computation yields

$$\begin{aligned} (\text{id} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)}) \circ (\text{id} + \lambda \Delta_{S_0}^R \circ V^{(1)}) &= \\ &= \text{id} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)} + \lambda \Delta_{S_0}^R \circ V^{(1)} - \lambda^2 \Delta_{S_{\lambda V}}^R \circ V^{(1)} \circ \Delta_{S_0}^R \circ V^{(1)}. \end{aligned}$$

Since it holds that $\lambda V^{(1)}(\phi) = (P_{\lambda V} - P_0)\phi$, for all $\phi \in \mathcal{E}(\mathcal{M})$, we obtain

$$\begin{aligned} \lambda^2 \Delta_{S_{\lambda V}}^R \circ V^{(1)} \circ \Delta_{S_0}^R \circ V^{(1)} &= \lambda \Delta_{S_{\lambda V}}^R \circ (P_{\lambda V} - P_0) \circ \Delta_{S_0}^R \circ V^{(1)} = \\ &= \lambda \Delta_{S_0}^R \circ V^{(1)} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)}, \end{aligned}$$

which exactly cancels the second and third term in the expression above. Hence, we have proved that

$$(\text{id} - \lambda \Delta_{S_{\lambda V}}^R \circ V^{(1)}) \circ (\text{id} + \lambda \Delta_{S_0}^R \circ V^{(1)}) = \text{id}.$$

An analogous computation shows also that

$$(\text{id} + \lambda \Delta_{S_0}^R \circ V^{(1)}) \circ r_{\lambda V} = \text{id}.$$

□

Remark 2.24. *The infrared cutoff χ in Proposition 2.7 entails that the interacting term is confined in a compact subset of the spacetime. This is needed to regularise the theory, avoiding infrared divergences in the perturbative expansion. However, to extract physically meaningful results, the so-called adiabatic limit $\chi \rightarrow 1$ has to be considered.*

Remark 2.25. *The specific case of quadratic interacting term in the Lagrangian allows us to find a convenient perturbative representation of the Møller map. As a matter of fact, Proposition 2.7 entails that we can write*

$$r_{\lambda V} = (\text{id} + \lambda \Delta_{S_0}^R \circ V^{(1)})^{-1}.$$

This is particularly useful since it allows us to represent $r_{\lambda V}$ in terms of the retarded Green operator of the free theory and of the Fréchet derivative of the interacting potential, without the need to explicitly compute the retarded Green operator of the interacting theory.

We can furthermore express the Møller map as a formal power series, called Neumann series, to obtain

$$r_{\lambda V} = \sum_{k=0}^{\infty} (-\lambda)^k (\Delta_{S_0}^R \circ V^{(1)})^k.$$

Additionally, if the underlying background is the Minkowski spacetime, the resulting Neumann series can be shown to converge uniformly on any compact set for interactions at most quadratic in the configuration. We stress that, in general, within the pAQFT framework, λ is treated as a formal parameter, so the series is understood, unless otherwise stated, as a formal power series in λ .

Heretofore, the action of the Møller maps is defined on the configuration space of the theory. Yet, since in the algebraic framework, the key objects are functionals rather than field configurations, we shall now extend its definition to elements of the observable algebra. This allows us to identify interacting classical observables with formal power series in the coupling parameter.

Definition 2.35. *Let $(\mathcal{M}, g)$ be a globally hyperbolic manifold as per Definition 2.6 and let $S_0, S_{\lambda V}$ be two actions as per Definition 2.21 such that*

$$S_{\lambda V} = S_0 + \lambda V, \quad V \in \mathcal{F}_{\text{loc}}(\mathcal{M}), \lambda \in \mathbb{R}.$$

*We define the **retarded Møller map** on the space of microcausal functionals via pullback of the map in Definition 2.34:*

$$\mathcal{R}_{\lambda V} : \mathcal{F}_{\mu\text{c}}(\mathcal{M}) \rightarrow \mathcal{F}_{\mu\text{c}}(\mathcal{M})[[\lambda]],$$

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$$(\mathcal{R}_{\lambda V} F)(\phi) \doteq F(r_{\lambda V}(\phi)), \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \forall F \in \mathcal{F}_{\mu c}(\mathcal{M}).$$

Here $\mathcal{F}_{\mu c}(\mathcal{M})[[\lambda]]$ denotes the space of microcausal functionals as per Definition 2.16 seen as formal power series in λ . We analogously define the **advanced Møller map** $\mathcal{A}_{\lambda V} : \mathcal{F}_{\mu c}(\mathcal{M}) \rightarrow \mathcal{F}_{\mu c}(\mathcal{M})[[\lambda]]$.

As highlighted in the previous discussion, the retarded and advanced Green operators play a fundamental rôle in the description of the Møller maps. The following proposition outlines how the free and interacting Green operators are related for any choice of interaction.

Proposition 2.8. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let S_0 be an action as per Definition 2.21. Moreover, if P_0 denotes the normally hyperbolic operator induced by the second-order Euler-Lagrange derivative of S_0 , let $\Delta_{S_0}^A$ denote its advanced Green operator as per Definition 2.24. Additionally, let $V \in \mathcal{F}_{loc}(\mathcal{M})$ be a local functional as per Definition 2.18 and $\lambda \in \mathbb{R}$ a constant parameter such that the second-order Euler-Lagrange derivative of*

$$S_{\lambda V} \doteq S_0 + \lambda V,$$

yields a normally hyperbolic operator

$$P_{\lambda V}(\phi) = P_0 + \lambda V^{(2)}(\phi),$$

for every $\phi \in \mathcal{E}(\mathcal{M})$. Then, denoting by $\Delta_{S_{\lambda V}}^A(\phi)$ the advanced Green operator associated to $P_{\lambda V}(\phi)$, it holds that

$$\Delta_{S_{\lambda V}}^A(\phi)(\psi) = \Delta_{S_0}^A(\psi) + \sum_{k=1}^{\infty} (-\lambda)^k \left(\Delta_{S_0}^A \circ V^{(2)}(\phi) \right)^k \Delta_{S_0}^A(\psi), \quad \forall \psi \in \mathcal{D}(\mathcal{M}). \quad (2.36)$$

Here the series is understood as a formal power series in λ . An analogous result holds for the retarded Green operator.

Proof. Since the operator $P_{\lambda V}(\phi)$ is normally hyperbolic, Proposition 2.3 guarantees existence and uniqueness of the advanced Green operator $\Delta_{S_{\lambda V}}^A(\phi)$. Thus, it holds that

$$P_{\lambda V}(\phi) \Delta_{S_{\lambda V}}^A(\phi) \psi = P_0 \Delta_{S_{\lambda V}}^A(\phi) \psi + \lambda V^{(2)}(\phi) \Delta_{S_{\lambda V}}^A(\phi) \psi = \psi, \quad \psi \in \mathcal{D}(\mathcal{M}).$$

We can rewrite this expression to isolate P_0 as

$$P_0 \Delta_{S_{\lambda V}}^A(\phi) \psi = \psi - \lambda V^{(2)}(\phi) \Delta_{S_{\lambda V}}^A(\phi) \psi.$$

We can then apply the advanced Green operator $\Delta_{S_0}^A$ to both terms to obtain

$$\Delta_{S_{\lambda V}}^A(\phi)\psi = \Delta_{S_0}^A(\psi) - \lambda \Delta_{S_0}^A(V^{(2)}(\phi)(\Delta_{S_{\lambda V}}^A(\phi)\psi)).$$

Thus, the zeroth-order term in λ in the Neumann expansion (2.36) is $\Delta_{S_0}^A$. We can then obtain the sought expression by iterating the substitution of the left-hand side into the right-hand side. For example, at first order in λ , we obtain

$$\begin{aligned} \Delta_{S_{\lambda V}}^A(\phi)\psi &= \Delta_{S_0}^A(\psi) - \lambda \Delta_{S_0}^A(V^{(2)}(\phi)(\Delta_{S_0}^A(\psi) - \lambda \Delta_{S_0}^A(V^{(2)}(\phi)(\Delta_{S_{\lambda V}}^A(\phi)\psi))) = \\ &= \Delta_{S_0}^A(\psi) - \lambda \Delta_{S_0}^A(V^{(2)}(\phi)(\Delta_{S_0}^A(\psi))) + \lambda^2 \Delta_{S_0}^A(V^{(2)}(\phi)(\Delta_{S_{\lambda V}}^A(\phi)(\psi))). \end{aligned}$$

The desired expression is obtained via an iteration procedure order by order in λ . $\square$

We now state a proposition that gives the perturbative expansion of the Møller maps and provides a recursive formula for computing interacting observables.

Proposition 2.9. *Let $\mathcal{F}_{loc}(\mathcal{M})$ be the space of local functionals as per Definition 2.18 on a globally hyperbolic spacetime $(\mathcal{M}, g)$ as per Definition 2.6 and let $S_0, S_{\lambda V}$ be two actions as per Definition 2.21 such that*

$$S_{\lambda V} = S_0 + \lambda V, \quad V \in \mathcal{F}_{loc}(\mathcal{M}), \lambda \in \mathbb{R}.$$

Then, the retarded Møller map $\mathcal{R}_{\lambda V}$ as per Definition 2.35 satisfies

$$\mathcal{R}_{\lambda V} F = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \mathcal{R}_k(V^{\otimes k}; F), \quad \forall F \in \mathcal{F}_{\mu c}(\mathcal{M})$$

where the coefficients $\mathcal{R}_k(V^{\otimes k}; F)$ satisfy, for all $\phi \in \mathcal{E}(\mathcal{M})$, the recursion relations

$$\begin{aligned} &\mathcal{R}_{k+1}(V^{\otimes(k+1)}, F)(\phi) \\ &= - \sum_{l=0}^k \binom{k}{l} \mathcal{R}_l \left(V^{\otimes l}, \int_{\mathcal{M}^2} d\mu_x d\mu_y \frac{\delta V}{\delta \phi}(x) \Delta_{S_0}^{A(k-l)}(\phi)(x, y) \frac{\delta F}{\delta \phi}(y) \right) (\phi), \\ &\Delta_{S_0}^{A(n)}(\phi)(x, y) \doteq \frac{d^n}{d\lambda^n} \Delta_{S_{\lambda V}}^A(\phi)(x, y) \Big|_{\lambda=0}. \end{aligned}$$

where $\Delta_{S_0}^A(x, y)$ denotes the integral kernel of the advanced propagator as per Definition 2.24 associated to the free action S_0 , while $\frac{\delta F}{\delta \phi}(x)$ denotes the integral kernel of the Fréchet derivative of F as per Definition 2.14 at ϕ . In addition, $\Delta_{S_{\lambda V}}^A(\phi)$ is defined as in Proposition 2.8 and its derivatives are computed by means of the expansion in Equation (2.36). An analogous result holds for the advanced Møller map $\mathcal{A}_{\lambda V}$, with the advanced and retarded Green operators interchanged.

For a proof of this result, we refer to [Rej16, Prop. 4.10].

Example 2.7. *As an example, let us consider the free action of a Klein-Gordon field as in Equation (2.12) and a quadratic interacting potential:*

$$\lambda V_h(\phi) = \frac{\lambda}{2} \int_{\mathcal{M}} d\mu_x h(x) \phi^2(x), \quad \phi \in \mathcal{E}(\mathcal{M}), h \in \mathcal{D}(\mathcal{M}).$$

Let us consider the smeared field observable $\Phi_f \in \mathcal{F}_{loc}(\mathcal{M})$, $f \in \mathcal{D}(\mathcal{M})$, as per Example 2.2, and let us compute the first-order correction due to the quadratic interacting potential. On account of Proposition 2.9, we have the following formal expansion for the interacting field observable

$$\mathcal{R}_{\lambda V_h} \Phi_f = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \mathcal{R}_k(V_h^{\otimes k}; \Phi_f),$$

where the $\mathcal{R}_0$ map is nothing but the identity on $\mathcal{F}_{loc}(\mathcal{M})$. The first order correction reads

$$\mathcal{R}_1(V_h; \Phi_f) = -\mathcal{R}_0 \left(V_h; \int_{\mathcal{M}^2} d\mu_x d\mu_y \frac{\delta V_h}{\delta \phi}(x) \Delta_{S_0}^A(x, y) \frac{\delta \Phi_f}{\delta \phi}(y) \right).$$

On account of examples 2.2 and 2.3, the Fréchet derivatives of the potential and the observable read

$$\begin{aligned} \Phi_f^{(1)}(\phi)(y) &= f(y), \\ V_h^{(1)}(\phi)(x) &= h(x) \phi(x). \end{aligned}$$

Thus, it holds that

$$\mathcal{R}_1(V_h; \Phi_f)(\phi) = - \int_{\mathcal{M}^2} d\mu_x d\mu_y \phi(x) h(x) \Delta_{S_0}^A(x, y) f(y), \quad \forall \phi \in \mathcal{E}(\mathcal{M}).$$

Hence, we obtain the following result:

$$\mathcal{R}_{\lambda V_h} \Phi_f = \Phi_f - \lambda \Phi_{h \Delta_{S_0}^A(f)} + \mathcal{O}(\lambda^2).$$

Before passing on to the quantization of the Møller maps, we discuss how the classical Møller maps relate to the Poisson structure of the algebra of observables. As a matter of fact, given the splitting of the total action into a free part and an interacting potential, we can endow the space of microcausal functionals with two distinct Peierls brackets, namely, $\{\cdot, \cdot\}_{S_0}$ and $\{\cdot, \cdot\}_{S_{\lambda V}}$, see Definition 2.28. The following proposition shows the intertwining property of the Møller maps with respect to these structures.

Proposition 2.10. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $S_0, S_{\lambda V}$ be two actions as per Definition 2.21 such that*

$$S_{\lambda V} = S_0 + \lambda V.$$

Additionally, let $\mathcal{F}_{\mu c, pol}(\mathcal{M})$ be the set of microcausal functionals of polynomial type as per Definition 2.16. If $\{\cdot, \cdot\}_{S_0}$ and $\{\cdot, \cdot\}_{S_{\lambda V}}$ denote the Peierls brackets, as per Definition 2.28 associated to S_0 and $S_{\lambda V}$, respectively, and if $\mathcal{R}_{\lambda V}$ denotes the Møller map as per Definition 2.35, it holds that

$$\{\mathcal{R}_{\lambda V} F, \mathcal{R}_{\lambda V} G\}_{S_0} = \mathcal{R}_{\lambda V}(\{F, G\}_{S_{\lambda V}}), \quad \forall F, G \in \mathcal{F}_{\mu c, pol}(\mathcal{M}).$$

An analogous result holds for the advanced Møller map $a_{\lambda V}$.

We refer to [DF03, Prop. 2] for a proof.

2.2.7 Interacting quantum field theory

This section is devoted to the construction of an interacting quantum field theory within the pAQFT framework. Specifically, we shall define the quantum counterpart of the retarded Møller map introduced in Section 2.2.6, namely the Bogoliubov map. Similarly to how the quantization of the free theory can be understood as a deformation of the classical algebra of observables, via the definition of the deformed product in Equation (2.22), within our framework the interacting theory is constructed as another deformation of the free theory. The Bogoliubov map involves a new product of the algebra, called *time-ordered product*.

We shall start by introducing this product on the subalgebra of regular functionals. This intermediate step will allow us to discuss the main properties of the time-ordered product via explicit formulae. Then, we will present its extension to local functionals, where a notion of renormalisation must be introduced.

It is worth mentioning that the time-ordered products can be characterized axiomatically, see, *e.g.*, [HW01] and [HW02] for a detailed overview. Here, however, we limit ourselves to detailing its explicit construction which is better suited for computations.

Definition 2.36. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $(\mathcal{F}_{reg}(\mathcal{M}), \star_H, *)$ be the unital $*$ -algebra of regular functionals as per Definition 2.17. Here $\star_H$ is the deformed product in Equation (2.24), where the rôle of deforming bidistribution is played by H , see Definition 2.31. Then we call **time-ordered product** on $\mathcal{F}_{reg}(\mathcal{M})$ a map*

$$\cdot_{\mathcal{T}} : \mathcal{F}_{reg}(\mathcal{M}) \times \mathcal{F}_{reg}(\mathcal{M}) \rightarrow \mathcal{F}_{reg}(\mathcal{M})[[\hbar]], \quad (2.37)$$

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where $\mathcal{F}_{\text{reg}}(\mathcal{M})[[\hbar]]$ denotes the space of regular functionals regarded as formal power series in $\hbar$. The map in Equation (2.37) is such that, for any pair of regular functionals $A, B \in \mathcal{F}_{\text{reg}}(\mathcal{M})$, it holds that

$$A \cdot_{\mathcal{T}} B = B \cdot_{\mathcal{T}} A,$$

and

$$A \cdot_{\mathcal{T}} B = A \star_H B, \quad \text{if } A \succeq B$$

Here $A \succeq B$ denotes that there exists a Cauchy surface $\Sigma \subset \mathcal{M}$ as per Definition 2.6 separating the support of A and B and such that $\text{supp}(B) \subset J^-(\Sigma)$ while $\text{supp}(A) \subset J^+(\Sigma)$. Here $J^\pm(\Sigma)$ denotes the causal future (+) or past (−) of Σ as per Definition 2.4 while $\text{supp}(A)$ is the spacetime support of A as per Definition 2.15.

For regular functionals, these properties completely determine the time-ordered product, as shown in [GHP15]. In particular, the time-ordered product of regular functionals can be expanded as

$$A \cdot_{\mathcal{T}} B(\phi) = \sum_{k=0}^{\infty} \frac{\hbar^k}{k!} \langle A^{(k)}(\phi), H_F^{\otimes k} B^{(k)}(\phi) \rangle, \quad \forall \phi \in \mathcal{E}(\mathcal{M}), \forall A, B \in \mathcal{F}_{\text{reg}}(\mathcal{M}), \quad (2.38)$$

where the right-hand side is well-defined on account of the microlocal properties of regular functionals. Here H_F denotes the *Feynman parametrix*, which is a bidistribution whose integral kernel reads

$$H_F(x, y) = H(x, y) + i\Delta^A(x, y),$$

where $H(x, y)$ is a Hadamard parametrix as per Definition 2.31 while $\Delta^A(x, y)$ denotes the integral kernel of the advanced Green operator as per Definition 2.24.

We can directly verify that the product in Equation (2.38) satisfies the properties in Definition 2.36. Let us start by showing that the Feynman parametrix is a symmetric bidistribution. A direct computation yields

$$\begin{aligned} H_F(x, y) &= H(x, y) + i\Delta^A(x, y) = H(x, y) + i\Delta^R(y, x) \\ &= H(y, x) - i\Delta_S(y, x) + i\Delta^R(y, x) = H(y, x) + i\Delta^A(y, x) = H_F(y, x). \end{aligned}$$

Here we used that the formal adjoint of the advanced propagator is the retarded one and the fact that $H(x, y) - H(y, x) = i\Delta_S(x, y)$. Thus, if we

express any term in Equation (2.38) in terms of integral kernels, we obtain

$$\begin{aligned}
 \langle A^{(k)}(\phi), H_F^{\otimes k} B^{(k)}(\phi) \rangle &= \\
 &= \int_{\mathcal{M}^{2k}} d\mu_{x_1} \dots d\mu_{y_k} A^{(k)}(\phi)(x) H_F(x_1, y_1) \dots H_F(x_k, y_k) B^{(k)}(\phi)(y) \\
 &= \int_{\mathcal{M}^{2k}} d\mu_{x_1} \dots d\mu_{y_k} B^{(k)}(\phi)(y) H_F(y_1, x_1) \dots H_F(y_k, x_k) A^{(k)}(\phi)(x) \\
 &= \langle B^{(k)}(\phi), H_F^{\otimes k} A^{(k)}(\phi) \rangle.
 \end{aligned}$$

Here we used the short-hand notation $x = (x_1, \dots, x_k)$ and equivalently for y . Moreover, let us suppose that $A \succeq B$ as in Definition 2.36. Then, it holds that

$$\langle A^{(1)}(\phi), \Delta^A B^{(1)} \rangle = \int_{\mathcal{M}^\infty} d\mu_x d\mu_y A^{(1)}(\phi)(x) \Delta^A(x, y) B^{(1)}(\phi)(y) = 0,$$

for all $\phi \in \mathcal{E}(\mathcal{M})$. This is because, on account of Definition 2.15, it holds that $\text{supp}(A^{(1)}(\phi)) \subset \text{supp}(A)$ and thus, if $x \in \text{supp}(A^{(1)}(\phi))$ and $y \in \text{supp}(B^{(1)}(\phi))$, then it holds that $x \notin J^-(y)$. This is incompatible with $(x, y) \in \text{supp}(\Delta^A)$, for which $x \in J^-(y)$. Hence, if $A \succeq B$, the pairing with Δ^A vanishes. Furthermore, it holds that

$$\begin{aligned}
 \langle A^{(1)}(\phi), H_F B^{(1)}(\phi) \rangle &= \langle A^{(1)}(\phi), H B^{(1)}(\phi) \rangle + i \langle A^{(1)}(\phi), \Delta^A B^{(1)}(\phi) \rangle = \\
 &= \langle A^{(1)}(\phi), H B^{(1)}(\phi) \rangle.
 \end{aligned}$$

By an inductive argument, this simplification holds for all $k \in \mathbb{N}$ and thus the Feynman parametrix defines a time-ordered product as per Definition 2.36.

It is possible to give a local characterization of the Feynman parametrix, similarly to what we did for the Hadamard parametrix in Definition 2.31.

Definition 2.37. *Let $(\mathcal{M}, g)$ be a 4-dimensional globally hyperbolic spacetime as per Definition 2.6 and let $H \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be a Hadamard parametrix as per Definition 2.31. Moreover, let $p \in \mathcal{M}$ and let $\mathcal{O} \subset \mathcal{M}$ be a geodesically convex open neighborhood of p . Then, for any $x, y \in \mathcal{O}$ the integral kernel of the Feynman parametrix reads:*

$$H_F(x, y) = \lim_{\varepsilon \rightarrow 0^+} \frac{i}{8\pi^2} \left[\frac{U(x, y)}{\sigma_{F, \varepsilon}(x, y)} + V(x, y) \ln \frac{\sigma_{F, \varepsilon}(x, y)}{\lambda^2} \right] + W(x, y). \quad (2.39)$$

Here the smooth functions $U, V, W \in \mathcal{E}(\mathcal{O} \times \mathcal{O})$ are the same functions that appear in Equation (2.27), while $\sigma_{F, \varepsilon}(x, y) = \sigma(x, y) + i\varepsilon$, $\varepsilon > 0$, where $\sigma(x, y)$ denotes the halved squared geodesic distance. Additionally, $\lambda > 0$ is a reference length scale.

Note that, until now, we have defined the time-ordered product only for regular functionals. Since all physically-relevant observables are represented as local functionals, we would like to extend the construction to this class of functionals. To this end, it is necessary to analyse the singular behaviour of the Feynman parametrix. In particular, on account of the results in [RV96],[Rad96] and [DH72], it holds that the wavefront set, as per Definition A.4, of the Feynman parametrix in Definition 2.37 reads

$$\text{WF}(H_F) = \{(x, \xi_x; y, -\xi_y) \in \mathring{T}^*(\mathcal{M} \times \mathcal{M}) \mid (x, \xi_x) \sim_F (y, \xi_y)\} \cup \text{WF}(\delta_2).$$

Here $\mathring{T}^*(\mathcal{M} \times \mathcal{M}) \doteq T^*(\mathcal{M} \times \mathcal{M}) \setminus \{0\}$ denotes the punctured cotangent bundle of $\mathcal{M} \times \mathcal{M}$, while the equivalence relation $(x, \xi_x) \sim_F (y, \xi_y)$ means that there exists a null-geodesic γ connecting x and y such that ξ_x is tangent to γ at x while ξ_y is the parallel transport of ξ_x along γ . Additionally, if $y \in J^-(x)$ then ξ_x is past-directed, while, if $y \in J^+(x)$, then ξ_x is future-directed. Furthermore,

$$\text{WF}(\delta_2) = \{(x, k; x, -k) \in \mathring{T}(\mathcal{M} \times \mathcal{M}) \mid x \in \mathcal{M}, k \in \mathring{T}_x \mathcal{M}\},$$

is the wavefront set of the Dirac delta distribution supported on the diagonal of $\mathcal{M} \times \mathcal{M}$.

This result highlights a first problem in the extension of the time-ordered product to $\mathcal{F}_{\text{loc}}(\mathcal{M})$, as the form of the wavefront set of H_F is such that the powers H_F^k , $k \in \mathbb{N}$, are not well-defined distribution. This is due to the presence of the term $\text{WF}(\delta_2)$, which causes H_F^k to be ill-defined, according to Hörmander's criterion for the multiplication of distributions, see Theorem A.4, on the thin diagonal $\text{Diag}_k \subset \mathcal{M}^k$. Hence, if we consider two local functionals $A, B \in \mathcal{F}_{\text{loc}}(\mathcal{M})$ with overlapping support and try to apply Equation (2.38), the second-order term yields, at a formal level,

$$\begin{aligned} \langle A^{(2)}(\phi), H_F^{\otimes 2} B^{(2)}(\phi) \rangle &= \\ &= \int_{M^4} d\mu_{x_1} \dots d\mu_{y_2} A^{(2)}(\phi)(x_1, x_2) H_F(x_1, y_1) H_F(x_2, y_2) B^{(2)}(\phi)(y_1, y_2) = \\ &= \int_{\mathcal{M}^2} d\mu_x d\mu_y A^{(2)}(\phi)(x, x) H_F^2(x, y) B^{(2)}(\phi)(y, y). \end{aligned} \quad (2.40)$$

Here we used that, for any local functional $A \in \mathcal{F}_{\text{loc}}(\mathcal{M})$, it holds that $\text{supp}(A^{(2)}(\phi)) \subset \text{Diag}_2$ for all $\phi \in \mathcal{E}(\mathcal{M})$. Note that, on account of the previous discussion, Equation (2.40) is ill-defined.

In order to circumvent this problem, we first observe that the powers of the Feynman parametrix H_F^k , $k \in \mathbb{N}$, are well-defined distribution on $\mathcal{M}^2 \setminus \text{Diag}_2$. Hence, we can apply microlocal techniques in order to establish whether it is possible to extend H_F^k to obtain a well-defined distribution

also at the diagonal. This extension problem is referred to as *renormalization* within the pAQFT framework. We shall adopt the approach presented in [BF00], which is based on the theory of homogeneous distributions first formulated by Hörmander in [Hör98, Sec. 3.2].

The idea is that, given a submanifold $\mathcal{N} \subset \mathcal{M}^n$, one can associate to every distribution in $\mathcal{D}'(\mathcal{M}^n \setminus \mathcal{N})$ two quantities, namely, the *scaling degree*, see Definition A.6, and the **degree of divergence**, see Definition A.7, which characterize the behaviour of the distribution at the submanifold and allow one to determine whether an extension exists and whether it is unique. In Appendix A.2 we present a succinct overview of the tools necessary, while we refer the interested reader to [BF00] for a detailed overview.

As an example, let us conclude this section by showing this procedure for the case of the square of the Feynman parametrix H_F^2 . For simplicity, let us work on Minkowski spacetime $\mathbb{M}^4 \equiv (\mathbb{R}^4, \eta)$, although the whole discussion can be generalised to any 4-dimensional globally hyperbolic spacetime $\mathcal{M}$.

By translational invariance of Minkowski spacetime, we can rewrite Equation (2.39) as

$$H_F(x - y) = \frac{i}{8\pi^2} \left[\frac{U(x - y)}{\sigma(x - y)} + V(x - y) \ln \left(\frac{\sigma(x - y)}{\lambda^2} \right) \right].$$

Here we have neglected the smooth function W since it does not contribute to the singular structure of the parametrix, as well as the ε -regularisation as we consider two points x, y away from the diagonal. Note that, throughout the following, we shall regard the Feynman parametrix as being dependent on the single variable $z \doteq x - y \in \mathbb{R}^4$. Hence, H_F is a well-defined distribution in $\mathcal{D}'(\mathbb{R}^4 \setminus \{0\})$.

Additionally, note that U, V are smooth functions and therefore they do not contribute to the singular structure of H_F , while $\ln \frac{\sigma}{\lambda^2}$ is a locally integrable function and therefore it generates a well-defined distribution in $\mathcal{D}'(\mathbb{R}^4)$. Thus, in order to establish whether H_F can be extended to a distribution in $\mathcal{D}'(\mathbb{R}^4)$, we need to compute the scaling degree at the origin, as per Definition A.6, of the distribution generated by σ^{-1} . Let us observe that, for any $\zeta > 0$ it holds that

$$\sigma^{-1}(\zeta(x - y)) = \frac{2}{(\zeta(x - y))^2} = \zeta^{-2} \frac{2}{(x - y)^2} = \zeta^{-2} \sigma^{-1}(x - y).$$

Therefore, the distribution generated by σ^{-1} is homogeneous of degree -2 as per Definition A.5. Hence, on account of Remark A.7, the scaling degree of the distribution generated by σ^{-1} reads $sd_{\sigma^{-1}} = 2$. Thus, on account of Theorem A.5, we can uniquely extend H_F to a distribution in $\mathcal{D}'(\mathbb{R}^4)$.

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Turning to the analysis of H_F^2 , formally the square of the Feynman parametrix reads

$$\begin{aligned} H_F^2(x-y) = & \frac{U(x-y)}{\sigma^2(x-y)} + 2 \frac{V(x-y)U(x-y)}{\sigma(x-y)} \ln \left(\frac{\sigma(x-y)}{\lambda^2} \right) \\ & + V^2(x-y) \ln^2 \left(\frac{\sigma(x-y)}{\lambda^2} \right). \end{aligned}$$

Here we once again omitted the smooth terms and the ε -regularisation as we are considering points away from the diagonal.

Note that the function $\ln^2 \left(\frac{\sigma(x-y)}{\lambda^2} \right)$ is locally integrable and therefore generates a distribution in $\mathcal{D}'(\mathbb{R}^4)$. Additionally, if we introduce the change of coordinates from $z = (t, x_1, x_2, x_3)$ to the hyperbolic coordinates

$$\begin{cases} t = \rho \cosh \chi \\ x_1 = \rho \sinh \chi \cos \theta \\ x_2 = \rho \sinh \chi \sin \theta \cos \varphi \\ x_3 = \rho \sinh \chi \sin \theta \sin \varphi \end{cases}, \quad \rho > 0, \chi \in [0, \infty), (\theta, \varphi) \in \mathbb{S}^2,$$

we obtain that $\sigma(x-y) = \rho^2$. Thus, the second term is proportional to $\frac{2 \ln \rho}{\rho^2}$, which is a locally integrable function if we consider that, under this change of coordinates, the volume measure is proportional to $\rho^3 d\rho$.

It remains to analyse the first term proportional to $\sigma^{-2}(x-y)$. Since the distribution generated by σ^{-1} is homogeneous of degree -2 , as highlighted above, the one generated by σ^{-2} is homogeneous of degree -4 . Hence, it holds that $sd_{\sigma^{-2}} = 4$. Thus, we can apply Theorem A.6 to conclude that it is possible to extend the square of the Feynman parametrix H_F^2 to a distribution in $\mathcal{D}'(\mathbb{R}^4)$. However, differently from the case of the H_F , the extension is not unique and, denoting by H_F^2 and $(H'_F)^2$ two admissible extensions, it holds that

$$H_F^2(x-y) = (H'_F)^2(x-y) + c\delta(x-y),$$

Thus, for this particular extension problem, two prescriptions preserving the scaling degree differ by a distribution proportional to the Dirac delta distribution δ_2 supported on the thin diagonal of $\mathbb{R}^4 \times \mathbb{R}^4$. While mathematically any extension preserving the scaling degree is a valid distribution, we can restrict the choice by imposing physically motivated constraints, such as local covariance and the preservation of local symmetries. Among the possible renormalisation schemes, for the scalar field theory we are considering, it is possible to make contact with the Minimal Subtraction (MS) scheme, which is usually adopted in theories where there is no reference mass. As expected,

this approach turns out to be equivalent to that obtained in dimensional regularisation. For an in-depth overview and for the explicit computations of the renormalised Feynman parametrix and its powers within this renormalisation scheme, we refer the interested reader to [GHP15].

This construction allows us to extend the definition of the time-ordered product to the algebra of local functionals $\mathcal{F}_{\text{loc}}(\mathcal{M})$. In the following, we shall still denote this extension by $\cdot_{\mathcal{T}}$, with the renormalisation procedure understood to have been carried out. We have all the data necessary to introduce the main tools necessary for the perturbative analysis of an interacting quantum field theory.

Definition 2.38. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $V \in \mathcal{F}_{\text{loc}}(\mathcal{M})$ be a local functional as per Definition 2.18 representing an interacting potential. Moreover, let $\lambda \in \mathbb{R}$ be the coupling constant of the theory. We call the **S-matrix** the map*

$$S : \lambda \mathcal{F}_{\text{loc}}(\mathcal{M}) \rightarrow \mathcal{F}_{\mu\text{c}}(\mathcal{M})[[\lambda]]$$

$$S(\lambda V) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\lambda}{\hbar} \right)^n \underbrace{V \cdot_{\mathcal{T}} \cdots \cdot_{\mathcal{T}} V}_{n \text{ times}}.$$

Here $\mathcal{F}_{\mu\text{c}}(\mathcal{M})[[\lambda]]$ denotes the space of microcausal functionals as per Definition 2.16, which are a formal power series in λ . Furthermore $\cdot_{\mathcal{T}}$ denotes the extension of the time-ordered product in Definition 2.36 to the space of local functionals.

The S-matrix is the structure that encodes the perturbative effect of the interaction and it provides the basic tool for constructing interacting observables. It is possible to construct an inverse, in the sense of formal power series, of the S-matrix with respect to the deformed product $\star_H$ of the algebra as per Equation (2.22). In order to give an explicit representation, we start by defining the *Dyson parametrix*, which is the formal adjoint of the Feynman parametrix, as per Definition 2.37, with respect to the standard pairing between smooth functions and compactly supported, smooth functions. At the level of integral kernels it reads

$$H_{AF}(x, y) \doteq (H_F)^*(x, y) = H(x, y) - i\Delta^R(x, y).$$

Here $H(x, y)$ denotes the integral kernel of a Hadamard parametrix as per Definition 2.31 while $\Delta^R(x, y)$ denotes the integral kernel of the retarded propagator as per Definition 2.24. Furthermore, the symmetry of the Feynman propagator entails that of the Dyson one. By choosing H_{AF} as deforming

bidistribution in Equation (2.22), we obtain another product which is called *anti time-ordered product*, which we shall denote by $\cdot_{\overline{\mathcal{T}}}$. Similarly to the case of the Feynman propagator, in order to extend it to local functionals it is necessary to carry out a renormalisation procedure. However, once a renormalisation scheme has been selected for the Feynman propagator, it can be consequently extended to the Dyson one.

After introducing the anti time-ordered product $\cdot_{\overline{\mathcal{T}}}$, we can write the inverse of S-matrix, with respect to the product $\star_H$, as

$$S(\lambda V)^{\star^{-1}} \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\lambda}{\hbar} \right)^n \underbrace{V \cdot_{\overline{\mathcal{T}}} \dots \cdot_{\overline{\mathcal{T}}} V}_{n \text{ times}}, \quad \lambda V \in \lambda \mathcal{F}_{\text{loc}}(\mathcal{M}). \quad (2.41)$$

By direct computation it can be shown that

$$S(\lambda V) \star_H S^{\star^{-1}}(\lambda V) = S^{\star^{-1}}(\lambda V) \star_H S(\lambda V) = \mathbf{1},$$

where $\mathbf{1}$ denotes the unit of the algebra.

The definition of the S-matrix and of its inverse allows us to introduce the Bogoliubov map, which will be one of the main tools we shall use in the rest of our work.

Definition 2.39. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\lambda V \in \mathcal{F}_{\text{loc}}(\mathcal{M})$, $\lambda \in \mathbb{R}$, be a local functional, as per Definition 2.18, representing an interacting potential. Additionally, let $\cdot_{\overline{\mathcal{T}}}$ denote the extension of the time-ordered product as per Definition 2.36 to $\mathcal{F}_{\text{loc}}(\mathcal{M})$, and let $\star_H$ denote the product in Equation (2.24). Here the deforming bidistribution is a Hadamard parametrix H as per Definition 2.31. Then, we define the **Bogoliubov map** as*

$$R_{\lambda V} : \mathcal{F}_{\text{loc}}(\mathcal{M}) \rightarrow \mathcal{F}_{\mu c}(\mathcal{M})[[\lambda]]$$

$$R_{\lambda V}(F) = S^{\star^{-1}}(\lambda V) \star_H (S(\lambda V) \cdot_{\overline{\mathcal{T}}} F), \quad \lambda V \in \mathcal{F}_{\text{loc}}(\mathcal{M}), \forall F \in \mathcal{F}_{\text{loc}}(\mathcal{M}). \quad (2.42)$$

Here $S(\lambda V)$ is the S-matrix, as per Definition 2.38, while $S^{\star^{-1}}(\lambda V)$ is its inverse as per Equation (2.41). Additionally, $\mathcal{F}_{\mu c}(\mathcal{M})[[\lambda]]$ denotes the space of microcausal functionals, as per Definition 2.16, constructed as power series in λ .

The map introduced above allows us to construct interacting observables as formal power series in the coupling constant for an interacting quantum field theory and it represents the quantisation of the Møller map introduced in Section 2.2.6.

Example 2.8. *As an example of application of the Bogoliubov map, let us compute explicitly the first order corrections in the coupling constant λ to the square field observable $\Phi_f^2 \in \mathcal{F}_{loc}(\mathcal{M})$, $f \in \mathcal{D}(\mathcal{M})$ for an interacting potential of the form*

$$\lambda V(\phi) = \frac{\lambda}{4!} \int_{\mathcal{M}} d\mu_x h(x) \phi^4(x), \quad \phi \in \mathcal{E}(\mathcal{M}), h \in \mathcal{D}(\mathcal{M}), \lambda \in \mathbb{R}.$$

We assume that a renormalisation procedure for the Feynman and Dyson propagators H_F, H_{AF} and their powers has been carried out. Let us compute, up to order $\mathcal{O}(\lambda)$, the expansion of the S -matrix in Definition 2.38

$$S(\lambda V) = \mathbb{I} + \frac{i\lambda}{\hbar} V + \mathcal{O}(\lambda^2),$$

$$S^{\star-1}(\lambda V) = \mathbb{I} - \frac{i\lambda}{\hbar} V + \mathcal{O}(\lambda^2).$$

Thus, Definition 2.39 entails

$$R_{\lambda V}(\Phi_f^2) = \left(\mathbb{I} - \frac{i\lambda}{\hbar} V + \mathcal{O}(\lambda^2) \right) \star_H \left(\left(\mathbb{I} + \frac{i\lambda}{\hbar} V + \mathcal{O}(\lambda^2) \right) \cdot_{\mathcal{T}} \Phi_f^2 \right).$$

Neglecting higher-order terms we obtain

$$R_{\lambda V}(\Phi_f^2) = \Phi_f^2 + \frac{i\lambda}{\hbar} (V \cdot_{\mathcal{T}} \Phi_f^2 - V \star_H \Phi_f^2) + \mathcal{O}(\lambda^2).$$

Hence, in order to compute the first-order correction we must compute the time-ordered product $V \cdot_{\mathcal{T}} \Phi_f^2$. Applying Equation (2.38) yields, for all $\phi \in \mathcal{E}(\mathcal{M})$,

$$\begin{aligned} (V \cdot_{\mathcal{T}} \Phi_f^2)(\phi) &= V(\phi) \Phi_f^2(\phi) + \hbar \langle V^{(1)}(\phi), H_F(\Phi_f^2)^{(1)}(\phi) \rangle \\ &\quad + \frac{\hbar^2}{2} \langle V^{(2)}(\phi), H_F^{\otimes 2}(\Phi_f^2)^{(2)}(\phi) \rangle. \end{aligned}$$

On account of Example 2.3, the Fréchet derivatives, as per Definition 2.14, of the squared field observable Φ_f^2 at ϕ read

$$\Phi_f^{(1)}(\phi)(x) = 2f(x)\phi(x), \quad \Phi_f^{(2)}(\phi)(x_1, x_2) = 2f(x_1)\delta(x_1, x_2).$$

Here $\delta(x_1, x_2)$ denotes the integral kernel of the Dirac delta distribution supported on the thin diagonal of $\mathcal{M} \times \mathcal{M}$.

By direct computation, the Fréchet derivatives of the interacting potential V read, at the level of integral kernels

$$V^{(1)}(\phi)(y) = \frac{1}{6} h(y) \phi^3(y), \quad V^{(2)}(\phi)(y_1, y_2) = \frac{1}{2} h(y_1) \phi^2(y_1) \delta(y_1, y_2).$$

Thus, the time-ordered product between V and Φ_f^2 reads, at a formal level

$$(V \cdot_{\mathcal{T}} \Phi_f^2)(\phi) = V(\phi)\Phi_f^2(\phi) + \frac{\hbar}{3} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x)\phi(x)H_F(x,y)h(y)\phi^3(y) \\ + \frac{\hbar^2}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x)H_F^2(x,y)h(y)\phi^2(y).$$

In order to compute the first order corrections, it is necessary to evaluate also $V \star_H \Phi_f^2$. However, since the product is formally defined by an analogous expression obtained by substituting the Feynman parametrix H_F with the Hadamard parametrix H , we obtain

$$(V \star_H \Phi_f^2)(\phi) = V(\phi)\Phi_f^2(\phi) + \frac{\hbar}{3} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x)\phi(x)H(x,y)h(y)\phi^3(y) \\ + \frac{\hbar^2}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x)H^2(x,y)h(y)\phi^2(y).$$

Hence, the first order correction in λ for the squared field functional reads

$$R_{\lambda V}(\Phi_f^2)(\phi) = \Phi_f^2(\phi) + \\ \frac{i\lambda}{\hbar} \left(\frac{\hbar}{3} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x)\phi(x) (H_F(x,y) - H(x,y)) h(y)\phi^3(y) \right. \\ \left. + \frac{\hbar^2}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) (H_F^2(x,y) - H^2(x,y)) h(y)\phi^2(y) \right) + \mathcal{O}(\lambda^2) = \\ = \Phi_f^2(\phi) - \frac{\lambda}{3} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x)\phi(x)\Delta^A(x,y)h(y)\phi^3(y) + \\ + \frac{i\hbar}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) (H_F^2(x,y) - H^2(x,y)) h(y)\phi^2(y) + \mathcal{O}(\lambda^2).$$

Here we used that, by definition, it holds that $H_F(x,y) - H(x,y) = i\Delta^A(x,y)$, where $\Delta^A(x,y)$ is the advanced propagator as per Definition 2.24.

Given the fact that the Bogoliubov map $R_{\lambda V}$ as per Definition 2.39 is the quantum counterpart of the Møller map $\mathcal{R}_{\lambda V}$ as per Definition 2.35, it is natural to wonder whether some classical limit exists where these two maps actually coincide. In order to answer this question, let us notice that the free observables of the underlying locally and covariant algebra, as per Definition 2.32, are constructed as formal power series in the deformation parameter $\hbar$. This holds due to the definition of the deformed product $\star_H$. Since negative powers of $\hbar$ appear in the definition of $S(\lambda V)$, the interacting observables obtained by means of the Bogoliubov map are both formal power series in λ and Laurent series in $\hbar$. The classical limit is obtained by imposing $\hbar \rightarrow 0$,

being $\hbar$ the deformation parameter linked to the quantisation of the theory. This is however, in principle problematic, as negative powers of $\hbar$ in the expression of $R_{\lambda V}(F)$ would entail the presence of divergent terms. The following proposition states that this is not the case, as no negative power of $\hbar$ appear in the formal expansion of the Bogoliubov map.

Proposition 2.11. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\lambda V \in \mathcal{F}_{loc}(\mathcal{M})$, $\lambda \in \mathbb{R}$, a local functional, as per Definition 2.18, representing an interacting potential. Moreover, let $R_{\lambda V}$ be the Bogoliubov map as per Definition 2.39. Then, the formal expansion of $R_{\lambda V}(F)$ contains no negative power of $\hbar$ for all $F \in \mathcal{F}_{loc}(\mathcal{M})$.*

For a proof of this result, we refer to [Rej16, Prop. 6.1] and [BDR23, Prop. 4.3].

Having ensured that no negative powers of $\hbar$ appears inside the Bogoliubov map, we state a proposition that highlights the link between the Møller map $\mathcal{R}_{\lambda V}$ in Definition 2.35 and the Bogoliubov map $R_{\lambda V}$.

Proposition 2.12. *Let $(\mathcal{M}, g)$ be a globally hyperbolic spacetime as per Definition 2.6 and let $\lambda V \in \mathcal{F}_{loc}(\mathcal{M})$, $\lambda \in \mathbb{R}$, be a local functional, as per Definition 2.18, representing an interacting potential. Moreover, let $R_{\lambda V}$ be the Bogoliubov map as per Definition 2.39 and let $\mathcal{R}_{\lambda V}$ be the retarded Møller map as per Definition 2.35. Then, it holds that*

$$R_{\lambda V}(F)|_{\hbar=0} = \mathcal{R}_{\lambda V}(F), \quad \forall F \in \mathcal{F}_{loc}(\mathcal{M}).$$

For a proof of this proposition, we refer to [Rej16, Prop. 6.2].

2.2.8 Quantum algebra on the boundary

The goal of this section is to introduce the quantum algebra of observables at the conformal null boundary $\mathcal{I}^+$ of an asymptotically flat spacetime as per Definition 2.8. Furthermore, we introduce the bulk-to-boundary map that projects observables from the locally covariant algebra of the theory to counterparts on $\mathcal{I}^+$. Note that, in order to construct an algebra of observables, the construction of the bulk algebra that we carried out in Section 2.2.2 cannot be transferred directly to $\mathcal{I}^+$. The reason is that the induced metric is degenerate rather than Lorentzian. Hence, there is no analogue, for example, of a Hadamard parametrix on $\mathcal{I}^+$. Moreover, the bulk-to-boundary map is defined by composing bulk observables with the causal propagator of the theory, and its image need not have compact support in $\mathcal{I}^+$. In fact, the support may reach also future timelike infinity i^+ , as for a generic curved,

asymptotically flat spacetime Huygens' principle does not hold. Hence, we construct a different class of functionals that is suitably defined in order to represent the asymptotic observables at $\mathcal{I}^+$. The following discussion is mainly based on [DMP17] and [DPP11].

Before introducing the boundary algebra and its properties, let us fix the notation. We shall consider a globally hyperbolic spacetime $(\mathcal{M}, g)$, as per Definition 2.6, which is asymptotically flat at future null and timelike infinity as per Definition 2.8. We shall denote by $\widetilde{\mathcal{M}}$ the unphysical spacetime in which $\mathcal{M}$ is embedded via a conformal transformation, and we identify $\mathcal{M}$ with its image under the embedding $\iota : \mathcal{M} \rightarrow \widetilde{\mathcal{M}}$.

Additionally, we shall denote the boundary of $\mathcal{M}$ by $\mathcal{C} = \partial J^-(i^+; \widetilde{\mathcal{M}})$, where $J^-(i^+; \widetilde{\mathcal{M}})$ denotes the causal past of future timelike infinity i^+ with respect to the causal structure of $\widetilde{\mathcal{M}}$. It can be decomposed into

$$\mathcal{C} = \mathcal{I}^+ \cup \{i^+\}.$$

Here $\mathcal{I}^+$ denotes future null infinity which, in the Bondi coordinates (u, θ, ϕ) introduced in Section 2.1.2, is diffeomorphic to $\mathbb{R} \times \mathbb{S}^2$, while i^+ is future timelike infinity.

Let us start our discussion by introducing the building blocks necessary to construct the boundary algebra. Here we report Definition [DMP17, Def. 5.2.1] adapted to the case at hand.

Definition 2.40. *Let $(\mathcal{M}, g)$ be a globally hyperbolic and asymptotically flat spacetime at future timelike and null infinity as per Definitions 2.6 and 2.8. Moreover, let us denote by $\mathcal{C} = \mathcal{I}^+ \cup \{i^+\}$ the boundary $\partial\mathcal{M}$ under the conformal embedding of $\mathcal{M}$ in Definition 2.8 and let $\mathcal{D}'(\mathcal{I}^+)$ be the space of distributions as per Definition A.1. Then, we denote by $\mathcal{F}^n$, $n \in \mathbb{N}$, the set of distributions $F_n \in \mathcal{D}'((\mathcal{I}^+)^n)$ such that:*

- *The closure on $\mathcal{C}^n$ of $\text{supp}(F_n)$ is compact, where $\text{supp}(F_n)$ is the support of F_n as per Definition A.1,*
- *it holds that*

$$\text{WF}(F_n) \subseteq \{(x, \xi) \in (\mathring{T}^* \mathcal{I}^+)^n \mid (x, \xi) \notin (\overline{V}_n^+ \cup \overline{V}_n^-), (x, \xi) \notin S_n\}.$$

Here $\text{WF}(F_n)$ denotes the wavefront set of F_n as per Definition A.4, while we used the shorthand notation $(x; \xi) = (x_1, \dots, x_n; \xi_1, \dots, \xi_n)$. Additionally $\mathring{T}^*(\mathcal{I}^+)^n = T^*(\mathcal{I}^+)^n \setminus \{0\}$ is the punctured cotangent space. Furthermore, $(x, \xi) \in \overline{V}_n^+$ if, for every i , either $\xi_i = 0$ or $(\xi_i)_u > 0$, and analogously for $\overline{V}_n^-$. Furthermore, $(x, \xi) \in S_n$ if there exists an index i such that $\xi_i \neq 0$ and $(\xi_i)_u = 0$,

- The distribution F_n can be factorised into the tensor product of a smooth function and an element of $\mathcal{F}^{n-1}$ when localised in a neighbourhood of i^+ .

Remark 2.26. The support condition in Definition 2.40 is not restrictive. For a compact set $\mathcal{K} \subset \mathcal{M}$, its causal future $J^+(\mathcal{K})$ is past compact, namely, for any point $p \in \widetilde{\mathcal{M}}$, it holds that $J^-(p) \cap J^+(\mathcal{K})$ is compact in $\widetilde{\mathcal{M}}$. Any observable supported in $\mathcal{K}$ will be mapped to a counterpart supported in $J^+(\mathcal{K}) \cap \mathcal{C}$, which is a closed subset of $J^+(\mathcal{K}) \cap J^-(i^+)$ and therefore compactly supported in $\mathcal{C}$.

Remark 2.27. The third condition in Definition 2.40 entails that all singularities are localised away from i^+ . This is not a restrictive condition as it can be verified by applying the propagation of singularity theorem, cfr. [Hör98, Sec. 8.3]. In particular, for the bulk-to-boundary map that we shall introduce below, this states that singular directions of a distribution in the bulk propagate along null curves. Therefore they reach $\mathcal{I}^+$ rather than i^+ .

We are now ready to introduce the algebra of boundary observables

Definition 2.41. Let $(\mathcal{M}, g)$ be a globally hyperbolic, as per Definition 2.6, and asymptotically flat spacetime as per Definition 2.8. Moreover, let us denote by $\mathcal{C} = \mathcal{I}^+ \cup \{i^+\}$ the conformal boundary of $\mathcal{M}$ and let $\mathcal{F}^n$, $n \in \mathbb{N}$, be the functional spaces introduced in Definition 2.40. We call **extended algebra of boundary observables** the unital $*$ -algebra, as per Definition B.2, $(\mathcal{A}_e(\mathcal{I}^+), *, \star_\omega)$. Here, the space $\mathcal{A}_e(\mathcal{I}^+)$ is

$$\mathcal{A}_e(\mathcal{I}^+) = \bigoplus_{n=0}^{\infty} \mathcal{F}_s^n, \quad \mathcal{F}^0 = \mathbb{C},$$

where $\mathcal{F}_s^n$ denotes the subset of $\mathcal{F}^n$ of symmetric distributions admitting only a finite number of terms are considered. Furthermore, the involution $*$ is defined as

$$F_n^*(f_1 \otimes \cdots \otimes f_n) = \overline{F_n(f_n \otimes \cdots \otimes f_1)}, \quad \forall f_1, \dots, f_n \in \mathcal{D}(\mathcal{I}^+), \forall F \in \mathcal{F}_s^n.$$

For every element $F \in \mathcal{A}_e(\mathcal{I}^+)$ we set

$$F(f) = \sum_{k=0}^N \frac{1}{k!} F_k(f^{\otimes k}), \quad F_k \in \mathcal{F}^k, f \in \mathcal{D}(\mathcal{I}^+).$$

The product $\star_\omega$ is defined as

$$(F \star_\omega G)(f) = \sum_{n=0}^{\infty} \frac{1}{n!} \langle F^{(n)}(f), \omega_{\mathcal{I}}^{\otimes n} G^{(n)}(f) \rangle, \quad \forall f \in \mathcal{D}(\mathcal{I}^+), \forall F, G \in \mathcal{A}_e(\mathcal{I}^+).$$

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Here the bidistribution $\omega_{\mathcal{J}} \in \mathcal{D}'(\mathcal{J}^+ \times \mathcal{J}^+)$ reads, at the level of integral kernel,

$$\omega_{\mathcal{J}}(u, u', s, s') = \lim_{\varepsilon \rightarrow 0^+} \frac{\delta(s, s')}{(u - u' - i\varepsilon)^2}, \quad s, s' \in \mathbb{S}^2, u, u' \in \mathbb{R},$$

where the limit $\lim_{\varepsilon \rightarrow 0^+}$ has to be taken in the topology of $\mathcal{D}'(\mathcal{J}^+ \times \mathcal{J}^+)$. Moreover, $F^{(n)}(f)$ denotes the Fréchet derivative of order n of the functional F .

Remark 2.28. The specific form of the integral kernel of $\omega_{\mathcal{J}}$ in Definition 2.41 is obtained by imposing BMS-invariance to the kinematical configurations on $\mathcal{J}^+$. Furthermore, its pullback under the bulk-to-boundary map we shall construct below yields a bidistribution which is of Hadamard form as per Definition 2.31. This result is of particular relevance since, given the uniqueness of $\omega_{\mathcal{J}}$, we obtain a way of selecting a distinguished Hadamard bidistribution H for the bulk theory. For a detailed analysis we refer to [DMP17, Sec. 4].

Note that the wavefront set condition in Definition 2.40 entails that the product in Definition 2.41 is well defined on account of Theorem A.4. For an explicit proof we refer to [DPP11, Prop. 3.5].

Additionally, note that if we had considered the algebra of local functionals as per Definition 2.18 on the manifold $\mathcal{J}^+$, the wavefront set condition would not be satisfied and therefore the product of the algebra would have been ill-defined.

Once the bulk and boundary algebra have been defined, we proceed by introducing the bulk-to-boundary map that defines the projection of observables from the bulk to $\mathcal{J}^+$.

Theorem 2.4. Let $(\mathcal{M}, g)$ be a globally hyperbolic, as per Definition 2.6, and asymptotically flat spacetime as per Definition 2.8. Moreover, let $\mathcal{C} = \mathcal{J}^+ \cup \{i^+\}$ denote the conformal boundary of $\mathcal{M}$. Additionally, let $\mathcal{A}_H(\mathcal{M})$ be the quantum microcausal algebra as per Definition 2.30 and let $\mathcal{A}_e(\mathcal{J}^+)$ be the extended boundary algebra as per Definition 2.41. Then, there exists a unit preserving $*$ -homomorphism between $\mathcal{A}_H(\mathcal{M})$ and $\mathcal{A}_e(\mathcal{J}^+)$

$$\Gamma : \mathcal{A}_H(\mathcal{M}) \rightarrow \mathcal{A}_e(\mathcal{J}^+).$$

Additionally, let S be the action of a massless, conformally coupled scalar field as introduced in Example 2.4 and let Δ_S be the associated causal propagator as per Definition 2.25. Then, if $\Omega \in \mathcal{E}(\widetilde{\mathcal{M}})$ denotes the conformal factor

while $\widetilde{\Delta}_S$ denotes the causal propagator for the Klein-Gordon action on $\widetilde{\mathcal{M}}$, it holds that

$$\Gamma(F) = \sum_{k=0}^N \frac{1}{k!} (\widetilde{\Delta}_S \Omega^{-3})^{\otimes k} (F_k) \big|_{\mathcal{J}^+} \in \mathcal{A}_e(\mathcal{J}^+). \quad (2.43)$$

Here $F_k \in \mathcal{E}'(\mathcal{M}^k)$ are the compactly supported distributions as per Definition A.2 introduced in Remark 2.6.

For a complete proof of this theorem we refer to [DPP11, Th. 3.1]. However, given the relevance of this result, we shall give here an outline of the procedure. Each term in Equation (2.43) has to be understood as the product of distributions

$$\iota^* \widetilde{\Delta}_S^{\otimes k} \cdot (1 \otimes (\Omega^{-3})^{\otimes k} F_k).$$

Here ι^* denotes the pullback of the causal propagator by means of the embedding $\iota : \mathcal{J}^+ \times \widetilde{\mathcal{M}} \hookrightarrow \widetilde{\mathcal{M}} \times \widetilde{\mathcal{M}}$, while 1 is the distribution generated by the constant function 1 on $(\mathcal{J}^+)^k$. The integral kernel of this expression reads

$$\widetilde{\Delta}_S(v_1, x_1) \Omega^{-3}(x_1) \dots \widetilde{\Delta}_S(v_k, x_k) \Omega^{-3}(x_k) F_k(x_1, \dots, x_k), \quad (2.44)$$

where $x_i \in \mathcal{M}, v_i \in \mathcal{J}^+, \forall i = 1 \dots, k$. We smear this distribution with $\psi \in \mathcal{E}(\mathcal{M}^k)$ such that $\psi|_{\text{supp}(F_k)} = 1$. Here $\text{supp}(F_k)$ is the support of the distribution F_k as per Definition A.1.

The proof consists in showing that the pullback of $\widetilde{\Delta}_S$ to the boundary and the product of distributions in Equation (2.44) is well-defined, as well as verifying that the resulting functional on $\mathcal{J}^+$ lies in the boundary algebra $\mathcal{A}_e(\mathcal{J}^+)$.

Let us start by discussing the restriction of the causal propagator $\widetilde{\Delta}_S$. Note that the set of normals of ι , as introduced in Theorem A.2, satisfies

$$N_\iota \subset \{(x_1, \xi_1; x_2, \xi_2) \in T^*(\widetilde{\mathcal{M}} \times \widetilde{\mathcal{M}}) \mid x_1 \in \mathcal{J}^+, \xi_1 = (\xi_1)_u du, (\xi_1)_u \in \mathbb{R}\},$$

and that, denoting the right-hand side by M_ι , $M_\iota \cap \text{WF}(\widetilde{\Delta}_S) = \emptyset$, see [DPP11, Th. 3.1]. Hence, we can apply Theorem A.2 in order restrict the causal propagator to a distribution on $\mathcal{J}^+ \times \widetilde{\mathcal{M}}$.

On account of Theorem A.3, it holds that

$$\text{WF}(1 \otimes (\Omega^{-3})^{\otimes k} F_k) \subset \{0\} \times \text{WF}(F_k), \quad (2.45)$$

where $\{0\}$ denotes the zero section in $T^*(\mathcal{J}^+)^k$. This is due to 1 being a distribution generated by a smooth function and, thus, $\text{WF}(1) = \emptyset$. Furthermore, since F_k is compactly supported in $\mathcal{M}^k$, it holds that

$$(\Omega^{-3})^{\otimes k} F_k = (\Omega^{-3})^{\otimes k} \eta F_k, \quad \eta \in \mathcal{D}(\mathcal{M}^k), \eta|_{\text{supp}(F_k)} = 1.$$

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Thus, since Ω is nowhere vanishing inside $\mathcal{M}$, the function $(\Omega^{-3})^{\otimes k} \eta$ is smooth, non-vanishing on the support of F_k and compactly supported. Therefore, it holds that

$$\text{WF}((\Omega^{-3})^{\otimes k} \eta F_k) = \text{WF}(F_k).$$

Thus, any element in $\text{WF}(1 \otimes (\Omega^{-3})^{\otimes k} F_k)$ is of the form

$$(v, 0; y, \beta) = (v_1, \dots, v_k, 0, \dots, 0; y_1, \dots, y_k, \beta_1, \dots, \beta_k),$$

where $(y_1, \dots, y_k, \beta_1, \dots, \beta_k) \in \text{WF}(F_k)$, $v_1, \dots, v_k \in \mathcal{I}^+$. Moreover, as shown in [DPP11, Th. 3.1], the wavefront set of the pullback via ι of the causal propagator reads

$$\text{WF}(\iota^* \widetilde{\Delta}_S) = \{(u, \xi; x, -\zeta) \in T^*(\mathcal{I}^+ \times M) \setminus \{0\} \mid (u, \xi) \sim (x, \zeta)\}, \quad (2.46)$$

where the relation $(u, \xi) \sim (x, \zeta)$ means that the points u and x are connected by a null geodesic γ , ζ is tangent to γ at x and ξ is the parallel transport of ζ along γ . We apply once more Theorem A.3 to infer that

$$\text{WF}\left((\iota^* \widetilde{\Delta})^{\otimes k}\right) \subset \text{WF}(\iota^* \widetilde{\Delta})^{\times k}. \quad (2.47)$$

Thus, any element of $\text{WF}\left((\iota^* \widetilde{\Delta})^{\otimes k}\right)$ is of the form

$$(u, \xi; x, \zeta) = (u_1, \dots, u_k, \xi_1, \dots, \xi_k; x_1, \dots, x_k, \zeta_1, \dots, \zeta_k),$$

where it holds that $(u_i, \xi_i) \sim (x_i, \zeta_i)$ for all $i = 1 \dots k$. Let us now consider $(u, \xi; x, \zeta) \in \text{WF}(\iota^* \widetilde{\Delta}_S^{\otimes k})$ and $(v, 0; y, \beta) \in \text{WF}(1 \otimes (\Omega^{-3})^{\otimes k} F_k)$ such that $u_i = v_i$, $x_i = y_i \forall i = 1, \dots, k$. Since the covectors $\xi_1, \dots, \xi_k$ are non-vanishing, being the parallel transport of $\zeta_1, \dots, \zeta_k$ and $\zeta_i \neq 0$ for all i , the sum $(\xi_1, \dots, \xi_k, \zeta_1, \dots, \zeta_k) + (0, \dots, 0, \beta_1, \dots, \beta_k)$ is non zero. Thus, $\{0\} \notin \text{WF}(\iota^* \widetilde{\Delta}^{\otimes k}) + \text{WF}(1^{\otimes k} \otimes F_k)$. The product is well defined on account of Theorem A.4. Moreover, the wavefront set of the distribution obtained by partial evaluation with the function ψ satisfies the wavefront set properties and smoothness condition in Definition 2.40.

Remark 2.29. *Let us consider the field observable $\Phi_f \in \mathcal{A}_{loc}(\mathcal{M})$, $f \in \mathcal{D}(\mathcal{M})$, as in Example 2.2. If we apply the map Γ introduced in Theorem 2.4, the projected functional $\Gamma(\Phi_f)$ reads*

$$\widetilde{\Delta}_S(\Omega^{-3} f)|_{\mathcal{I}^+},$$

where $\widetilde{\Delta}_S$ is the causal propagator of the unphysical spacetime $\widetilde{\mathcal{M}}$.

Chapter 3

Projection of massive scalar fields

The construction developed in Section 2.2.8 is restricted to a massless, conformally coupled scalar field theory. The goal of this chapter is to extend this construction to the case of a massive theory, focusing in particular on the analysis of the massive scalar field observable. Massive scalar fields play a central rôle in physically relevant models, most notably in the Higgs sector of the Standard Model. The Higgs mechanism is based on the spontaneous breaking of the electroweak symmetry, generating masses for the electroweak bosons and fermions. For a detailed analysis of the Higgs mechanism, we refer to [Hig64; EB64].

The main difficulty in treating massive fields lies in the fact that the conformal invariance of the equation of motion is lost and it appears a singular potential in the conformally transformed equation.

To address this issue, we employ the *Principle of perturbative agreement* which states that every quadratic mass term in the Lagrangian can be equivalently seen as either part of the free theory or as an interacting term. For a detailed overview of this topic, we refer to [DHP17]. By choosing to interpret the mass term as an interacting potential, we can apply the perturbative tools developed in Section 2.2.6 in order to represent the massive field observable as a formal power series in the coupling constant, which, in this context, is linked to the mass of the field. Once the perturbative series is obtained, it will be possible to define a projection map for the massive field observable to the future null infinity $\mathcal{I}^+$ similarly to what we did in Section 2.2.8 for the massless field.

Let us start by fixing the preliminary notations and conventions. We shall work on Minkowski spacetime $\mathbb{M}^4$ which, as shown in Section 2.1.2, is conformally embedded in the Einstein static universe $\mathcal{M}_{\text{esu}} \simeq \mathbb{R} \times \mathbb{S}^3$. The

conformal boundary can be decomposed as

$$\mathcal{C} = \mathcal{I}^+ \cup \mathcal{I}^- \cup i^+ \cup i^- \cup i_0.$$

Here $i^\pm$ represents future/past timelike infinity and i_0 represents spatial infinity. On the Einstein static universe, we choose the global coordinates $(\tau, \rho, \omega) \in \mathbb{R} \times [0, \pi] \times \mathbb{S}^2$, as defined in Section 2.1.2, so that the line element of the metric g_{esu} of $\mathcal{M}_{\text{esu}}$ reads

$$ds^2 = -d\tau^2 + d\rho^2 + \sin^2 \rho d\mathbb{S}^2(\omega).$$

Furthermore, on the Minkowski spacetime we consider the free theory induced by the generalised Lagrangian, as per Definition 2.20,

$$\mathcal{L}(\chi)(\phi) = -\frac{1}{2} \int_{\mathcal{M}} d^4x \chi(x) \eta^{\mu\nu}(x) \nabla_\mu \phi(x) \nabla_\nu \phi(x).$$

Here $\phi \in \mathcal{E}(\mathbb{M}^4)$, while $\chi \in \mathcal{D}(\mathbb{M}^4)$ is some smooth, compactly supported cutoff function.

The Cauchy problem associated to the equation of motion induced by this Lagrangian, as per Definition 2.23, reads

$$\begin{cases} P_0 \phi \doteq \square_\eta \phi = 0, \\ \phi|_\Sigma = \phi_0, \quad n^\mu \nabla_\mu \phi|_\Sigma = \phi_1, \quad (\phi_0, \phi_1) \in \mathcal{D}(\Sigma) \oplus \mathcal{D}(\Sigma) \end{cases} \quad (3.1)$$

Here $\square_\eta = \eta^{\mu\nu} \nabla_\mu \nabla_\nu$ is the d'Alembert operator built out of the Minkowski metric with signature $(-, +, +, +)$, Σ is any spacelike Cauchy surface as per Definition 2.6, while n^μ is the unit, outward-pointing normal vector to Σ .

If we apply the conformal embedding $\iota : \mathbb{M}^4 \hookrightarrow \mathcal{M}_{\text{esu}}$, the Cauchy problem becomes

$$\begin{cases} \tilde{P}_0 \Phi \doteq (\square_{g_{\text{esu}}} - 1) \Phi = 0, \\ \Phi|_{\Sigma'} = \Phi_0, \quad n^\mu \nabla_\mu \Phi|_{\Sigma'} = \Phi_1, \quad (\Phi_0, \Phi_1) \in \mathcal{D}(\Sigma') \oplus \mathcal{D}(\Sigma') \end{cases} \quad (3.2)$$

Here Σ' is any spacelike Cauchy hypersurface of $\mathcal{M}_{\text{esu}}$. This initial value problem in the literature is also known as the *conformal wave equation* given its conformal invariance.

Additionally, we shall denote by $\Delta^{A,R}$ the advanced and retarded Green operators, as per Definition 2.24, associated to P_0 and by $\tilde{\Delta}^{A/R}$ the ones associated with $\tilde{P}_0$, and similarly for the causal propagators, as per Definition 2.25, Δ_S and $\tilde{\Delta}_S$. On account of the principle of perturbative agreement, we consider the interacting theory with interacting potential

$$m^2 V(\phi) = -\frac{m^2}{2} \int_{\mathbb{M}^4} d\mu_x h(x) \phi^2(x), \quad h \in \mathcal{D}(\mathbb{M}^4), \phi \in \mathcal{E}(\mathbb{M}^4), m^2 > 0.$$

On account of the discussion in Section 2.2.6, the massive field observable is obtained by applying the classical retarded Møller map $\mathcal{R}_{m^2V}$ as per Definition 2.35 to the free observable $\Phi_f \in \mathcal{A}_{\text{loc}}(\mathbb{M}^4)$, $f \in \mathcal{D}(\mathbb{M}^4)$, as introduced in Example 2.2.

By definition, it holds that

$$\mathcal{R}_{m^2V}(\Phi_f)(\phi) = \Phi_f(r_{m^2V}(\phi)), \quad \forall \phi \in \mathcal{E}(\mathbb{M}^4),$$

where r_{m^2V} denotes the retarded Møller map acting on configurations as per Definition 2.34. On account of Remark 2.25, it holds that

$$r_{m^2V}(\phi) = \sum_{k=0}^{\infty} (m^2)^k (\Delta^R \circ h)^k(\phi),$$

where we used that the linear map induced by the first Fréchet derivative of the interacting potential as per Definition 2.14 reads $V^{(1)}(\psi)(x) = -h(x)\psi(x)$ for all $\psi \in \mathcal{E}(\mathbb{M}^4)$.

Hence, we obtain the following expansion

$$\mathcal{R}_{m^2V}(\Phi_f)(\phi) = \Phi_f \left(\sum_{k=0}^{\infty} (m^2)^k (\Delta^R \circ h)^k(\phi) \right),$$

where the series on the right-hand side, as we will later show, is convergent in the topology of smooth functions as per Definition 2.12. In order to express the functional itself as a formal power series, we observe that

$$\Phi_f((\Delta^R \circ h)\phi) = \langle f, \Delta^R(h\phi) \rangle = \langle h\Delta^A(f), \phi \rangle,$$

where $\langle \cdot, \cdot \rangle$ denotes the standard distributional pairing between $\mathcal{D}(\mathbb{M}^4) \hookrightarrow \mathcal{E}'(\mathbb{M}^4)$ and $\mathcal{E}(\mathbb{M}^4)$ as in Equation (2.18) and we used that the formal adjoint of the retarded Green operator with respect to that pairing is the advanced one. Here $\mathcal{E}'(\mathbb{M}^4)$ denotes the space of compactly supported distributions as per Definition A.2.

Furthermore, by induction, it holds that, for all $k > 1$,

$$\Phi_f((\Delta^R \circ h)^k(\phi)) = \langle f, (\Delta^R \circ h)^k(\phi) \rangle = \langle h(\Delta^A \circ h)^{k-1} \Delta^A(f), \phi \rangle.$$

Hence, we conclude that the massive field $\mathcal{R}_{m^2V}(\Phi_f)$ is the functional generated by the following formal series

$$\begin{aligned} \mathcal{R}_{m^2V}(\Phi_f) &= f + h \sum_{k=1}^{\infty} (m^2)^k (\Delta^A \circ h)^{k-1} \Delta^A(f) \\ &= f + m^2 h \sum_{n=0}^{\infty} (m^2)^n (\Delta^A \circ h)^n \Delta^A(f), \end{aligned} \tag{3.3}$$

where, with a slight abuse of notation, we identified the functional with the function that generates it. Note that the series in Equation (3.3) is formally equivalent to the Møller series in Remark 2.25 applied to the smooth function $\Delta^A(f)$, the only difference being the presence of the advanced Green operator in place of the retarded one. The following proposition proves that, on the Minkowski background, this is a convergent series.

Proposition 3.1. *Let $(\mathbb{M}^4, \eta)$ be the 4-dimensional Minkowski spacetime and let $P_0 = \square_\eta$ be the d’Alambert operator constructed out of η . Furthermore, let $\Delta^{A/R}$ be the advanced/retarded Green operator associated to P_0 as per Definition 2.24. Then, for any $h \in \mathcal{D}(\mathbb{M}^4)$ and $\phi \in \mathcal{E}(\mathbb{M}^4)$, the series*

$$\sum_{n=0}^{\infty} (\Delta^{A/R} \circ h)^n \phi, \quad (3.4)$$

is convergent in the topology of $\mathcal{E}(\mathbb{M}^4)$ as per Definition 2.12.

For a proof, we refer to [DHP17, Appendix B].

Once we have obtained an explicit form for the massive field observable in the Minkowski spacetime, we can proceed to the analysis of its projection to future null infinity $\mathcal{I}^+$. Let us rearrange the terms in Equation (3.3) as

$$\mathcal{R}_{m^2V}(\Phi_f) = \sum_{n=0}^{\infty} (m^2)^n (h \circ \Delta^A)^n(f). \quad (3.5)$$

Note that each term of the series is the functional generated by a smooth, compactly supported function in $\mathbb{M}^4$. Therefore, each term is a regular functional as per Definition 2.17 and thus lies in the free algebra $\mathcal{A}_{\text{loc}}(\mathbb{M}^4)$ as per Definition 2.32. On account of Theorem 2.4, we can therefore independently project each term of the series to the future null boundary and therefore obtain a series representing the asymptotic behaviour of the massive field observable. The main problem we have to face in this section is to determine whether the resulting boundary series is just a formal power series or it is converging. In the latter case, we can define the projected massive field observable as the functional in the boundary algebra $\mathcal{A}_e(\mathcal{I}^+)$ as per Definition 2.41 generated by a function on $\mathcal{I}^+$ which lies in a suitable functional space.

Let us start by writing the formal expression of the projected massive field observable obtained by applying to each term in the Møller series of Φ_f the map Γ introduced in Theorem 2.4

$$\Gamma(\mathcal{R}_{m^2V}\Phi_f) \doteq \sum_{n=0}^{\infty} (m^2)^n \widetilde{\Delta}_S (\Omega^{-3}(h \circ \Delta^A)^n(f)) \big|_{\mathcal{I}^+}. \quad (3.6)$$

Here $\widehat{\Delta}_S$ denotes the causal propagator as per Definition 2.25 of the operator $\widetilde{P}_0$.

Note that each term of the series can be decomposed as

$$\widetilde{\Delta}_S(\psi) = \widetilde{\Delta}_R(\psi) - \widetilde{\Delta}_A(\psi),$$

for a suitable smooth, compactly supported function $\psi \in \mathcal{D}(\mathbb{M}^4)$. On account of the support properties of the advanced and retarded Green operators in Definition 2.24, it holds that

$$\widetilde{\Delta}_A(\psi)|_{\mathcal{I}^+} = 0, \quad \forall \psi \in \mathcal{D}(\mathbb{M}^4).$$

Hence, we can equivalently write

$$\Gamma(\mathcal{R}_{m^2V}\Phi_f) = \sum_{n=0}^{\infty} (m^2)^n \widetilde{\Delta}_R(\Omega^{-3}(h \circ \Delta^A)^n(f))|_{\mathcal{I}^+}. \quad (3.7)$$

Here $\Omega \in \mathcal{E}(\mathcal{M}_{\text{esu}})$ is the conformal factor of the conformal embedding $\mathbb{M}^4 \hookrightarrow \mathcal{M}_{\text{esu}}$.

The crucial observation is that each term in Equation (3.7) is the restriction of a function that satisfies the following initial value problem in $\mathcal{M}_{\text{esu}}$

$$\begin{cases} \widetilde{P}_0 \widetilde{\Delta}_R(\psi) = \psi \\ \widetilde{\Delta}_R(\psi)|_{\mathcal{I}^-} = 0 \end{cases}. \quad (3.8)$$

This is an initial value problem with initial data assigned on a null hypersurface rather than a spacelike one and is therefore called *Goursat problem*.

We shall therefore apply suitable norm estimates derived from the analysis of the Goursat problem in the Einstein static universe in order to prove the convergence of the series in Equation (3.7). We shall here briefly outline the main definitions and results, referring to [BSZ90] for a complete overview of the Goursat problem in $\mathcal{M}_{\text{esu}}$.

Let us start by considering that, for any fixed $\tau \in \mathbb{R}$, the Cauchy hypersurface $\Sigma_\tau = \{\tau\} \times \mathbb{S}^3 \subset \mathcal{M}_{\text{esu}}$ is diffeomorphic to the 3-sphere $\mathbb{S}^3$. Therefore, the initial value problem in Equation (3.2) requires initial data to be assigned on a 3-sphere. We proceed by enlarging the space of initial data from that of smooth, compactly supported functions to a larger functional space that ensures that the resulting solution of the problem yields a finite energy, namely

$$H(S) = H^1(\mathbb{S}^3) \oplus L^2(\mathbb{S}^3), \quad (3.9)$$

which is the direct sum of the first Sobolev space and the L^2 space on $\mathbb{S}^3$. The space $H(S)$ is called the *finite-energy space*. This is an Hilbert space,

being the direct sum of two Hilbert spaces, whose scalar product is given by:

$$\langle \Phi_1 \oplus \Phi_2, \Psi_1 \oplus \Psi_2 \rangle_{H(S)} \doteq \langle \Phi_1, A\Psi_1 \rangle_{L^2(S)} + \langle \Phi_2, \Psi_2 \rangle_{L^2(S)}, \quad A = (-\Delta_{\mathbb{S}^3} + 1). \quad (3.10)$$

Here $\Delta_{\mathbb{S}^3}$ denotes the Laplacian operator on $\mathbb{S}^3$ while $\langle \cdot, \cdot \rangle_{L^2(S)}$ is the usual inner product in the space of square integrable functions on S . This product induces the following norm on $H(S)$

$$\|\Phi_1 \oplus \Phi_2\|_{H(S)} \doteq \left(\langle \Phi_1, A\Phi_1 \rangle_{L^2(S)} + \|\Phi_2\|_{L^2(S)}^2 \right)^{\frac{1}{2}}. \quad (3.11)$$

We now define the set of all finite-energy solutions for the massless equation of motion

Definition 3.1. *Let $(\mathcal{M}_{esu}, g_{esu})$ be the Einstein static universe introduced in Section 2.1.2 with global coordinates $(\tau, \rho, \omega) \in \mathbb{R} \times [0, \pi] \times \mathbb{S}^2$ and let $H(S)$ be the finite-energy space as per Equation (3.9). Then, we say that $\phi : \mathcal{M}_{esu} \rightarrow \mathbb{R}$ is a **finite-energy solution** of the conformal wave equation if*

$$\begin{cases} (\square_{g_{esu}} - 1)\phi = 0 \\ \phi(\tau, \cdot) \oplus \partial_\tau \phi(\tau, \cdot) \in H(S), \quad \tau \in \mathbb{R} \end{cases}.$$

We denote by H the space of finite-energy solutions. Furthermore, we define an inner product on H

$$\langle \phi, \psi \rangle_E = \langle \phi(\tau, \cdot) \oplus \partial_\tau \phi(\tau, \cdot), \psi(\tau, \cdot) \oplus \partial_\tau \psi(\tau, \cdot) \rangle_{H(S)}, \quad \forall \phi, \psi \in H, \tau \in \mathbb{R}.$$

This inner product induces a norm on H , called **energy norm**, as follows

$$\|\phi\|_E = \|\phi(\tau, \cdot) \oplus \partial_\tau \phi(\tau, \cdot)\|_{H(S)}, \quad \phi \in H.$$

Additionally, we denote by H_∞ the set of all $\phi \in H$ such that $\phi(\tau, \cdot) \oplus \partial_\tau \phi(\tau, \cdot) \in \mathcal{E}(S) \oplus \mathcal{E}(S)$ for some $\tau \in \mathbb{R}$.

Remark 3.1. *Although it may appear that the definition of the norm of finite-energy solutions is dependent of the choice of $\tau \in \mathbb{R}$, it can be proven that, for solutions of the conformal wave equation, $\|\phi\|_E$ is constant for all possible values of τ , see [BSZ90, Sec. 3].*

As already mentioned, we are interested in studying the initial value problem with initial data assigned on a lightcone, rather than constant Einstein-time surfaces. Lightcones in the Einstein static universe are identified by a real parameter $t \in \mathbb{R}$ and are defined in the following way

$$C_t = \{(\tau, \rho, \omega) \in \mathbb{R} \times [0, \pi] \times \mathbb{S}^2 \mid \tau \pm \rho = t \in \mathbb{R}\}. \quad (3.12)$$

Note that every lightcone $C_t \in \mathcal{M}_{\text{esu}}$ can be identified with $\mathbb{S}^3$. Our goal is to identify the equivalent initial value space for the Goursat problem to $H(S)$. To this end, we begin by showing that the energy norm, as per Definition 3.1, of a finite-energy solution ϕ can equivalently be characterised in terms of its restriction to a lightcone. We refer to [BSZ90, Proposition 4] for a proof of this result.

Proposition 3.2. *Let $(\mathcal{M}_{\text{esu}}, g_{\text{esu}})$ be the Einstein static universe introduced in Section 2.1.2 and let H_∞ be the set of all smooth, finite-energy solutions as per Definition 3.1. Furthermore, let $C_t \subset \mathcal{M}_{\text{esu}}$, $t \in \mathbb{R}$, be a lightcone as per Equation (3.12). Then, it holds that, for all $\phi, \psi \in H_\infty$,*

$$\langle \phi, \psi \rangle_E = \int_{C_t} d\mu_x \phi|_{C_t}(x) (-\Delta_{\mathbb{S}^3} + 1) \psi|_{C_t}(x) \quad (3.13)$$

Here $\langle \cdot, \cdot \rangle_E$ denotes the inner product in H as per Definition 3.1. Furthermore, $\phi|_{C_t}$ denotes the restriction to C_t of ϕ , while $\Delta_{\mathbb{S}^3}$ denotes the Laplace operator on $\mathbb{S}^3$. Here the integral is considered with respect to the standard volume measure of $\mathbb{S}^3$ denoted by $d\mu_x$.

A direct consequence of Proposition 3.2 is that, for any smooth, finite-energy solution $\phi \in H_\infty$, its restriction to any lightcone C_t , $t \in \mathbb{R}$, lies in the first order Sobolev space $H^1(C_t)$. This holds true on account of the fact that the right-hand side of Equation (3.13) is equivalent to the Sobolev norm on $\mathbb{S}^3$. Furthermore, since this map is isometric with respect to the respective inner products, it can be uniquely extended to a map

$$U : H \rightarrow H^1(C_t).$$

The following theorem makes this observation precise and shows that the inverse holds, namely, every function in $H^1(C_t)$ is the restriction to the lightcone of some finite-energy solution.

Proposition 3.3. *Let $(\mathcal{M}_{\text{esu}}, g_{\text{esu}})$ be the Einstein static universe and let H be the finite-energy solution space to the conformal wave equation as per Definition 3.1. Furthermore, let $H^1(C_t)$ denote the first-order Sobolev space on the lightcone C_t , $t \in \mathbb{R}$ as per Equation (3.12). Then the map*

$$U : H \rightarrow H^1(C)$$

$$\phi \mapsto \phi|_{C_t},$$

is an isometric bijection with respect to the inner products $\langle \cdot, \cdot \rangle_E$ as per Definition 3.1 and the inner product on $H^1(C)$ defined by the right-hand side of Equation (3.13).

For a proof of this result, we refer to [BSZ90, Prop. 5, Th. 8].

Remark 3.2. *Propositions 3.3 and 3.2 entail that, for any pair of functions $\Phi, \Psi \in H^1(C_t)$, the inner product defined on the right-hand side of Equation (3.13) between Φ and Ψ yields the same result as the inner product defined on H , as in Definition 3.1, between the corresponding finite-energy solutions. Hence, on account of this 1 to 1 correspondence, we shall equivalently use the symbol $\|\cdot\|_E$ to denote the induced norm both on H and on $H^1(C_t)$.*

On account of Proposition 3.3, we regard $H^1(C_t)$ as the natural functional space to assign initial data for the Goursat problem and, for this reason, in the following we shall refer to it also as the *space of Goursat data*.

The following result gives a norm estimate for the solutions to the Goursat problem that will allow us to prove the convergence of the series in Equation (3.7).

Lemma 3.1. *Let $(\mathcal{M}_{esu}, g_{esu})$ be the Einstein static universe and let $C_t, C_{t'}$, $t, t' \in \mathbb{R}$, $t' > t$, two lightcones. Additionally, let $D(t, t') \subset \mathcal{M}_{esu}$ denote the region bounded by C_t and $C_{t'}$. Let $f \in \mathcal{E}(\mathcal{M}_{esu})$ be a smooth function supported inside $D(t, t')$ and let $\Phi_0 \in H^1(C_t) \cap \mathcal{E}(C_t)$ be a smooth Goursat data. Then, there exists a unique smooth solution $\phi : \mathcal{M}_{esu} \rightarrow \mathbb{R}$ to the Goursat problem*

$$\begin{cases} (\square_{g_{esu}} - 1)\phi = f \\ \phi|_{C_t} = \Phi_0 \end{cases}. \quad (3.14)$$

Here, $\square_{g_{esu}} = g_{esu}^{\mu\nu} \nabla_\mu \nabla_\nu$ is the D'Alembert operator on the Einstein static universe. Moreover, it holds that

$$\|\phi|_{C_{t'}} - e^{(t'-t)L} \phi|_{C_t}\|_E \leq c((t' - t) + \pi)^{\frac{1}{2}} \|f\|_{L^2(\mathcal{M}_{esu})}, \quad c > 0.$$

Here $\|\cdot\|_E$ denotes the norm on $H^1(C_{t'})$ as per Remark 3.2, while $\|\cdot\|_{L^2(\mathcal{M}_{esu})}$ denotes the standard L^2 norm with respect to the metric induced measure in $\mathcal{M}_{esu}$. Furthermore, L is the closure in $H^1(C_t)$ of the operator

$$L_0 \Phi = \sin \rho \int_0^\rho \sin \rho' (-\Delta_{\mathbb{S}^3} + 1) \Phi \, d\rho', \quad \Phi \in H^1(C_t) \cap \mathcal{E}(C_t).$$

For a proof of this theorem, we refer to [BSZ90, Lemma 10].

We can now prove the main result of this section, namely, convergence of the series in Equation (3.7).

Proposition 3.4. *In the aforementioned setting, the series*

$$\Gamma(\mathcal{R}_{m^2V} \Phi_f) = \sum_{k=0}^{\infty} (m^2)^k \tilde{\Delta}^R \left(\Omega^{-3} (h \circ \Delta^A)^k (f) \right) |_{\mathcal{I}^+}, \quad (3.15)$$

is convergent in the topology induced by the energy norm in $H^1(C_\pi)$ as per Remark (3.2).

Proof. Let us start by observing that, on account of the discussion in Section 2.1.2, the conformal boundary of $\mathbb{M}^4$ with respect to the conformal embedding $\iota : \mathbb{M}^4 \rightarrow \mathcal{M}_{\text{esu}}$ is $\partial\mathbb{M}^4 = C_\pi \cup C_{-\pi}$. In particular, it holds that $\mathcal{I}^+ \subset C_\pi$. Additionally, in Minkowski spacetime, the retarded Green operator's integral kernel for a massless scalar theory is supported exclusively on lightlike-separated points, see [Sch89, Sec. 2.3]. As a consequence, since $\mathcal{I}^+$ is the accumulation set of all null geodesics in Minkowski spacetime, the function $\widetilde{\Delta}^R(\Omega^{-3}\chi) \in \mathcal{E}(\mathcal{M}_{\text{esu}})$ never reaches future timelike infinity i^+ for all $\chi \in \mathcal{D}(\mathbb{M}^4)$. Hence, it holds that

$$\widetilde{\Delta}^R(\Omega^{-3}\chi)|_{\mathcal{I}^+} = \widetilde{\Delta}^R(\Omega^{-3}\chi)|_{C_\pi}.$$

Additionally, it holds that $\widetilde{\Delta}^R(\Omega^{-3}\chi)|_{C_{-\pi}} = 0$ since the retarded Green operator propagates only in the causal future of $\text{supp}(\chi)$. Hence, by the definition of the retarded Green operator, it holds that

$$\begin{cases} (\square_{g_{\text{esu}}} - 1)\widetilde{\Delta}^R(\Omega^{-3}\chi) = \chi \\ \widetilde{\Delta}^R(\Omega^{-3}\chi)|_{C_{-\pi}} = 0 \end{cases}.$$

Therefore the k -th term of Equation (3.15) is the restriction of a smooth solution of the Goursat problem with smooth initial data on $C_{-\pi}$. Furthermore, the source is a compactly supported smooth function supported inside $\mathbb{M}^4$, which in turn is contained in the region bounded by C_π and $C_{-\pi}$. Therefore, on account of Lemma 3.1, it holds that

$$\|\widetilde{\Delta}^R(\Omega^{-3}(h \circ \Delta^A)^k(f))\|_{\mathcal{I}^+} \|_E \leq c\sqrt{2\pi} \|\Omega^{-3}(h \circ \Delta^A)^k(f)\|_{L^2(\mathcal{M}_{\text{ESU}}; d\mu_{\text{ESU}})}, \quad (3.16)$$

Here we have made the measure with respect to which we consider the L^2 norm explicit. Let now $K \subset \mathbb{M}^4$ be a compact set such that $\text{supp}(f), \text{supp}(h) \subset K$ and let us analyse the case $k = 0$ and $k > 0$ separately. By imposing $k = 0$ in Equation (3.16) we obtain

$$\begin{aligned} \|\Omega^{-3}f\|_{L^2(\mathcal{M}_{\text{esu}}; d\mu_{\text{esu}})} &= \left(\int_{\mathcal{M}_{\text{esu}}} d\mu_{\text{esu}} |\Omega^{-3}f|^2 \right)^{\frac{1}{2}} = \\ &= \left(\int_{\mathbb{M}^4} d^4x \, \Omega^4 \Omega^{-6} |f|^2 \right)^{\frac{1}{2}} \leq \|f\|_{L^\infty(K)} \|\Omega^{-1}\|_{L^2(K; d\mu_{\mathbb{M}^4})}. \end{aligned} \quad (3.17)$$

Here the second equality is obtained by changing the global coordinates $(\tau, \rho, \omega) \in \mathbb{R} \times [0, \pi] \times \mathbb{S}^2$ of the Einstein static universe with the standard cartesian coordinates on Minkowski spacetime. Note that the last term is finite since the function Ω is strictly positive on any compact set of $\mathbb{M}^4$ and f is a bounded function, being smooth and compactly supported.

Let now $k > 0$. By direct computation, it holds that

$$\begin{aligned} \|\Omega^{-3}(h \circ \Delta^A)^k(f)\|_{L^2(\mathcal{M}_{\text{esu}}; d\mu_{\text{esu}})} &= \left(\int_{\mathcal{M}_{\text{esu}}} d\mu_{\text{esu}} \Omega^{-6} |(h \circ \Delta^A)^k(f)|^2 \right)^{\frac{1}{2}} = \\ &= \left(\int_{\mathbb{M}^4} d^4x \Omega^4 \Omega^{-6} |(h \circ \Delta^A)^k(f)|^2 \right)^{\frac{1}{2}} \leq \\ &\leq \|(\Delta^A \circ h)^{k-1} \Delta^A(f)\|_{L^\infty(K)} \|\Omega^{-1}h\|_{L^2(K; d\mu_{\mathbb{M}^4})}. \end{aligned} \quad (3.18)$$

Therefore we obtain the following estimate for the boundary series:

$$\begin{aligned} \|\Gamma(\mathcal{R}_{m^2V}\Phi_f)\|_E &\leq c_0 \|f\|_{L^\infty(K)} + \sum_{k=1}^{\infty} c_k \|(\Delta^A \circ h)^{k-1} \Delta^A(f)\|_{L^\infty(K)}, \\ c_k &= (m^2)^k c \sqrt{2\pi} \max\{\|\Omega^{-1}h\|_{L^2(K; d\mu_{\mathbb{M}^4})}, \|\Omega^{-1}\|_{L^2(K; d\mu_{\mathbb{M}^4})}\}. \end{aligned} \quad (3.19)$$

Note that each term of the form $(\Delta^A \circ h)^{k-1} \Delta^A(f)$ is the term of order $k-1$ in the advanced Møller expansion of $a_{m^2V}(\Delta^A(f))$, where a_{m^2V} denotes the advanced Møller map on the space of configurations as per Definition 2.34 for a quadratic interacting potential. This follows on account of Remark 2.25 by exchanging the retarded with the advanced Møller map. Therefore, we shall now show that we can further estimate the uniform norm of this function on K to obtain the sought result. To this end, let us consider a compact set in $\mathbb{M}^4$ of the form $K' = [t_0, t_1] \times \Sigma$, where $t_0, t_1 \in \mathbb{R}$ and Σ is some compact spacelike hypersurface such that $K \subset K'$. Then, we define the following norm on the set of smooth, spacelike compact functions $\mathcal{E}_{\text{sc}}(\mathbb{M}^4)$:

$\|\widehat{\psi}\|_{1,\infty} = \sup_{t \in [t_0, t_1]} \|\widehat{\psi}(t, \cdot)\|_1$, where $\widehat{\cdot}$ denotes the Fourier transform with respect to the spatial coordinates and $\|\cdot\|_1$ denotes the $L^1(\mathbb{R}^3)$ norm. Note that this norm allows to estimate the uniform norm of ψ , namely,

$$\|\psi\|_{L^\infty(K)} \leq \|\widehat{\psi}\|_{1,\infty}.$$

This can be shown by writing

$$\psi(t, \mathbf{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} d^3\mathbf{k} \widehat{\psi}(t, \mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}},$$

on account of the properties of the Fourier transform, see [Hör98, Chap. 7].

It holds that

$$|\psi(t, \mathbf{x})| \leq \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} d^3\mathbf{k} |\widehat{\psi}(t, \mathbf{k})| = \|\widehat{\psi}(t, \cdot)\|_1, \quad \forall \mathbf{x} \in \mathbb{R}^3,$$

and taking the supremum over $\mathbf{x} \in \Sigma$ and $t \in [t_0, t_1]$ we obtain the desired estimate for the uniform norm of ψ .

In [DHP17, Appendix B] it is proved that the following chain of inequalities holds

$$\begin{aligned} \|(\Delta^A \circ h)^{k-1} \Delta^A(f)\|_{L^\infty(K)} &\leq \frac{1}{(2\pi)^{\frac{3}{2}}} \|(\Delta^A \circ h)^{k-1} \Delta^A(f)\|_{1,\infty} \\ &\leq b_{k-1} \frac{(t_1 - t_0)^{2(k-1)} \|\widehat{h}\|_{1,\infty}^{k-1}}{(k-1)!} \|\widehat{\Delta^A(f)}\|_{1,\infty}. \end{aligned} \quad (3.20)$$

Here $b_{k-1} > 0$ are constants arising from the normalisation of the Fourier transform.

Thus we conclude that

$$\|\Gamma(\mathcal{R}_{m^2V}\Phi_f)\|_E \leq c_0 \|f\|_{L^\infty(K)} + \sum_{k=1}^{\infty} c_k b_{k-1} \frac{(t_1 - t_0)^{2(k-1)} \|\widehat{h}\|_{1,\infty}^{(k-1)}}{(k-1)!} \|\widehat{\Delta^A(f)}\|_{1,\infty}. \quad (3.21)$$

This series is convergent since the constants b_{k-1} and c_k grow at most exponentially with k , and therefore are dominated by the factorial $(k-1)!$ in the denominator. $\square$

This result shows that the massive field observable $\mathcal{R}_{m^2V}\Phi_f$ can be projected, on the Minkowski background, to the future null infinity and that the projected observable is not merely a formal power series but it is convergent in the energy norm. Therefore, it defines a boundary observable in $\mathcal{A}_e(\mathcal{I}^+)$.

Remark 3.3. *Note that the estimate in Equation (3.21) fails if the infrared cutoff function h is replaced by the constant function 1 on $\mathbb{M}^4$. Thus, the procedure outlined in this chapter does not yield a projection of the massive field observable in the adiabatic limit $h \rightarrow 1$. However, information about the local behaviour of the theory can be obtained by setting the function h to be equal to 1 in some relatively compact set of Minkowski spacetime.*

Chapter 4

Projection of the Stress-Energy tensor

The goal of this chapter is to investigate how the bulk-to-boundary map introduced in Section 2.2.8 can be extended to the study of an interacting theory. The projection map Γ to $\mathcal{I}^+$ provides a useful tool for describing scattering processes on asymptotically flat spacetimes in a manifestly covariant way. In quantum field theory on Minkowski spacetime, scattering is usually formulated by assuming that interacting fields become asymptotically free at large times and by expressing interacting observables perturbatively in terms of the corresponding free theory. On a generic curved background, however, such a formulation is less natural, since it relies on the choice of a preferred time coordinate and therefore breaks manifest covariance of the theory. A more natural approach, from this perspective, consists in studying the asymptotic behaviour of physical observables as they approach future null infinity. Therefore, one follows the evolution of the system along causal directions without relying on a distinguished set of coordinates. As an application of this idea, in this chapter we compute the projection to $\mathcal{I}^+$ of the stress-energy tensor $T_{\mu\nu}$ in the presence of a quartic interaction in the bulk at first order in perturbation theory. The stress-energy tensor plays a pivotal rôle in the description of a physical theory, as it describes the distribution of energy and momentum of the field and it acts as the matter source in Einstein's field equations.

The starting point of our analysis is the perturbative construction of interacting observables in pAQFT. As discussed in Section 2.2.7, the Bogoliubov map $R_{\lambda V}$, as per Definition 2.39, associates with an observable of the free algebra $F \in \mathcal{A}_{\text{loc}}(\mathcal{M})$, as per Definition 2.32, a formal power series in the

coupling constant $\lambda \in \mathbb{R}$. Writing

$$R_{\lambda V}(F) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} R_n(V; F), \quad (4.1)$$

each coefficient $R_n(V; F)$ is an element of the free algebra and therefore, by Theorem 2.4, it admits a well-defined projection to $\mathcal{J}^+$. This suggests defining the projection of the observable order by order in perturbation theory:

$$\Gamma[R_{\lambda V}(F)] \doteq \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \Gamma[R_n(V; F)]. \quad (4.2)$$

The stress-energy tensor of any field theory can be explicitly computed from the underlying action, as per Definition 2.21. To start with, we consider the action for a massless, conformally coupled scalar field on a 4-dimensional globally hyperbolic, asymptotically flat spacetime $(\mathcal{M}, g)$, as per Definitions 2.6 and 2.8, which reads

$$S(\phi; g) = -\frac{1}{2} \int_{\mathcal{M}} d\mu_x f(x) \left[g^{\mu\nu} \nabla_{\mu} \phi \nabla_{\nu} \phi + \frac{R}{6} \phi^2 \right], \quad \phi \in \mathcal{E}(\mathcal{M}), f \in \mathcal{D}(\mathcal{M}). \quad (4.3)$$

Here $d\mu_x$ is the metric-induced volume form. Note that here we have made the dependence of the action on the metric explicit. The stress-energy tensor can be computed via the defining relation

$$T_{\mu\nu} = -\frac{2}{\sqrt{|g|}} \frac{\delta S}{\delta g^{\mu\nu}}, \quad (4.4)$$

where $|g|$ is the absolute value of the determinant of the metric and $\frac{\delta S}{\delta g^{\mu\nu}}$ denotes the Fréchet derivative of the action with respect to a variation in the metric, see Definition 2.14.

A direct computation yields, for all $\phi \in \mathcal{E}(\mathcal{M})$,

$$\begin{aligned} T_{\mu\nu, f}(\phi) &= \int_{\mathcal{M}} d\mu_x f(x) \left(\nabla_{\mu} \phi(x) \nabla_{\nu} \phi(x) - \frac{1}{2} g_{\mu\nu}(x) \nabla^{\sigma} \phi(x) \nabla_{\sigma} \phi(x) \right. \\ &\quad \left. + \frac{1}{6} [G_{\mu\nu} + g_{\mu\nu} \square - \nabla_{\mu} \nabla_{\nu}] \phi^2 \right), \end{aligned} \quad (4.5)$$

where $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R$ is the Einstein tensor while ∇_{μ} is the component of the Levi-Civita connection in an arbitrary but fixed coordinate chart of $\mathcal{M}$. From the definition of stress-energy tensor, two important properties arise, namely, it is divergence-free and, at least for the classical theory, traceless when evaluated at on-shell configurations. We state a proposition proving these properties. We refer to [Mor03, Sec. 2] for a proof and for an in-depth analysis of the stress-energy tensor.

Proposition 4.1. *Let $(\mathcal{M}, g)$ be a 4-dimensional globally hyperbolic spacetime as per Definition 2.6 and let us consider the action S , as per Definition 2.21, in Equation (4.3). Moreover, let $\mathcal{E}_S(\mathcal{M})$ denote the solution space of the equation of motion induced by S as per Definition 2.23. Additionally, let $T_{\mu\nu, f} \in \mathcal{F}_{loc}(\mathcal{M})$ be the stress-energy tensor as per Equation (4.5). Then, the following hold*

- *The stress-energy tensor is conserved on-shell, namely,*

$$\nabla^\mu T_{\mu\nu, f}(\phi) = 0, \quad \forall \phi \in \mathcal{E}_S(\mathcal{M}).$$

- *The stress-energy tensor is on-shell traceless, namely,*

$$T_f(\phi) \doteq g^{\mu\nu} T_{\mu\nu, f}(\phi) = 0 \quad \forall \phi \in \mathcal{E}_S(\mathcal{M}).$$

This proposition entails that we are free to add to the stress-energy tensor any term of the form

$$\eta(g_{\mu\nu}\Phi P_0\Phi)_f(\phi) = \eta \int_{\mathcal{M}} d\mu_x g_{\mu\nu}(x) f(x) \phi(x) P_0 \phi(x), \quad \eta \in \mathbb{R}, \quad (4.6)$$

where $P_0 = \square_g - \frac{R}{6}$ is the operator ruling the equation of motion of the free theory and $\phi \in \mathcal{E}(\mathcal{M})$. As a matter of fact, since every on-shell field satisfies the equation of motion

$$P_0 \phi = 0,$$

this additional contribution and its trace vanish for on-shell configurations and therefore leaves the stress-energy tensor conserved and traceless.

Even though in principle any real value of η is admissible, when we proceed to analyse the quantisation of the theory, we have to consider the effects of the normal ordering, as per Remark 2.20, on the stress-energy tensor. Heuristically, the Wick ordered observable $:T_{\mu\nu, f}:$ yields additional contributions linked to the contraction of the fields. These additional terms need to be neither conserved nor traceless. Therefore they give a possibly non-vanishing contribution to the divergence and to the trace of the stress-energy tensor even when considered on-shell. The next theorem shows that, for $\eta = \frac{1}{3}$, we recover the on-shell conservation of the stress-energy tensor also at the quantum level.

Theorem 4.1. *Let (M, g) be a 4-dimensional globally hyperbolic spacetime as per Definition 2.6 and let $H \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be a Hadamard parametrix as per Definition 2.31. Additionally, let $\mathcal{A}_{loc}(\mathcal{M})$ be the locally covariant algebra*

as per Definition 2.32 and let $\mathcal{A}_H(\mathcal{M})$ be the quantum microcausal algebra as per Definition 2.30. Moreover, let H_{0+} be the singular part of H and let

$$\alpha_{-H_{0+}} : \mathcal{A}_{loc}(\mathcal{M}) \rightarrow \mathcal{A}_H(\mathcal{M})$$

$$F \mapsto \alpha_{-H_{0+}}(F) \doteq :F:,$$

be the map that identifies the abstract Wick ordering as per Remark 2.20. Then, if $T_{\mu\nu,f} \in \mathcal{A}_{loc}(\mathcal{M})$ is the stress-energy tensor as per Equation (4.5) and

$$:T_{\mu\nu,f}^{(\eta)}: \doteq :T_{\mu\nu,f}: + \eta :g_{\mu\nu}(\Phi P_0 \Phi)_f:,$$

where the last term on the right-hand side is the normal-ordering of the functional in Equation (4.6), then it holds that

- $\nabla^\mu :T_{\mu\nu,f}^{(\frac{1}{3})}:(\phi) = 0$ for all $\phi \in \mathcal{E}_S(\mathcal{M})$ if and only if $\eta = \frac{1}{3}$. Here $\mathcal{E}_S(\mathcal{M})$ is the solution space of the equation of motion as per Definition 2.23.
- Let $x \in \mathcal{M}$ and let $\mathcal{O} \subset \mathcal{M}$ be a geodesically convex normal neighborhood of x . If $V_1 \in \mathcal{E}(\mathcal{O} \times \mathcal{O})$ denotes the Hadamard coefficient as per Equation (2.29), it holds that

$$g^{\mu\nu} :T_{\mu\nu,f}^{(\frac{1}{3})}:(\phi) = \frac{1}{4\pi^2} \int_{\mathcal{M}} d\mu_x f(x) V_1(x, x), \quad \forall \phi \in \mathcal{E}_S(\mathcal{M}).$$

For a proof of this theorem, we refer to [Mor03, Th. 3.2]. On account of the result above, in the following we shall work with the following form for the stress-energy tensor of the free theory

$$\begin{aligned} T_{\mu\nu,f} = & (\nabla_\mu \Phi \nabla_\nu \Phi)_f - \frac{1}{2} (g_{\mu\nu} \nabla^\sigma \Phi \nabla_\sigma \Phi)_f + \frac{1}{6} ([G_{\mu\nu} + g_{\mu\nu} \square - \nabla_\mu \nabla_\nu] \Phi^2)_f \\ & + \frac{1}{3} (g_{\mu\nu} \Phi P_0 \Phi)_f, \end{aligned} \quad (4.7)$$

where we see that each term is of the form

$$(K \Phi K' \Phi)_f(\phi) = \int_{\mathcal{M}} d\mu_x f(x) K \phi(x) K' \phi(x), \quad \forall \phi \in \mathcal{E}(\mathcal{M}). \quad (4.8)$$

for suitable differential operators K, K' of finite order. Furthermore, note that the following equalities hold

$$\square \phi^2 = g^{\mu\nu} \nabla_\mu \nabla_\nu \phi^2 = 2g^{\mu\nu} \nabla_\nu \phi \nabla_\mu \phi + 2\phi \square \phi,$$

$$\nabla_\mu \nabla_\nu \phi^2 = 2\nabla_\mu \phi \nabla_\nu \phi + 2\phi \nabla_\mu \nabla_\nu \phi.$$

Hence, we can rewrite the stress-energy tensor as

$$\begin{aligned}
T_{\mu\nu,f} = & (\nabla_\mu \Phi \nabla_\nu \Phi)_f - \frac{1}{2} (g_{\mu\nu} \nabla^\sigma \Phi \nabla_\sigma \Phi)_f \\
& + \frac{1}{6} ((G_{\mu\nu} \Phi^2)_f + 2(g_{\mu\nu} \nabla_\sigma \Phi \nabla^\sigma \Phi + g_{\mu\nu} \Phi \square \Phi)_f \\
& - 2(\nabla_\nu \Phi \nabla_\mu \Phi + \Phi \nabla_\mu \nabla_\nu \Phi)_f) + \frac{1}{3} (g_{\mu\nu} \Phi P_0 \Phi)_f.
\end{aligned} \tag{4.9}$$

By direct inspection of the integral kernel of the functionals in Equation (4.8), we conclude that it is indeed a local functional as per Definition 2.18 and therefore $T_{\mu\nu,f} \in \mathcal{F}_{\text{loc}}(\mathcal{M})$.

In order to compute the interacting corrections to the stress-energy tensor, we introduce an interaction potential $\lambda V_h \in \mathcal{F}_{\text{loc}}(\mathcal{M})$ of the form

$$\lambda V_h(\phi) = \frac{\lambda}{4!} \int_{\mathcal{M}} d\mu_x \phi^4(x) h(x), \quad h \in \mathcal{D}(\mathcal{M}). \tag{4.10}$$

On account of the discussion of Section 2.2.7, to compute the interacting stress-energy tensor, we apply the Bogoliubov map, as per Definition 2.39, which reads

$$R_{\lambda V_h}(T_{\mu\nu,f}) = S^{\star-1}(\lambda V_h) \star_H (S(\lambda V_h) \cdot_{\mathcal{T}} T_{\mu\nu,f}). \tag{4.11}$$

Here H denotes a Hadamard parametrix as per Definition 2.31, $\star_H$ denotes the deformed product as per Equation (2.22) while $\cdot_{\mathcal{T}}$ is the time-ordered product as per Definition 2.36. Moreover, $S(\lambda V_h)$ is the S-matrix, as per Definition 2.38, and $S^{\star-1}(\lambda V_h)$ is its inverse with respect to the product $\star_H$ as per Equation (2.41).

Note that here we have the time-ordered product between local functionals and therefore a renormalisation procedure has to be accounted for. By following the contents of Section 2.2.7, in the remainder of this chapter we will also assume that a suitable extension of the Feynman parametrix, as per Definition 2.37, and its powers to the thin diagonal of $\mathcal{M} \times \mathcal{M}$ has been selected.

The expansion of the S-matrix and its inverse yields, at first order in perturbation theory,

$$R_{\lambda V_h}(T_{\mu\nu,f})(\phi) = T_{\mu\nu,f}(\phi) + \frac{i\lambda}{\hbar} (V_h \cdot_{\mathcal{T}} T_{\mu\nu,f} - V_h \star_H T_{\mu\nu,f})(\phi) + \mathcal{O}(\lambda^2), \tag{4.12}$$

In order to compute the deformed product in the first-order correction of the interacting potential, the following lemma is useful.

Lemma 4.1. *Let $(\mathcal{M}, g)$ be 4-dimensional globally hyperbolic spacetime as per Definition 2.6 and let*

$$\begin{cases} K = a_0(x) \nabla_{\mu_1} \dots \nabla_{\mu_i}, & a_0 \in \mathcal{E}(\mathcal{M}) \\ K' = a_1(x) \nabla_{\nu_1} \dots \nabla_{\nu_j}, & a_1 \in \mathcal{E}(\mathcal{M}) \end{cases},$$

be two finite-order differential operators, where ∇_{μ_i} denotes the component in some coordinate chart of the Levi-Civita connection ∇ . Additionally, let $\mathcal{G} \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be a bidistribution as per Definition A.1 whose integral kernel is $\mathcal{G}(x, y)$ and let $\star_{\mathcal{G}}$ be the associated deformed product as per Equation (2.22). Furthermore, let $V_h \in \mathcal{F}_{loc}(\mathcal{M})$, $h \in \mathcal{D}(\mathcal{M})$, be the interaction potential as per Equation (4.10) and let $(K\Phi K'\Phi)_f$, $f \in \mathcal{D}(\mathcal{M})$, be the functional as per Equation (4.8). Then, it holds that, for all $\phi \in \mathcal{E}(\mathcal{M})$,

$$\begin{aligned} V_h \star_{\mathcal{G}} (K\Phi K'\Phi)_f(\phi) &= V_h(\phi) (K\Phi K'\Phi)_f(\phi) \\ &+ \frac{\hbar}{6} \int_{\mathcal{M}^2} d\mu_x d\mu_y h(x) f(y) \phi^3(x) [K\mathcal{G}(x, y) K'\phi(y) + K\phi(y) K'\mathcal{G}(x, y)] \\ &+ \frac{\hbar^2}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y h(x) f(y) \phi^2(x) K\mathcal{G}(x, y) K'\mathcal{G}(x, y). \end{aligned} \quad (4.13)$$

For a proof of this result we refer to [CDG25, Lemma 4.2].

On account of it, we can compute the time-ordered product and the $\star_H$ product between V_h and $T_{\mu\nu, f}$:

$$\begin{aligned} V_h \cdot_{\mathcal{T}} T_{\mu\nu, f}(\phi) &= V_h(\phi) T_{\mu\nu, f}(\phi) + \frac{\hbar}{6} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \phi^3(x) \\ &\left[\frac{2}{3} \nabla_{\mu}^{(y)} H_F(x, y) \nabla_{\nu} \phi(y) + \frac{2}{3} \nabla_{\nu}^{(y)} H_F(x, y) \nabla_{\mu} \phi(y) \right. \\ &\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_{\sigma}^{(y)} H_F(x, y) \nabla^{\sigma} \phi(y) - \frac{1}{6} g_{\mu\nu}(y) \nabla^{\sigma, (y)} H_F(x, y) \nabla_{\sigma} \phi(y) \\ &\quad + \frac{1}{3} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) H_F(x, y) \phi(y) + \frac{2}{3} \phi(y) \square^{(y)} H_F(x, y) \\ &\quad \left. + \frac{2}{3} g_{\mu\nu}(y) H_F(x, y) \square \phi(y) - \frac{1}{3} \phi(y) \nabla_{\nu}^{(y)} \nabla_{\mu}^{(y)} H_F(x, y) - \frac{1}{3} H_F(x, y) \nabla_{\nu} \nabla_{\mu} \phi(y) \right] \\ &+ \frac{\hbar^2}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \phi^2(x) \left[\frac{2}{3} \nabla_{\mu}^{(y)} H_F(x, y) \nabla_{\nu}^{(y)} H_F(x, y) \right. \\ &\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_{\sigma}^{(y)} H_F(x, y) \nabla^{\sigma, (y)} H_F(x, y) + \frac{1}{6} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) H_F^2(x, y) \\ &\quad \left. + \frac{2}{3} g_{\mu\nu}(y) H_F(x, y) \square^{(y)} H_F(x, y) - \frac{1}{3} H_F(x, y) \nabla_{\mu}^{(y)} \nabla_{\nu}^{(y)} H_F(x, y) \right], \end{aligned} \quad (4.14)$$

while the $\star$ -product yields

$$\begin{aligned}
V_h \star_H T_{\mu\nu,f}(\phi) &= V_h(\phi) T_{\mu\nu,f}(\phi) + \frac{\hbar}{6} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \phi^3(x) \\
&\left[\frac{2}{3} \nabla_\mu^{(y)} H(x, y) \nabla_\nu \phi(y) + \frac{2}{3} \nabla_\nu^{(y)} H(x, y) \nabla_\mu \phi(y) \right. \\
&\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H(x, y) \nabla^\sigma \phi(y) - \frac{1}{6} g_{\mu\nu}(y) \nabla^{\sigma,(y)} H(x, y) \nabla_\sigma \phi(y) \\
&\quad + \frac{1}{3} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) H(x, y) \phi(y) + \frac{2}{3} \phi(y) \square^{(y)} H(x, y) \\
&\quad \left. + \frac{2}{3} g_{\mu\nu}(y) H(x, y) \square \phi(y) - \frac{1}{3} \phi(y) \nabla_\nu^{(y)} \nabla_\mu^{(y)} H(x, y) - \frac{1}{3} H(x, y) \nabla_\nu \nabla_\mu \phi(y) \right] \\
&+ \frac{\hbar^2}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \phi^2(x) \left[\frac{2}{3} \nabla_\mu^{(y)} H(x, y) \nabla_\nu^{(y)} H(x, y) \right. \\
&\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H(x, y) \nabla^{\sigma,(y)} H(x, y) + \frac{1}{6} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) H^2(x, y) \\
&\quad \left. + \frac{2}{3} g_{\mu\nu}(y) H(x, y) \square^{(y)} H(x, y) - \frac{1}{3} H(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H(x, y) \right]. \tag{4.15}
\end{aligned}$$

In order to obtain the first-order correction of the stress-energy tensor we compute the difference $V_h \cdot_{\mathcal{T}} T_{\mu\nu,f} - V_h \star_H T_{\mu\nu,f}$. Note that the terms of order $\hbar^0$ cancel out. Additionally, all terms of order $\hbar$ in Equation (4.15) are formally equal to the ones in Equation (4.14), the only difference being the presence of the Hadamard parametrix H in place of the Feynman one H_F . Furthermore, the integrand in each expression is linear in H and H_F . Additionally, by definition of the Feynman parametrix, it holds that $H_F(x, y) - H(x, y) = i\Delta_A(x, y)$, where $\Delta_A(x, y)$ is the integral kernel of the advanced Green operator as per Definition 2.24. Thus, the resulting first-order correction to the stress-energy tensor reads

$$\begin{aligned}
\frac{i\lambda}{\hbar} (V_h \cdot_{\mathcal{T}} T_{\mu\nu,f} - V_h \star_H T_{\mu\nu,f})(\phi) &= -\frac{\lambda}{6} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \phi^3(x) \\
&\left[\frac{2}{3} \nabla_\mu^{(y)} \Delta_A(x, y) \nabla_\nu \phi(y) + \frac{2}{3} \nabla_\nu^{(y)} \Delta_A(x, y) \nabla_\mu \phi(y) \right. \\
&\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} \Delta_A(x, y) \nabla^\sigma \phi(y) - \frac{1}{6} g_{\mu\nu}(y) \nabla^{\sigma,(y)} \Delta_A(x, y) \nabla_\sigma \phi(y) \\
&\quad + \frac{1}{3} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) \Delta_A(x, y) \phi(y) + \frac{2}{3} \phi(y) \square^{(y)} \Delta_A(x, y) \\
&\quad \left. + \frac{2}{3} g_{\mu\nu}(y) \Delta_A(x, y) \square \phi(y) - \frac{1}{3} \phi(y) \nabla_\nu^{(y)} \nabla_\mu^{(y)} \Delta_A(x, y) - \frac{1}{3} \Delta_A(x, y) \nabla_\nu \nabla_\mu \phi(y) \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{i\hbar\lambda}{2} \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \phi^2(x) \left[\frac{2}{3} \nabla_\mu^{(y)} H_F(x, y) \nabla_\nu^{(y)} H_F(x, y) \right. \\
& - \frac{2}{3} \nabla_\mu^{(y)} H(x, y) \nabla_\nu^{(y)} H(x, y) - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H_F(x, y) \nabla^{\sigma, (y)} H_F(x, y) \\
& + \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H(x, y) \nabla^{\sigma, (y)} H(x, y) \\
& + \frac{1}{6} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) (H_F^2(x, y) - H^2(x, y)) \\
& + \frac{2}{3} g_{\mu\nu}(y) H_F(x, y) \square^{(y)} H_F(x, y) - \frac{2}{3} g_{\mu\nu}(y) H(x, y) \square^{(y)} H(x, y) \\
& \left. - \frac{1}{3} H_F(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H_F(x, y) + \frac{1}{3} H(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H(x, y) \right]. \quad (4.16)
\end{aligned}$$

We shall now proceed to compute the projection to $\mathcal{J}^+$ of the free stress-energy tensor and its first-order correction.

In order to compute explicitly the action of Γ on these terms, we need to express these functionals in terms of their integral kernel, on account of Remark 2.6. To this end, let us denote by $F_1, F_2 \in \mathcal{F}_{\mu c}(\mathcal{M})$ the functionals such that

$$\frac{i\lambda}{\hbar} (V_h \cdot_{\mathcal{T}} T_{\mu\nu, f} - V_h \star_H T_{\mu\nu, f})(\phi) = -\frac{\lambda}{6} F_1(\phi) + \frac{i\lambda\hbar}{2} F_2(\phi). \quad (4.17)$$

Starting from $T_{\mu\nu, f}$, as in Equation (4.9), its evaluation on $\phi \in \mathcal{E}(\mathcal{M})$ reads

$$\begin{aligned}
T_{\mu\nu, f}(\phi) &= \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) \delta(x, y) D_{\mu\nu'} \phi(x) \phi(y) \\
D_{\mu\nu'} &= \nabla_\mu^{(x)} \nabla_\nu^{(y)} - \frac{1}{2} g_{\mu\nu} \nabla_\sigma^{(x)} \nabla^{\sigma, (y)} + \frac{1}{6} (G_{\mu\nu} + 2g_{\mu\nu}(\square^{(x)} + \nabla_\sigma^{(x)} \nabla^{\sigma, (y)})) \\
&\quad - 2(\nabla_\mu^{(x)} \nabla_\nu^{(x)} + \nabla_\mu^{(x)} \nabla_\nu^{(y)}) + \frac{1}{3} g_{\mu\nu} P_0^{(x)}. \quad (4.18)
\end{aligned}$$

Here $\delta(x, y)$ is the integral kernel of the Dirac delta distribution supported on the diagonal of $\mathcal{M} \times \mathcal{M}$. Hence, the stress-energy tensor can be expressed as a compactly supported bidistribution whose integral kernel reads

$$T_{\mu\nu, f}(x, y) = D_{\mu\nu'}^* f(x) \delta(x, y),$$

where $D_{\mu\nu'}^*$ represents the formal adjoint of the operator $D_{\mu\nu'}$ in Equation (4.18) with respect to the dual pairing.

Similarly, the kernels of F_1 and F_2 are

$$\begin{aligned}
F_1(x_1, x_2, x_3, x_4) = & \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \delta(x, x_1) \delta(x, x_2) \delta(x, x_3) \\
& \left[-\frac{2}{3} \nabla_\mu^{(y)} \Delta_A(x, y) \nabla_\nu^{(y)} \delta(y, x_4) - \frac{2}{3} \nabla_\nu^{(y)} \Delta_A(x, y) \nabla_\mu^{(y)} \delta(y, x_4) \right. \\
& + \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} \Delta_A(x, y) \nabla^{\sigma, (y)} \delta(y, x_4) \\
& + \frac{1}{6} g_{\mu\nu}(y) \nabla^{\sigma, (y)} \Delta_A(x, y) \nabla_\sigma^{(y)} \delta(y, x_4) \\
& + \frac{1}{3} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) \Delta_A(x, y) \delta(y, x_4) \\
& + \frac{2}{3} g_{\mu\nu}(y) \delta(y, x_4) \square^{(y)} \Delta_A(x, y) \\
& + \frac{2}{3} g_{\mu\nu}(y) \Delta_A(x, y) \square^{(y)} \delta(y, x_4) - \frac{1}{3} \delta(y, x_4) \nabla_\nu^{(y)} \nabla_\mu^{(y)} \Delta_A(x, y) \\
& \left. - \frac{1}{3} \Delta_A(x, y) \nabla_\nu^{(y)} \nabla_\mu^{(y)} \delta(y, x_4) \right], \tag{4.19}
\end{aligned}$$

$$\begin{aligned}
F_2(x_1, x_2) = & \int_{\mathcal{M}^2} d\mu_x d\mu_y \delta(x, x_1) \delta(x, x_2) f(y) h(x) \\
& \left[\frac{2}{3} \nabla_\mu^{(y)} H_F(x, y) \nabla_\nu^{(y)} H_F(x, y) - \frac{2}{3} \nabla_\mu^{(y)} H(x, y) \nabla_\nu^{(y)} H(x, y) \right. \\
& - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H_F(x, y) \nabla^{\sigma, (y)} H_F(x, y) + \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H \nabla^{\sigma, (y)} H(x, y) \\
& + \frac{1}{6} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) (H_F^2(x, y) - H^2(x, y)) \\
& + \frac{2}{3} g_{\mu\nu}(y) H_F(x, y) \square^{(y)} H_F(x, y) - \frac{2}{3} g_{\mu\nu}(y) H(x, y) \square^{(y)} H(x, y) \\
& \left. - \frac{1}{3} H_F(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H_F(x, y) + \frac{1}{3} H(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H(x, y) \right]. \tag{4.20}
\end{aligned}$$

On account of Theorem 2.4, each of these functionals can be projected to $\mathcal{I}^+$ as follows. Following the definition of asymptotically flat spacetime in Section 2.1.2, let us consider the unphysical spacetime $(\widetilde{\mathcal{M}}, \widetilde{g})$ and let $\widetilde{\Delta}_S$ be the causal propagator, as per Definition 2.25, for the massless, conformally coupled Klein-Gordon operator $\widetilde{P}_0 \doteq \widetilde{g}^{\mu\nu} \widetilde{\nabla}_\mu \widetilde{\nabla}_\nu - \frac{\widetilde{R}}{6}$. Here $\widetilde{\nabla}_\mu$ denotes the component, in an arbitrary but fixed coordinate chart, of the Levi-Civita connection on $\widetilde{\mathcal{M}}$. Furthermore, we denote by $\iota^* \widetilde{\Delta}_S$ the pullback of the causal propagator induced by the map $\iota : \mathcal{I}^+ \times \widetilde{\mathcal{M}} \rightarrow \widetilde{\mathcal{M}} \times \widetilde{\mathcal{M}}$ and let

$\Omega \in \mathcal{E}(\widetilde{\mathcal{M}})$ be the conformal factor of the transformation. The projection to $\mathcal{I}^+$ is given by the following multiplication of distributions

$$\Gamma[F_k] = (\iota^* \widetilde{\Delta}_S)^{\otimes k} \cdot (1 \otimes (\Omega^{-3})^{\otimes k} F_k), \quad F_k \in \mathcal{E}'(\widetilde{\mathcal{M}}^k),$$

where $1 \in \mathcal{D}'((\mathcal{I}^+)^k)$ is the distribution generated by the constant function 1. We smear the resulting functional with a smooth, compactly supported function $\eta \in \mathcal{D}(\widetilde{\mathcal{M}}^k)$ such that $\eta|_{\text{supp}(F_k)} \equiv 1$, where $\text{supp}(F_k)$ denotes the support of F_k as per Definition A.1. Let us work at the level of integral kernels for the projected functionals and let $u_1, \dots, u_4 \in \mathcal{I}^+$.

The projection of the free stress-energy tensor reads

$$\begin{aligned} \Gamma[T_{\mu\nu,f}](u_1, u_2) &= \\ &= \int_{\mathcal{M}^2} d\mu_x d\mu_y \widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x) \widetilde{\Delta}_S(u_2, y) \Omega^{-3}(y) D_{\mu\nu}^* f(x) \delta(x, y) = \\ &= \int_{\mathcal{M}^2} d\mu_x d\mu_y f(x) \delta(x, y) D_{\mu\nu}(\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x) \widetilde{\Delta}_S(u_2, y) \Omega^{-3}(y)) = \\ &= \int_{\mathcal{M}} d\mu_x f(x) \frac{1}{2} (\nabla_\mu^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \nabla_\nu^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \\ &\quad + \nabla_\nu^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \nabla_\mu^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x))) \\ &\quad - \frac{1}{2} g_{\mu\nu}(x) (\nabla^{\sigma,(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \nabla_\sigma^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x))) \\ &\quad + \frac{1}{6} \left[(G_{\mu\nu}(x) - \frac{R(x)}{3} g_{\mu\nu}(x)) \widetilde{\Delta}_S(u_1, x) \widetilde{\Delta}_S(u_2, x) \Omega^{-6}(x) \right. \\ &\quad + 2g_{\mu\nu}(x) \nabla_\sigma^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \nabla^{\sigma,(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \\ &\quad + 2g_{\mu\nu}(x) (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \square^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \\ &\quad + 2g_{\mu\nu}(x) (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \square^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \\ &\quad - (\nabla_\mu^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \nabla_\nu^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \\ &\quad + (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \nabla_\mu^{(x)} \nabla_\nu^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \\ &\quad + \nabla_\mu^{(x)} (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \nabla_\nu^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \\ &\quad \left. + (\widetilde{\Delta}_S(u_2, x) \Omega^{-3}(x)) \nabla_\mu^{(x)} \nabla_\nu^{(x)} (\widetilde{\Delta}_S(u_1, x) \Omega^{-3}(x)) \right]. \end{aligned} \quad (4.21)$$

Remark 4.1. *Note that, even though the bulk stress-energy tensor is a local functional, as per Definition 2.18, its projection to $\mathcal{I}^+$ also has support outside the thin diagonal of $\mathcal{I}^+ \times \mathcal{I}^+$. This explains why the boundary algebra $\mathcal{A}_e(\mathcal{I}^+)$ in Definition 2.41 cannot be identified with that of local functionals on $\mathcal{I}^+$.*

If we proceed by computing the projection of the first-order correction terms F_1 and F_2 we obtain, by a direct computation

$$\begin{aligned}
\Gamma[F_1](u_1, u_2, u_3, u_4) &= \\
&= \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \widetilde{\Delta}_S(u_1, x) \widetilde{\Delta}_S(u_2, x) \widetilde{\Delta}_S(u_3, x) \Omega^{-9}(x) \\
&\quad \left[\frac{2}{3} \nabla_\mu^{(y)} \Delta_A(x, y) \nabla_\nu^{(y)} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \right. \\
&\quad + \frac{2}{3} \nabla_\nu^{(y)} \Delta_A(x, y) \nabla_\mu^{(y)} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \\
&\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} \Delta_A(x, y) \nabla^{\sigma, (y)} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \\
&\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla^{\sigma, (y)} \Delta_A(x, y) \nabla_\sigma^{(y)} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \\
&\quad + \frac{1}{3} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) \Delta_A(x, y) (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \\
&\quad + \frac{2}{3} g_{\mu\nu}(y) (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \square^{(y)} \Delta_A(x, y) \\
&\quad + \frac{2}{3} g_{\mu\nu}(y) \Delta_A(x, y) \square^{(y)} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \\
&\quad - \frac{1}{3} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \nabla_\nu^{(y)} \nabla_\mu^{(y)} \Delta_A(x, y) \\
&\quad \left. - \frac{1}{3} \Delta_A(x, y) \nabla_\nu^{(y)} \nabla_\mu^{(y)} (\widetilde{\Delta}_S(u_4, y) \Omega^{-3}(y)) \right]. \tag{4.22}
\end{aligned}$$

$$\begin{aligned}
\Gamma[F_2](u_1, u_2) &= \\
&= \int_{\mathcal{M}^2} d\mu_x d\mu_y f(y) h(x) \widetilde{\Delta}_S(u_1, x) \widetilde{\Delta}_S(u_2, x) \Omega^{-6}(x) \\
&\quad \left[\frac{2}{3} \nabla_\mu^{(y)} H_F(x, y) \nabla_\nu^{(y)} H_F(x, y) - \frac{2}{3} \nabla_\mu^{(y)} H(x, y) \nabla_\nu^{(y)} H(x, y) \right. \\
&\quad - \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H_F(x, y) \nabla^{\sigma, (y)} H_F(x, y) + \frac{1}{6} g_{\mu\nu}(y) \nabla_\sigma^{(y)} H \nabla^{\sigma, (y)} H(x, y) \\
&\quad + \frac{1}{6} \left(G_{\mu\nu}(y) - g_{\mu\nu}(y) \frac{R(y)}{3} \right) (H_F^2(x, y) - H^2(x, y)) \\
&\quad + \frac{2}{3} g_{\mu\nu}(y) H_F(x, y) \square^{(y)} H_F(x, y) - \frac{2}{3} g_{\mu\nu}(y) H(x, y) \square^{(y)} H(x, y) \\
&\quad \left. - \frac{1}{3} H_F(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H_F(x, y) + \frac{1}{3} H(x, y) \nabla_\mu^{(y)} \nabla_\nu^{(y)} H(x, y) \right]. \tag{4.23}
\end{aligned}$$

The results obtained in this chapter provide a concrete realization of how bulk interactions affect the asymptotic behaviour of physical observables. In particular, Equation (4.21) describes the asymptotic energy-momentum content of the field as it reaches future null infinity $\mathcal{I}^+$, while the additional contributions in Equations (4.22) and (4.23) encode the effect of a quartic bulk interaction on this asymptotic behaviour. More specifically, the contribution associated with F_1 represents the classical first-order correction induced by the interaction, whereas the F_2 term represents a genuinely quantum contribution, arising from the difference between the time-ordered and Hadamard products. Thus, already at first order in perturbation theory, the asymptotic observable retains information both about the classical interacting dynamics in the bulk and about the corresponding quantum fluctuations.

Beyond the explicit form of the projected observables, an important feature of the construction is the loss of locality under the bulk-to-boundary map. Although the original bulk observables are local, their images at null infinity are, in general, non-local. This behaviour is intrinsic to the definition of the map Γ , which propagates bulk information to the asymptotic boundary through the causal dynamics of the theory. In this respect, the construction may be regarded as a null-boundary counterpart of the *time-slice axiom*, as discussed in [DMP17, Sec. 5], which states that the algebra associated with a globally hyperbolic region containing a Cauchy surface is $*$ -isomorphic to the algebra of the full spacetime, even though such an isomorphism need not preserve the localization properties of the observables. For a detailed discussion of the time-slice axiom, we refer to [CF09].

In this sense, the calculations presented in this chapter illustrate how the algebraic description at null infinity can retain non-trivial information about interacting quantum dynamics in the bulk, thereby providing a first perturbative bridge between local quantum field theory in the interior and its asymptotic description at $\mathcal{I}^+$. The same strategy can, in principle, be applied order by order in perturbation theory and extended to different interaction potentials.

Chapter 5

Conclusion and Results

In this thesis, we investigated two perturbative extensions of the bulk-to-boundary correspondence for massless, conformally coupled scalar fields developed in [DMP06; DMP17] within the pAQFT framework. The first concerns the projection of the massive field observable, while the second addresses the asymptotic behaviour of interacting quantum observables. In both cases, our strategy was to use the perturbative tools of pAQFT to express the observables as formal power series in terms of observables of the free theory, for which a well-established bulk-to-boundary map is available.

For the massive case, we applied the principle of perturbative agreement, which allowed us to treat the mass term as a quadratic interaction of the massless theory. The retarded Møller map introduced in Section 2.2.6 yields a formal power series expansion in m^2 of the massive field observable. Each coefficient belongs to the algebra of the massless theory and it can therefore be projected to future null infinity. Specialising to Minkowski spacetime, energy estimates for the Goursat problem showed that the boundary series is convergent in the relevant energy space in the presence of a compactly supported infrared cutoff. This establishes a well-defined boundary projection for the massive field observable within this setting.

For an interacting theory, we composed the Bogoliubov map presented in Section 2.2.7 with the bulk-to-boundary map of the free theory introduced in Section 2.2.8 to obtain a perturbative expression for asymptotic observables. As an application, we considered a scalar theory with a quartic interaction potential and computed the projection at first order in the coupling constant λ of the stress-energy tensor. The resulting boundary observable separates into the free contribution, a classical first-order correction and a quantum correction. A notable feature of the bulk-to-boundary projection is the loss of locality: local observables in the bulk are generally projected to nonlocal boundary observables.

A possible further development of this work is a detailed analysis of the adiabatic limit for the massive case. Indeed, the estimate used in Chapter 3 to establish convergence of the boundary series does not extend to the adiabatic limit $\hbar \rightarrow 1$. Thus, a further analysis is required in order to obtain a global bulk-to-boundary construction for the massive theory in the absence of an infrared cutoff.

A further extension of this work concerns the analysis of a bulk-to-boundary correspondence for higher-spin fields. As a matter of fact, the formalism of pAQFT can be used to study also fermionic and gauge theories, *cfr.* [Rej16]. In this case, a direct counterpart of the deformed and time-ordered products is defined and a new set of parametrices, corresponding to the Hadamard and Feynman ones, needs to be introduced. A key element in the definition of the bulk-to-boundary correspondence was the conformal invariance of the equation of motion of the underlying free theory. Hence, in order to extend this framework to higher-spin fields, a systematic analysis of the conformal properties of the operator ruling the field dynamics and, if applicable, of their Green operators is required.

Finally, a further development concerns the analysis of the interplay between the bulk-to-boundary correspondence, the BMS group and the infrared structure of the theory. Since asymptotically flat spacetimes are naturally endowed with a set of asymptotic symmetries, one can associate suitable asymptotic charges with these symmetries. It would then be interesting to investigate the corresponding conservation laws for the boundary theory obtained via bulk-to-boundary correspondence and to determine whether information about the bulk dynamics is retained. These effects are deeply linked with the analysis of the infrared sectors of field theories and memory effects in gravitational scattering [Str14; SZ14; FPT26].

Appendix A

Theory of distributions

A.1 Microlocal analysis

Here we outline the basic definitions and results concerning the theory of distributions and microlocal analysis. We shall only present the tools we need here, and we refer to [Hör98] for a complete overview.

Definition A.1. Let $\Omega \subset \mathbb{R}^n$ be an open set and let $\mathcal{D}(\Omega)$ denote the space of compactly supported, smooth functions over Ω . We call the space of **distributions** the set of all sequentially continuous linear maps

$$u : \mathcal{D}(\Omega) \rightarrow \mathbb{C}.$$

That is, for every sequence $\{f_j\}_{j \in \mathbb{N}} \subset \mathcal{D}(\Omega)$ such that $f_j \rightarrow f \in \mathcal{D}(\Omega)$ in the topology of Definition 2.13, it holds that $u(f_j) \rightarrow u(f)$ in $\mathbb{C}$. We denote the space of distributions by $\mathcal{D}'(\Omega)$. We define the **support** of $u \in \mathcal{D}'(\Omega)$ as

$$\text{supp}(u) = \{x \in \Omega \mid \forall U \ni x, U \subset \Omega \text{ open } \exists f \in \mathcal{D}(\Omega), \text{supp}(f) \subset U, u(f) \neq 0\}.$$

Moreover, we define the **singular support** of u as

$$\text{sing supp}(u) = \Omega \setminus \{x \in \Omega \mid \exists U \subset \Omega \text{ open neighborhood of } x \text{ so that } u|_U \in \mathcal{E}(U)\}.$$

Remark A.1. Since we need to work on smooth manifolds, we need to generalise Definition A.1 to this case. The idea is that every smooth manifold is locally diffeomorphic to $\mathbb{R}^n$ and we can therefore define distributions locally on open coordinate charts and then glue them together by means of a partition of unity subordinated to the cover. More precisely, let us consider a manifold $\mathcal{M}$ and an atlas $(U_\alpha, \psi_\alpha)_{\alpha \in A}$, where A is some countable index set. Moreover, let $\{\rho_\alpha\}_{\alpha \in A}$ be a smooth partition of unity subordinated to that cover. Then,

a map $u : \mathcal{D}(\mathcal{M}) \rightarrow \mathbb{C}$ is said to be a distribution if there exists a collection of distributions $u_\alpha \in \mathcal{D}'(\psi_\alpha(U_\alpha))$ defined as above such that

$$u(f) = \sum_{\alpha \in A} u_\alpha(\rho_\alpha f \circ \psi_\alpha^{-1}), \quad f \in \mathcal{D}(\mathcal{M}).$$

For our purposes, it is necessary to enlarge the set of test functions to include field configurations, which need not be compactly supported. For this reason, we introduce the space of compactly supported distributions.

Definition A.2. Let $\Omega \subset \mathbb{R}^n$ be an open set and let $\mathcal{E}(\Omega)$ denote the space of real-valued, smooth functions over Ω . We call the space of **compactly supported distributions** the subset of $\mathcal{D}'(\Omega)$ consisting of all sequentially continuous linear maps

$$u : \mathcal{E}(\Omega) \rightarrow \mathbb{C},$$

with respect to the topology of $\mathcal{E}(\Omega)$ as per Definition 2.12. We denote the space of compactly supported distributions by $\mathcal{E}'(\Omega)$.

Moreover, we generalize this definition for a manifold $\mathcal{M}$ analogously to Remark A.1.

As a first result of the theory of distributions, we start by outlining the Schwartz kernel theorem, which is at the core of most of the calculations of this work.

Theorem A.1. Let $\Omega \subset \mathbb{R}^n$ and $\Omega' \subset \mathbb{R}^m$ be two open sets. Then there exists a 1:1 correspondence between the set of continuous linear operators $K : \mathcal{D}(\Omega) \rightarrow \mathcal{D}'(\Omega')$ and bi-distributions $\mathcal{K} \in \mathcal{D}'(\Omega \times \Omega')$ as per Definition A.1 such that

$$(K(f))(g) = \mathcal{K}(f \otimes g), \quad f \in \mathcal{D}(\Omega), g \in \mathcal{D}(\Omega').$$

For a proof, we refer to [Hör98, Th. 5.2.1].

Remark A.2. In the following, we shall adopt the useful notation for the kernel of the map K in Theorem A.1.

$$\mathcal{K}(f \otimes g) = \int_{\Omega \times \Omega'} d\mu_x d\mu_y f(x)g(y)\mathcal{K}(x, y), \quad f \in \mathcal{D}(\Omega), g \in \mathcal{D}(\Omega').$$

We emphasize, however, that the term $\mathcal{K}(x, y)$ called the **integral kernel**, need not be a well-defined function and therefore this has to be interpreted as a formal expression.

The wavefront set of a distribution, which we shall now define, identifies precisely where a distribution is singular and in which cotangent directions those singularities propagate. This allows us to study their singular behaviour and will play a pivotal rôle in the definition of the product of distributions.

Definition A.3. Let $\Omega \subset \mathbb{R}^n$ be an open set and let $\mathcal{D}'(\Omega)$ denote the space of distributions as per Definition A.1. We say that $(x_0, k_0) \in \Omega \times (\mathbb{R}^n \setminus \{0\})$ is a **regular directed point** if there exists $f \in \mathcal{D}(\Omega)$, $f(x_0) \neq 0$ such that, for all $n \in \mathbb{N}_0$ and for all k in an open conic neighborhood $V \subset \mathbb{R}^n \setminus \{0\}$ of k_0 , there exists a constant $C_n > 0$ satisfying:

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

Here $\widehat{fu}$ denotes the Fourier transform of the compactly supported distribution fu .

We define the **wavefront set** of u as the complement in $\Omega \times (\mathbb{R}^n \setminus \{0\})$ of the set of all regular directions.

The wavefront set enjoys several analytical properties. Here we recall the ones that will be relevant for our purposes.

Proposition A.1. Let $\Omega \subset \mathbb{R}^n$ be an open set and let $u \in \mathcal{D}'(\Omega)$ be a distribution as per Definition A.1. Moreover, let $\text{WF}(u)$ denote the wavefront set of u as per Definition A.3. Then, $\pi(\text{WF}(u)) = \text{sing supp}(u)$, where π is the projection to the first entry in $\Omega \times (\mathbb{R}^n \setminus \{0\})$ and $\text{sing supp}(u)$ denotes the singular support of u as per Definition A.1.

For a proof we refer to [Tay81, Prop. 1.1].

Remark A.3. Proposition A.1 entails that a distribution has empty wavefront set if and only if it is the linear functional generated by a smooth function.

Proposition A.2. Let $\Omega \subset \mathbb{R}^n$ be an open set and let $u \in \mathcal{D}'(\Omega)$ be a distribution as per Definition A.1. Moreover, let $P = \sum_{|\alpha| \leq m} c_\alpha \partial^\alpha$, $m \in \mathbb{N}$, $\alpha \in \mathbb{N}_0^n$ be a differential operator with smooth coefficients $c_\alpha \in C^\infty(\Omega)$. Then, it holds that

$$\text{WF}(Pu) \subseteq \text{WF}(u).$$

Here $\text{WF}(u)$ denotes the wavefront set of u as per Definition A.3.

For a proof, see [Tay81, Th. 1.6].

Theorem A.2. *Let $\Omega \subset \mathbb{R}^n$ and $U \subset \mathbb{R}^m$ be two open sets and let $\psi : U \rightarrow \Omega$ be a smooth map. We define the set of normals of ψ as*

$$N_\psi = \{(\psi(x), \xi) \in \Omega \times \mathbb{R}^n \setminus \{0\}, x \in U \mid {}^t\psi'(x)\xi = 0\}.$$

*Here ${}^t\psi'$ denotes the transpose of the Jacobian matrix of ψ at x . For any distribution $u \in \mathcal{D}'(\Omega)$ as per Definition A.1, the pullback $\psi^*u \doteq u \circ \psi$ can be uniquely defined as a distribution in $\mathcal{D}'(U)$ provided that $N_\psi \cap \text{WF}(u) = \emptyset$. Furthermore, denoting by $\text{WF}(u)$ the wavefront set of u as per Definition A.3, it holds that*

$$\text{WF}(\psi^*u) \subseteq \psi^* \text{WF}(u) = \{(\psi(x), {}^t\psi'(x)\xi) \in U \times \mathbb{R}^m \mid (x, \xi) \in \text{WF}(u)\}.$$

If $n = m$ and ψ is a diffeomorphism, then the inclusion becomes an equality.

For a proof, see [Hör98, Th. 8.2.4].

Theorem A.3. *Let $\Omega \subset \mathbb{R}^n$ and $\Omega' \subset \mathbb{R}^m$ be two open sets. For any two distributions $u \in \mathcal{D}'(\Omega)$ and $v \in \mathcal{D}'(\Omega')$ as per Definition A.1 it holds that*

$$\begin{aligned} \text{WF}(u \otimes v) \subseteq & (\text{WF}(u) \times \text{WF}(v)) \cup (\text{WF}(u) \times (\text{supp}(v) \times \{0\})) \cup \\ & ((\text{supp}(u) \times \{0\}) \times \text{WF}(v)). \end{aligned}$$

Here $\text{WF}(u)$ denotes the wavefront set of u as per Definition A.3.

For a proof of this theorem, we refer to [Hör98, Th. 8.2.9]. By combining Theorems A.2 and A.3, we obtain a criterion for the well-posedness of the product of distributions.

Theorem A.4. *Let $\Omega \subset \mathbb{R}^n$ be an open set and $u, v \in \mathcal{D}'(\Omega)$ be two distributions as per Definition A.1. Moreover, let WF denote the wavefront set as per Definition A.3. Then, the product $uv \doteq \delta^*(u \otimes v) \in \mathcal{D}'(\Omega)$ is well-defined if, for all $(x, \xi) \in \text{WF}(u)$ then $(x, -\xi) \notin \text{WF}(v)$. Here δ^* is the pullback of the diagonal map $\delta : \Omega \rightarrow \Omega \times \Omega$, $\delta(x) = (x, x)$. Moreover, it holds that*

$$\begin{aligned} \text{WF}(uv) \subset \{ & (x, \eta + \xi) \in \Omega \times (\mathbb{R}^n \setminus \{0\}) \mid (x, \xi) \in \text{WF}(u) \text{ or } \xi = 0, \\ & (x, \eta) \in \text{WF}(v) \text{ or } \eta = 0\}. \end{aligned}$$

For a proof, see [Hör98, Th. 8.2.10].

On account of Theorem A.2, we can generalize the wavefront set of a distribution to include distributions on manifold.

Definition A.4. Let $u \in \mathcal{D}'(\mathcal{M})$ be a distribution on a smooth, n -dimensional manifold $\mathcal{M}$. Let $(U_\alpha, \psi_\alpha)_{\alpha \in A}$ be a covering by coordinate charts, where A is some countable index set. Moreover, let $\{\rho_\alpha\}_{\alpha \in A}$ be a partition of unity subordinated to the cover. Then, the **wavefront set** of u is the set $\text{WF}(u) \subset T^*\mathcal{M} \setminus \{0\}$, denoted by the same symbol used in Definition A.3, defined as

$$\text{WF}(u) \doteq \bigcup_{\alpha \in A} \psi_\alpha^* \text{WF}(\rho_\alpha u \circ \psi_\alpha^{-1}).$$

Here $\psi_\alpha^* : \psi_\alpha(U_\alpha) \times \mathbb{R}^n \rightarrow T^*U_\alpha$ denotes the pullback induced on the cotangent bundle by the diffeomorphism ψ_α .

Remark A.4. Note that Definition A.4 may appear to depend on the choice of local charts. Although the Fourier transform of the local representative depends on the chosen coordinates, the rapid decay property in Definition A.3 is invariant under changes of coordinates. Hence the notion of regular directed point is coordinate-independent, making Definition A.4 well-posed.

A.2 Scaling degree

Here we outline the key results concerning the analysis of the scaling degree of distributions. This will play a pivotal rôle in the renormalization within the pAQFT framework and was first introduced by Steinmann in [Ste71] and later adapted to the language of microlocal analysis in [BF00]. We first present the results in the Euclidean space $\mathbb{R}^d$, and only later give the generalisation for arbitrary manifolds.

Let us start by defining the notion of *homogeneous distribution*.

Definition A.5. Let $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ be a distribution as per Definition A.1. We say that u is **homogeneous of degree a** if, for all $f \in \mathcal{D}(\mathbb{R}^d \setminus \{0\})$, then

$$u(f) = \lambda^{-a} u(f_\lambda), \quad f_\lambda(x) = \lambda^{-d} f\left(\frac{x}{\lambda}\right), \quad \forall \lambda > 0.$$

If the same holds true on the whole $\mathbb{R}^d$ we say that u is homogeneous of degree a on $\mathbb{R}^d$.

Remark A.5. Let us consider a distribution $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ and let us denote its integral kernel by $u(x)$. Then, u is homogeneous of degree a if and only if it holds that

$$u(\lambda x) = \lambda^a u(x), \quad \lambda > 0.$$

We proceed by introducing the main object of this section, namely, the *scaling degree* of a distribution, which quantifies the singular behaviour of a distribution near a point.

Definition A.6. Let $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ be a distribution as per Definition A.1. We call the **scaling degree** of u at the origin

$$sd_u \doteq \inf\{\omega \in \mathbb{R} \cup \{\pm\infty\} \mid \lim_{\lambda \rightarrow 0^+} \lambda^\omega u_\lambda = 0\}. \quad (\text{A.1})$$

Here the limit is taken in the topology of $\mathcal{D}'(\mathbb{R}^d \setminus \{0\})$, while u_λ is the distribution in $\mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ such that

$$u_\lambda(f) \doteq u(f_\lambda), \quad f_\lambda(x) = \lambda^{-d} f\left(\frac{x}{\lambda}\right),$$

for all $f \in \mathcal{D}(\mathbb{R}^d \setminus \{0\})$ and $\lambda > 0$.

Remark A.6. Definition A.6 can be generalised to any arbitrary point $x_0 \in \mathbb{R}^d$ in the following way. Let us consider a distribution $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{x_0\})$, then, its scaling degree at x_0 is defined analogously to Equation (A.1) with u_λ substituted by u_{λ, x_0} , which is the distribution such that

$$u_{\lambda, x_0}(f) \doteq u(f_{\lambda, x_0}), \quad f_{\lambda, x_0}(x) = \lambda^{-d} f\left(\frac{x - x_0}{\lambda}\right).$$

In the following, we shall denote the scaling degree of u at x_0 as $sd_u(x_0)$.

Additionally, for any distribution $v \in \mathcal{D}'(\mathbb{R}^d)$ we can analogously define its scaling degree $sd_v(x_0)$ for every point $x_0 \in \mathbb{R}^d$. In the following we shall use the following convention: for a distribution lying in $\mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ we denote its scaling degree at the origin simply by sd_u , while for a distribution in $\mathcal{D}'(\mathbb{R}^d)$ we shall explicitly indicate the point at which we are considering the scaling degree by writing $sd_v(x_0)$.

Remark A.7. Let us consider a homogeneous distribution of degree a $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ as per Definition A.5. Then, if we consider the distribution u_λ , $\lambda > 0$, in Definition A.6, we obtain that $u_\lambda = \lambda^a u$ and therefore, the distributional limit $\lim_{\lambda \rightarrow 0^+} \lambda^\omega u_\lambda = \lim_{\lambda \rightarrow 0^+} \lambda^{\omega+a} u$ vanishes for all $\omega > -a$. Therefore, for homogeneous distributions of order a , their scaling degree is $sd_u = -a$.

Proposition A.3. Let $u \in \mathcal{D}'(\mathbb{R}^d)$ be a distribution as per Definition A.1 and let $sd_u(x_0)$ denote its scaling degree at a point $x_0 \in \mathbb{R}^d$ as per Definition A.6 and on account of Remark A.6. Moreover, let $\alpha \in (\mathbb{N} \cup \{0\})^d$ be any multi-index and let $\psi \in \mathcal{E}(\mathbb{R}^d)$ be any smooth function. Then, it holds that

1. $sd_{\partial^{\alpha} u}(x_0) \leq sd_u(x_0) + |\alpha|$,
2. $sd_{(x-x_0)^{\alpha} u}(x_0) \leq sd_u(x_0) - |\alpha|$,

$$3. \quad sd_{\psi u}(x_0) \leq sd_u(x_0).$$

Moreover, if $t_1 \in \mathcal{D}'(\mathbb{R}^{d_1})$ and $t_2 \in \mathcal{D}'(\mathbb{R}^{d_2})$, then

$$sd_{t_1 \otimes t_2}(x_1, x_2) = sd_{t_1}(x_1) + sd_{t_2}(x_2).$$

Here $sd_{t_1 \otimes t_2}(x_1, x_2)$ denotes the scaling degree of the tensor product t_1, t_2 at the point $(x_1, x_2) \in \mathbb{R}^{d_1} \times \mathbb{R}^{d_2}$.

For a proof of this proposition, we refer to [BF00, Lemma 5.1].

Definition A.7. Let $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ be a distribution as per Definition A.1 and let sd_u denote its scaling degree at the origin. Then, we call the **divergence degree** of u at the origin the quantity

$$\rho_u \doteq d - sd_u.$$

Theorem A.5. Let $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ be a distribution as per Definition A.1 and let ρ_u denote its divergence degree at the origin as per Definition A.7. Then, if $\rho_u < 0$, there exists a unique distribution $\tilde{u} \in \mathcal{D}'(\mathbb{R}^d)$ such that:

- $sd_u = sd_{\tilde{u}}(0)$, where sd_u denotes the scaling degree of u at the origin as per Definition A.6,
- $u(f) = \tilde{u}(f)$ for all $f \in \mathcal{D}(\mathbb{R}^d \setminus \{0\})$.

For a proof of this theorem, we refer to [BF00, Th. 5.2].

Theorem A.5 shows that, whenever the divergence degree of a distribution is negative, then the distribution can be extended to the whole $\mathbb{R}^d$. However, some of the distributions relevant to this work, such as the Feynman parametrix, do not satisfy this condition. Hence, a further analysis is necessary in order to study the extension of distributions with nonnegative divergence degree.

Definition A.8. Let $\omega \in \mathbb{N} \cup \{0\} \doteq \mathbb{N}_0$ and let $\mathcal{D}(\mathbb{R}^d)$ be the space of compactly supported smooth functions. Then, we define

$$\mathcal{D}_\omega(\mathbb{R}^d) = \{f \in \mathcal{D}(\mathbb{R}^d) \mid \partial^\alpha f(0) = 0, \forall \alpha \in \mathbb{N}_0^d, |\alpha| \leq \omega\}. \quad (\text{A.2})$$

Additionally, for any collection $\{\mathfrak{w}_\beta\}_{\beta \in \mathbb{N}_0^d, |\beta| \leq \omega}$, $\mathfrak{w}_\beta \in \mathcal{D}(\mathbb{R}^d)$, such that $\partial^\alpha \mathfrak{w}_\beta(0) = \delta_\beta^\alpha$, where δ_β^α denotes the Kronecker delta, while $\alpha, \beta \in \mathbb{N}_0^d$ are some multi-indexes such that $|\alpha|, |\beta| \leq \omega$, we introduce the projection operator

$$W_{\mathfrak{w}_\beta} : \mathcal{D}(\mathbb{R}^d) \rightarrow \mathcal{D}_\omega(\mathbb{R}^d)$$

$$f \mapsto W_{\mathfrak{w}_\beta}(f) \doteq f - \sum_{\substack{\beta \in \mathbb{N}_0^d \\ |\beta| \leq \omega}} \mathfrak{w}_\beta \partial^\beta f(0).$$

Theorem A.6. *Let $u \in \mathcal{D}'(\mathbb{R}^d \setminus \{0\})$ be a distribution as per Definition A.1, while sd_u denotes its scaling degree at the origin as per Definition A.6 and ρ_u denotes its divergence degree at the origin as per Definition A.7. Then, if $0 \leq \rho_u < \infty$, for any collection of compactly-supported smooth functions $\{\mathfrak{w}_\beta\}_{\beta \in \mathbb{N}_0^d, |\beta| \leq sd_u}$, there exists a distribution $\tilde{u}_{\mathfrak{w}_\beta} \in \mathcal{D}'(\mathbb{R}^d)$ such that*

- $sd_u = sd_{\tilde{u}_{\mathfrak{w}_\beta}}(0)$,
- $u(f) = \tilde{u}_{\mathfrak{w}_\beta}(f)$ for all $f \in \mathcal{D}(\mathbb{R}^d \setminus \{0\})$.

For a proof we refer to [BF00, Th. 5.3].

Theorem A.6 shows that, when the divergence degree is finite and non-negative, extensions preserving the scaling degree still exist, but they are no longer unique. The resulting ambiguity corresponds to the freedom in choosing the renormalisation prescription.

The preceding results concern distributions singular at an isolated point. In the applications considered in this work, however, singularities appear on distinguished submanifolds, most notably on the thin diagonal $\text{Diag}_2 \subset \mathcal{M} \times \mathcal{M}$, rather than points in the Euclidean space. Therefore, we require an extension of the definition of scaling degree that can be applied to this more general scenario. To formulate this construction, we first introduce several geometric and microlocal notions.

Definition A.9. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $u \in \mathcal{D}'(\mathcal{M})$ be a distribution as per Definition A.1. Moreover, let $\mathcal{N} \subset \mathcal{M}$ be a submanifold. We say that u is **orthogonal** to $\mathcal{N}$ if, for all $(x, \xi) \in \text{WF}(u)$ such that $x \in \mathcal{N}$, it holds that*

$$\langle \xi, v \rangle = 0, \quad \forall v \in T_x \mathcal{N}.$$

Here $\text{WF}(u)$ denotes the wavefront set of u as per Definition A.4, while $\langle \cdot, \cdot \rangle$ denotes the canonical pairing between tangent and cotangent vectors.

Definition A.10. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{C}, \mathcal{N} \subset \mathcal{M}$ be two submanifolds. We say that $\mathcal{C}$ and $\mathcal{N}$ are **transversal**, if, for all $x \in \mathcal{C} \cap \mathcal{N}$, it holds that $T_x \mathcal{M} \simeq T_x \mathcal{N} \oplus T_x \mathcal{C}$. We denote two transversal submanifolds by $\mathcal{C} \pitchfork \mathcal{N}$.*

The next lemma shows how these two definitions allow one to define whether a distribution can be restricted to a submanifold, see [BF00, Lemma 6.1].

Lemma A.1. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$ be a submanifold. Moreover, let $u \in \mathcal{D}'(\mathcal{M})$ be a distribution as per Definition A.1 which is orthogonal to $\mathcal{N}$ as per Definition A.9. Then, for any submanifold $\mathcal{C} \subset \mathcal{M}$ which is transversal to $\mathcal{N}$ as per Definition A.10, the restriction $u|_{\mathcal{C}} \in \mathcal{D}'(\mathcal{C})$ is well defined.*

Definition A.11. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$. Let us consider $T_{\mathcal{N}}\mathcal{M} \doteq \bigcup_{x \in \mathcal{N}} T_x\mathcal{M}$ and let U be a star-shaped neighbourhood of the zero section $Z(T_{\mathcal{N}}\mathcal{M}) \doteq \{(x, 0) \in T\mathcal{M} \mid x \in \mathcal{N}\}$. Then, we call **admissible** a map*

$$\alpha : U \rightarrow \mathcal{N} \times \mathcal{M},$$

which is a diffeomorphism onto its image and such that

1. $\alpha(x, 0) = (x, x)$, $x \in \mathcal{N}$,
2. $\alpha(T\mathcal{N} \cap U) \subset \mathcal{N} \times \mathcal{N}$,
3. $\alpha(x, v) \in \{x\} \times \mathcal{M}$, $x \in \mathcal{N}$ and $v \in T_x\mathcal{M}$,
4. $d_v\alpha(x, \cdot)|_{v=0} = \text{id}_{T_x\mathcal{M}}$, where d_v denotes the tangent map.

Furthermore, we denote the set of admissibles by $\mathcal{Z}$.

Definition A.12. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$. Furthermore, let U be a star-shaped neighbourhood of the zero section $Z(T_{\mathcal{N}}\mathcal{M}) = \{(x, 0) \in T\mathcal{M} \mid x \in \mathcal{N}\}$. If $u \in \mathcal{D}'(\mathcal{M})$ is a distribution as per Definition A.1 and α is an admissible as per Definition A.11, then we define the following:*

- $u^\alpha = (1 \otimes u) \circ \alpha \in \mathcal{D}'(U)$, where the composition is to be understood as pullback of the distribution $(1 \otimes u)$ under the admissible α ,
- u_λ^α , $\lambda \in (0, 1]$, is the distribution whose integral kernel reads $u_\lambda^\alpha(x, v) = u^\alpha(x, \lambda v)$.

Before passing to the definition of scaling degree on manifolds, we recall that, given a smooth manifold $\mathcal{M}$ and a submanifold $\mathcal{N} \subset \mathcal{M}$, we define the conormal bundle of $\mathcal{N}$ as

$$N^*\mathcal{N} = \{(x, \xi) \in T^*\mathcal{M} \mid x \in \mathcal{N} \text{ and } \langle \xi, v \rangle = 0, \forall v \in T_x\mathcal{N}\}. \quad (\text{A.3})$$

Here we have identified $T_x\mathcal{N}$ with its image under the push forward of the inclusion $\iota : \mathcal{N} \rightarrow \mathcal{M}$.

Proposition A.4. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$. Moreover, let $u \in \mathcal{D}'(\mathcal{M})$ be a distribution as per Definition A.1 such that u is orthogonal to $\mathcal{N}$ as per Definition A.9. Moreover, let $Z(T_{\mathcal{N}}\mathcal{M})$ be the zero section as introduced in Definition A.11 and let U be a star-shaped neighbourhood of $Z(T_{\mathcal{N}}\mathcal{M})$. Then, there exists a closed conic set $\Gamma \subset (T^*U) \setminus \{0\}$ such that*

- $\Gamma \subset N^*(T\mathcal{N} \cap U)$. Here $N^*(T\mathcal{N} \cap U)$ denotes the conormal bundle of $T\mathcal{N} \cap U$ as per Equation (A.3),
- $\text{WF}(u_{\lambda}^{\alpha}) \subset \Gamma$, $\lambda \in (0, 1]$, where $\text{WF}(u_{\lambda}^{\alpha})$ denotes the wavefront set as per Definition A.4 of the distribution u_{λ}^{α} as in Definition A.12

For a proof of this result, see [BF00, Prop. 6.2].

We are now ready to give the definition of the *microlocal scaling degree*, which is the generalisation of Definition A.6 to manifolds.

Definition A.13. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$ be an embedded submanifold. Additionally, let $u \in \mathcal{D}'(\mathcal{M})$ be a distribution as per Definition A.1 and let $\alpha \in \mathcal{Z}$ be an admissible as per Definition A.11. Then, if Γ_0 is a closed conical subset of $N^*\mathcal{N} \setminus \{0\}$, where $N^*\mathcal{N}$ denotes the conormal bundle as in Equation (A.3), we say that u has **microlocal scaling degree** $\mu\text{sd}_{\mathcal{N}}^{\Gamma_0}(u, \alpha)$ at $\mathcal{N}$ with respect to Γ_0 if*

- *There exists a closed conic set $\Gamma \subset T^*(T_{\mathcal{N}}\mathcal{M}) \setminus \{0\}$ such that $\text{WF}(u_{\lambda}^{\alpha}) \subset \Gamma$ and $\Gamma|_{T\mathcal{N}} \subset \alpha^*(Z(T^*\mathcal{N}) \times \Gamma_0)$, where u_{λ}^{α} is the distribution introduced in Definition A.12, with $\lambda \in (0, 1]$, while $\text{WF}(u_{\lambda}^{\alpha})$ denotes its wavefront set as per Definition A.4. Moreover, α^* denotes the pullback induced by the admissible α ,*
- *It holds that*

$$\mu\text{sd}_{\mathcal{N}}^{\Gamma_0}(u, \alpha) = \inf\{\omega \in \mathbb{R} \mid \lim_{\lambda \rightarrow 0^+} \lambda^{\omega} u_{\lambda}^{\alpha} = 0\}. \quad (\text{A.4})$$

Here the limit is considered in the topology of distributions.

Remark A.8. *The microlocal scaling degree introduced in Definition A.13 is independent of the choice of the admissible α , although it depends essentially on the choice of the conic set Γ_0 . For further details, see [BF00, Sec. 6].*

Definition A.14. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$ be an embedded submanifold. Let $u \in \mathcal{D}'(\mathcal{M} \setminus \mathcal{N})$ be a distribution as per*

Definition A.1 and let $\chi \in \mathcal{E}(\mathcal{M})$ be a smooth function such that $\text{supp}(\chi) \cap \mathcal{N} = \emptyset$. For any admissible $\alpha \in \mathcal{Z}$ as per Definition A.11, we define

$$u_\lambda^\chi \doteq ((1 \otimes \chi) \circ \alpha) \cdot u_\lambda^\alpha \in \mathcal{D}'(U), \quad \lambda \in (0, 1].$$

Here U is a star-shaped neighbourhood of the zero section $Z(T_{\mathcal{N}\mathcal{M}})$ as introduced in Definition A.11, while 1 denotes the distribution generated by the constant function, u_λ^α is the distribution introduced in Definition A.12 and $\cdot$ denotes the product of distributions in $\mathcal{D}'(U)$.

Additionally, we can define the **scaling degree** of u at $\mathcal{N}$ as

$$sd_{\mathcal{N}}(u) \doteq \inf\{\omega \in \mathbb{R} \mid \lim_{\lambda \rightarrow 0^+} \lambda^\omega u_\lambda^\chi = 0\}. \quad (\text{A.5})$$

In particular, Equation (A.5) is independent of the choice of the smooth function χ as long as it satisfies $\text{supp}(\chi) \cap \mathcal{N} = \emptyset$.

We can now state the equivalent of Theorems A.5 and A.6 for distributions that are not defined at a submanifold $\mathcal{N}$.

Theorem A.7. *Let $\mathcal{M}$ be a d -dimensional smooth manifold and let $\mathcal{N} \subset \mathcal{M}$ be an embedded submanifold. Let $u_0 \in \mathcal{D}'(\mathcal{M} \setminus \mathcal{N})$ be a distribution as per Definition A.1. Let $sd_{\mathcal{N}}(u_0)$ denote the scaling degree at $\mathcal{N}$ of u_0 as per Definition A.14. Then, it holds that*

1. *If $sd_{\mathcal{N}}(u_0) < \text{codim}(\mathcal{N})$ then there exists a unique distribution $u \in \mathcal{D}'(\mathcal{M})$ such that*

$$u|_{\mathcal{M} \setminus \mathcal{N}} = u_0, \quad sd_{\mathcal{N}}(u_0) = sd_{\mathcal{N}}(u).$$

2. *If $\text{codim}(\mathcal{N}) \leq sd_{\mathcal{N}}(u_0) < \infty$, then there exists $\tilde{u} \in \mathcal{D}'(\mathcal{M})$ such that*

$$\tilde{u}|_{\mathcal{M} \setminus \mathcal{N}} = u_0, \quad sd_{\mathcal{N}}(u_0) = sd_{\mathcal{N}}(\tilde{u}).$$

Moreover, for any pair of admissible extensions $\tilde{u}_1, \tilde{u}_2$, it holds that

$$\tilde{u}_1 - \tilde{u}_2 = \sum_{k=0}^{\rho_{\mathcal{N}}(u_0)} c_k \delta_{\mathcal{N}}^{(k)}, \quad c_k \in \mathcal{E}(\mathcal{N}).$$

Here $\rho_{\mathcal{N}}(u_0) = \lfloor sd_{\mathcal{N}}(u_0) - \text{codim}(\mathcal{N}) \rfloor$ denotes the floor function applied to the difference between the scaling degree at $\mathcal{N}$ of u_0 and $\text{codim}(\mathcal{N}) = \dim(\mathcal{M}) - \dim(\mathcal{N})$. Additionally $\delta_{\mathcal{N}}^{(k)}$ denotes the k -th order derivative of the Dirac delta distribution supported at $\mathcal{N}$.

For a proof of this result, we refer to [BF00, Th. 6.9].

Appendix B

Algebras and their representations

This section is devoted to outlining the fundamental notions regarding algebras and their representations. We limit ourselves to discuss solely the notions needed in the rest of the work, referring to [Hal15] for a complete overview of representation theory.

Definition B.1. An **algebra** $\mathcal{A}$ over a field $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$ is a $\mathbb{K}$ -vector space endowed with a map

$$\begin{aligned} \cdot : \mathcal{A} \times \mathcal{A} &\rightarrow \mathcal{A} \\ (a, b) &\rightarrow ab, \end{aligned}$$

called *product*, such that:

1. $(ab)c = a(bc)$ for all $a, b, c \in \mathcal{A}$,
2. $(a + b)c = ac + bc$ for all $a, b, c \in \mathcal{A}$,
3. $\mu(ab) = (\mu a)b = a(\mu b)$ for all $a, b \in \mathcal{A}$ and for all $\mu \in \mathbb{K}$.

Moreover, we say that $\mathcal{A}$ is an **unital algebra** if there exists an element $\mathbf{1} \in \mathcal{A}$ such that

$$\mathbf{1}a = a\mathbf{1} = a, \quad \forall a \in \mathcal{A}.$$

The element $\mathbf{1}$ is called *unit element* of the algebra.

In order to identify observables with self-adjoint elements, we endow the algebra with an *involution*.

Definition B.2. We call **unital $\ast$ -algebra** a unital algebra $\mathcal{A}$ as per Definition B.1 over a field $\mathbb{K}$ endowed with an **involution**, namely, a map

$$\ast : \mathcal{A} \rightarrow \mathcal{A}$$

$$a \mapsto a^\ast,$$

such that

1. $(a^\ast)^\ast = a$ for all $a \in \mathcal{A}$,
2. $(\mu a + \nu b)^\ast = \bar{\mu} a^\ast + \bar{\nu} b^\ast$ for all $a, b \in \mathcal{A}$ and for all $\mu, \nu \in \mathbb{K}$,
3. $(ab)^\ast = b^\ast a^\ast$ for all $a, b \in \mathcal{A}$.

Definition B.3. Let $\mathcal{A}$ be an algebra as per Definition B.1. We say that a linear subspace $\mathcal{I} \subset \mathcal{A}$ is a **left ideal** if

$$a \cdot b \in \mathcal{I}, \quad \forall a \in \mathcal{I}, \forall b \in \mathcal{A}.$$

We define similarly a **right ideal**. Additionally, if $\mathcal{I}$ is both a left and right ideal, we say that it is a **(two-sided) ideal**.

Definition B.4. Let $(\mathcal{A}_1, \cdot_1)$ and $(\mathcal{A}_2, \cdot_2)$ be two algebras as per Definition B.1. We say that a map $\varphi : \mathcal{A}_1 \rightarrow \mathcal{A}_2$ is an **algebra homomorphism** if

$$\varphi(a \cdot_1 b) = \varphi(a) \cdot_2 \varphi(b), \quad \forall a, b \in \mathcal{A}_1.$$

If both $\mathcal{A}_1$ and $\mathcal{A}_2$ are unital, we additionally require that $\varphi(\mathbf{1}_1) = \mathbf{1}_2$. Moreover, if both $\mathcal{A}_1$ and $\mathcal{A}_2$ are $\ast$ -algebras as per Definition B.2 with involutions $\ast_1$ and $\ast_2$ respectively, we say that φ is a **$\ast$ -algebra homomorphism** if

$$\varphi(a^{\ast_1}) = \varphi(a)^{\ast_2}, \quad \forall a \in \mathcal{A}_1.$$

Representations allow us to realize abstract algebraic elements as operators on a Hilbert space.

Definition B.5. Let $(\mathcal{A}, \cdot, \ast)$ be a unital $\ast$ -algebra over $\mathbb{C}$ as per Definition B.2, with unit element $\mathbf{1} \in \mathcal{A}$. Let $\mathcal{H}$ be a complex Hilbert space, and let $\mathcal{D}$ be a dense subspace of $\mathcal{H}$. Moreover, let $\mathcal{L}(\mathcal{D})$ denote the algebra of all linear operators $T : \mathcal{D} \rightarrow \mathcal{D}$. A **$\ast$ -representation** of $\mathcal{A}$ with domain $\mathcal{D}$ is a map

$$\pi : \mathcal{A} \rightarrow \mathcal{L}(\mathcal{D})$$

such that:

-
1. $\pi(\mu a + \nu b) = \mu\pi(a) + \nu\pi(b)$ for all $a, b \in \mathcal{A}$ and $\mu, \nu \in \mathbb{C}$,
 2. $\pi(ab) = \pi(a)\pi(b)$ for all $a, b \in \mathcal{A}$, where $\pi(a)\pi(b)$ denotes the composition of the two operators,
 3. $\pi(\mathbf{1}) = \text{id}_{\mathcal{D}}$, where $\text{id}_{\mathcal{D}}$ denotes the identity operator on $\mathcal{D}$,
 4. $\pi(a^*) = \pi(a)^\dagger|_{\mathcal{D}}$, where $\pi(a)^\dagger$ denotes the hermitian adjoint of $\pi(a)$ with respect to the inner product of $\mathcal{H}$.

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