ALGEBRAIC STRUCTURE OF CLASSICAL FIELD THEORY: KINEMATICS AND LINEARIZED DYNAMICS FOR REAL SCALAR FIELDS

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Abstract. We describe the elements of a novel structural approach to classical field theory, inspired by recent developments in perturbative algebraic quantum field theory. This approach is local and focuses mainly on the observables over field configurations, given by certain spaces of functionals which are studied here in depth. The analysis of such functionals is characterized by a combination of geometric, analytic and algebraic elements which (1) make our approach closer to quantum field theory, (2) allow for a rigorous analytic refinement of many computational formulae from the functional formulation of classical field theory and (3) provide a new pathway towards understanding dynamics. Particular attention will be paid to aspects related to nonlinear hyperbolic partial differential equations and their linearizations.

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Contents

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1. Introduction

The longstanding problem of finding a coherent and systematic mathematical structure for classical field theories has been addressed in various ways. Among them, we quote two main lines of investigation: one based on (multi)symplectic geometry [22, 37, 42, 57], seeking a covariant generalization of Hamiltonian mechanics and that goes back to de Donder [29] and Weyl [90]; and the other based on the so-called formal theory of systems of partial differential equations [3, 62, 79, 85, 86], seeking a higher-order generalization of S. Lie's and É. Cartan's geometric approach to the analysis of integrability and symmetries of such systems. Both approaches have several points of contact and lead to a highly developed framework for the calculus of variations. As far as *relativistic* field theories are concerned, however, the solution spaces of the dynamics generated by the variational principle are essentially taken for granted and their properties are seldom studied in depth, a noteworthy exception being the approach of Christodoulou [24].

Physicists, on the other hand, are keen on formal functional methods [25, 30], tailored to the needs of (path-integral-based) quantum field theory, which are essentially a heuristic infinite-dimensional generalization of Lagrangian mechanics. To a certain extent, it is possible to make these latter methods rigorous (see for instance [1, 11]). However, in these approaches the field configuration spaces are usually modeled on Banach spaces, which provide a simple differential calculus but entail some physically undesirable restrictions on the allowed space-times and on the regularity of the allowed field configurations. Moreover, these approaches also tend to deemphasize aspects related to covariance and locality, which are central in any relativistic field theory since then Euler-Lagrange equations of motion are *differential* (expressing locality of the underlying variational principle) and *hyperbolic* (expressing finiteness of the propagation speed of dynamical effects).

Even more importantly, a pivotal aspect that none of the above approaches has addressed in a satisfactory manner is the characterization of *local observables*, as opposed to spaces of field configurations. This remark is the starting point of our present investigation. Namely, we contend that if one wants to study the structure of local observables in a *model-independent* fashion, one is inevitably led to an *algebraic* viewpoint. This is a deep lesson learned from quantum field theory [44], which however does not seem to have echoed back to classical field theory until quite recently, the only exception to our knowledge being [65]. This state of things has started to change due to the recent developments in perturbative algebraic quantum field theory [12, 15, 16, 17, 18, 34, 35]. This is a research program aiming at a mathematically precise understanding of perturbative quantum field theory and renormalization from an algebraic viewpoint – to wit, renormalized perturbative quantum field theory can be seen as a formal deformation of classical field theory, in a rather precise sense [12, 15, 34].

The key upshot of this program, which motivated the present work, is that it singles out the relevant class of observables for classical field theory from a few, physically reasonable requirements which, at the quantum level, are needed to restrict the class of allowed counterterms in renormalization. This serves as a starting point for a new, algebraic framework for classical (relativistic) field theory in its own right, which emphasizes from the very beginning the role of local observables and how they are affected by the dynamics. Presenting this framework in full detail is the objective of this paper. Let us now give an overview of its results.

As we shall see, local observables are represented by certain classes of functionals over the space of smooth field configurations. More precisely, the kinematical requirements on functionals in order to qualify as local observables lead, among other things, to a surprisingly simple structure for the local algebras they generate – for instance, these algebras, when suitably topologized, turn out to be *nuclear*, opening the way to a seamless composition of classical subsystems by means of tensor products [17].

A cornerstone of our approach concerns the treatment of *dynamics*. We do not impose any equations of motion directly on field configurations – that is, we adopt an *off-shell* viewpoint. We show that, on an infinitesimal level, the dynamics is implemented algebraically on local observables by means of a Poisson structure associated to certain Lagrangians, given in covariant form by the Peierls bracket [30, 37, 68, 75]. This bracket is a covariant generalization of the canonical Poisson bracket [11, 87], and has an unambiguous off-shell extension which however becomes degenerate. This degeneracy can be removed by taking the quotient of our local Poisson algebras of functionals modulo the ideal generated by the equations of motion, which turns out to be a *Poisson* ideal. As a consequence, the quotient algebra is a Poisson algebra as well when endowed with the bracket induced on the quotient by the Peierls bracket. The quotient amounts to imposing the equations of motion on field configurations pretty much in the spirit of algebraic geometry, and allows for a unified analysis of quantum anomalies as violations of identities following from the classical equations of motion due to perturbative quantization and renormalization [12, 34].

We conclude this introduction with a summary of the contents of the paper. In Section 2, we discuss the bare minimum of kinematical concepts underlying our approach. For simplicity, we will consider only *real scalar* fields, since the case when the fields live in a general fiber bundle poses a different set of questions, which demand a separate treatment (we shall have more to say about this in the final Section 5). In Subsection 2.1, we present a fair amount of background on Lorentzian geometry, vector bundles and jets, which is also used in Subsection 2.2 to give an overview of the geometric and topological properties of the space of smooth field configurations. In Subsection 2.3 we introduce suitable classes of functionals over this space and discuss their support and localization properties, so as to be able to proceed to a detailed analysis of infinitesimal (i.e. linearized) dynamics in Section 3; the full nonlinear dynamics is to be analyzed in a forthcoming paper. Euler-Lagrange equations are obtained from a class of local functionals parametrized by smooth, compactly supported functions f specifying the localization of these functionals in space-time. Such functionals are called *generalized Lagrangians*, examples of which are provided by integrals of Lagrangian densities multiplied by f over the space-time manifold (Subsection 3.1). We are mainly interested in those generalized Lagrangians which lead to (normally) hyperbolic Euler-Lagrange operators, which are discussed in Subsection 3.2. Therein we also define the Peierls bracket associated with such operators, and study its properties in depth. This bracket is shown to yield a Lie bracket in the space of so-called *microcausal* functionals, which are distinguished by the singularity structure of their functional derivatives. A particular highlight of this development is perhaps the first fully fledged and rigorous proof of the Jacobi identity for the Peierls bracket in the literature (Corollary 3.2.17), parts of which having previously appeared or been sketched in [12, 34, 53]. A thorough discussion of the topological and algebraic aspects of the *-algebras of microcausal functionals is carried out in Section 4, using the previous Sections as motivation. We show in Subsection 4.1 that the Lie bracket provided by the Peierls bracket is in fact a Poisson bracket; another noteworthy result, shown in Subsection 4.2, is that the (Poisson) *-algebras of microcausal functionals also bear a $\mathscr{C}^\infty$*-ring* structure [72], that is, they admit a sort of smooth functional calculus (Theorem 4.2.1), which leads to a number of interesting consequences. For example, one recovers some basic facts from commutative C*-algebra theory: the *-algebra of microcausal functionals over a domain of field configurations completely encodes the topology of this domain (Proposition 4.2.4 (i)) and one may even reconstruct the domain itself as the space of *-characters of the *-algebra (Proposition 4.2.4 (iii–iv)). Moreover, any open cover of the domain admits locally finite partitions of unity whose members belong to this *-algebra (Proposition 4.2.4 (ii)). Finally, in Subsection 4.3 we show that the ideal generated by a hyperbolic Euler-Lagrange equation is a Poisson *-ideal (Proposition 4.3.2) and therefore the quotient of the Poisson *-algebra of microcausal functionals modulo this ideal is again a Poisson *-algebra. Section 5 concludes our work by presenting some future prospects and challenges. Appendix A recalls basic concepts of differential calculus on locally convex topological vector spaces.

2. Kinematics

2.1. **Preliminaries.** Given nonvoid sets $A, A_1, \ldots, A_m$, we denote by $\mathbb{1} = \mathbb{1}_A : A \to A$ the *identity map* $\mathbb{1}_A(a) = a$, and by $\mathrm{pr}_{j_1,\ldots,j_k} : A_1 \times \cdots \times A_m \to A_{j_1} \times \cdots \times A_{j_k}$ the *canonical projection* $\mathrm{pr}_{j_1,\ldots,j_k}(a_1, \ldots, a_m) = (a_{j_1}, \ldots, a_{j_k})$, $1 \leq j_1 < j_2 < \cdots < j_k \leq m$. If $k = 1$, we say that pr_j is the *canonical projection onto the k-th factor*.

First of all, a small refresher on Lorentzian geometry to fix our notation and terminology (we basically follow [46, 87]). Let $(\mathscr{M}, g)$ be a *space-time*, that is, an oriented d-dimensional Lorentzian manifold. The underlying manifold $\mathscr{M}$ (called the *space-time manifold*) is assumed to be smooth, Hausdorff, paracompact and second countable (in particular, $\mathscr{M}$ has at most a countable number of connected components). By a *region* of $\mathscr{M}$ (or of $(\mathscr{M}, g)$) we mean any subset of $\mathscr{M}$ with nonvoid interior. The Lorentzian metric g on $T\mathscr{M}$ endows $\mathscr{M}$ with the volume element $\mathrm{d}\mu_g = \sqrt{|\det g|}\mathrm{d}x$, the Levi-Civita connection ∇, the lowering (resp. raising) musical isomorphisms $g^\flat : T\mathscr{M} \to T^*\mathscr{M}$ (resp. $g^\sharp : T\mathscr{M} \to T^*\mathscr{M}$) given by $g^\flat(X) \doteq g(X, \cdot)$ (resp. $g^\sharp(\xi) \doteq (g^\flat)^{-1}(\xi)$), and the inverse Lorentzian metric g^{-1} on $T^*\mathscr{M}$ given by $g^{-1}(\xi_1, \xi_2) \doteq \xi_1(g^\sharp(\xi_2))$. We occasionally write $g(T)$ (resp. $g^{-1}(\omega)$) with a single argument T (resp. ω), which is understood to be a contravariant (resp. covariant) tensor of rank two. We will use the chosen orientation to identify smooth densities with smooth d-forms. We adopt for g the signature convention that, for all $p \in \mathscr{M}$, the subspace of $T_p\mathscr{M}$ consisting of eigenvectors of $g(p)$ with *negative* eigenvalues is one-dimensional and therefore consists of *timelike* vectors. Recall that $X \in T_p\mathscr{M}$ is timelike (resp. null, causal, spacelike) if $g(X,X) < 0$ (resp. $= 0$, ≤ 0, > 0) – hence, the subspace of $T_p\mathscr{M}$ consisting of (spacelike) eigenvectors of $g(p)$ with positive eigenvalues is $(d-1)$-dimensional. We always assume that $\mathscr{M}$ is *time-oriented*, that is, there is a global timelike vector field T on $\mathscr{M}$ – we then say that a causal $X \in T_p\mathscr{M}$ is future (resp. past) directed if $g(X,T) < 0$ (resp. > 0).

Recall as well that, given an interval $I \subset \mathbb{R}$ with nonvoid interior, a (piecewise) smooth curve $\gamma : I \ni \lambda \to \gamma(\lambda) \in \mathscr{M}$ is said to be timelike (resp. null, causal, spacelike) if $g(\dot\gamma(\lambda), \dot\gamma(\lambda)) < 0$ (resp. $= 0$, ≤ 0, > 0) for all $\lambda \in I$ (such that γ is smooth at λ), and that a causal curve is said to be future (resp. past) directed if $g(\dot\gamma(\lambda), T) < 0$ (resp. > 0) for any $\lambda \in I$ as above and any future directed timelike $T \in T_{\gamma(\lambda)}\mathscr{M}$. This allows us to define the chronological (resp. causal) future / past $I^{+/-}(U,g)$ (resp. $J^{+/-}(U,g)$) of $U \subset \mathscr{M}$ as

$$\begin{aligned} I^{+/-}(U,g) \doteq \{p \in \mathscr{M} : \exists \gamma : [0,1] \to \mathscr{M} & \text{ piecewise smooth, future / past directed} \\ & \text{timelike such that } \gamma(0) \in U, \gamma(1) = p\} \ , \end{aligned}$$

$$\begin{aligned} J^{+/-}(U,g) \doteq \{p \in \mathscr{M} : \exists \gamma : [0,1] \to \mathscr{M} & \text{ piecewise smooth, future / past directed} \\ & \text{causal such that } \gamma(0) \in U, \gamma(1) = p\} \ . \end{aligned}$$

We also set $I^{+/-}(\{p\}, g) \doteq I^{+/-}(p,g)$ (resp. $J^{+/-}(\{p\}, g) \doteq J^{+/-}(p,g)$) for any $p \in \mathscr{M}$, and, given $U, V \subset \mathscr{M}$, we write $U \gg_g / \ll_g V$ (resp. $U \geq_g / \leq_g V$) whenever $U \subset I^{+/-}(V,g)$ (resp. $U \subset J^{+/-}(V,g)$). If $U = \{p\}$ (resp. $V = \{q\}$) for some $p, q \in \mathscr{M}$, we replace U (resp. V) by p (resp. q) in the above notation. Finally, we always assume that g is *globally hyperbolic*, that is, g is *causal* (which means that there is no causal $\gamma : [0,1] \to \mathscr{M}$ such that $\gamma(0) = \gamma(1)$) and given $p \leq_g q \in \mathscr{M}$, the set $J^+(p,g) \cap J^-(q,g)$ is *compact*. An useful, equivalent description of global hyperbolicity can be given as follows [7, 8, 9, 10]: there is a smooth, surjective function $\tau : \mathscr{M} \to \mathbb{R}$ such that $g^\sharp(\mathrm{d}\tau)$ is a future directed timelike vector field and $\Sigma^\tau_t \doteq \tau^{-1}(t)$ is a *Cauchy hypersurface* for $\mathscr{M}$ at each $t \in \mathbb{R}$, that is, Σ^τ_t is a codimension-one, smooth and boundary-less submanifold of $\mathscr{M}$ such that any inextendible causal curve[1] intersects Σ^τ_t exactly once. Such a τ is called a *Cauchy time function* with respect to $(\mathscr{M}, g)$. Moreover, if $(\mathscr{M}, g)$ has a Cauchy hypersurface Σ, one can build a Cauchy time function τ such that $\tau^{-1}(0) = \Sigma$ [10] – in particular, $\mathscr{M}$ must then be diffeomorphic to $\mathbb{R} \times \Sigma \cong \mathbb{R} \times \Sigma^\tau_t$ for any $t \in \mathbb{R}$.

Occasionally, we will need to work with smooth sections of vector bundles over the space-time manifold $\mathscr{M}$ or over Cartesian powers thereof. Recall, for the sake of fixing nomenclature, that a (real) *vector bundle* of rank D over $\mathscr{M}$ is given by a smooth surjective submersion $\pi : \mathscr{E} \to \mathscr{M}$ from the *total space* $\mathscr{E}$ to the *base* $\mathscr{M}$, called the *projection map*, such that there is an open covering $\{U_j\}_{j \in J}$ of $\mathscr{M}$ and for each $j \in J$ a smooth diffeomorphism $\psi_j : \pi^{-1}(U_j) \to U_j \times \mathbb{R}^D$ (called a *local trivialization* over U_j) such that $\psi_k \circ \psi_j^{-1}(x, \zeta) = (x, t_{kj}(x,\zeta)) = (x, T_{kj}(x)\zeta)$ for all $x \in U_j \cap U_k$, $j, k \in J$, where the *transition functions* $T_{kj} : U_j \cap U_k \to GL(D, \mathbb{R})$ are smooth.

[1] A causal (resp. timelike, null) curve $\gamma : I \to \mathscr{M}$ is said to be *inextendible* if there is no causal (resp. timelike, null) curve $\tilde\gamma : \tilde I \to \mathscr{M}$ such that $\tilde I \supsetneq I$ and $\tilde\gamma|_I = \gamma$.

The collection of pairs $\{(U_j, \psi_j)\}_{j\in J}$ is called a *vector bundle atlas* for π. We usually identify a vector bundle with its projection map. Given $U \subset \mathscr{M}$ open, we say that a local trivialization ψ over U is said to be π-*compatible* if for every $j \in J$ such that $U \cap U_j \neq \varnothing$ we have that $\psi \circ \psi_j^{-1}(x,\zeta) = (x, t_j(x,\zeta)) = (x, T_j(x)\zeta)$ where $T_j : U_j \cap U \to GL(D,\mathbb{R})$ is smooth. A map $\vec{\varphi} : \mathscr{M} \to \mathscr{E}$ is said to be a *section* of π if $\pi \circ \vec{\varphi} = \mathbb{1}_{\mathscr{M}}$. Notice that if, in the above discussion, we replace $\mathbb{R}^D$ by a manifold Q, and just demand that the smooth maps t_{kj} are diffeomorphisms of Q for each fixed $x \in U_j \cap U_k$ and the smooth maps t_j are diffeomorphisms of Q for each fixed $x \in U \cap U_j$ and π-compatible local trivialization ψ, $j,k \in J$, we get instead a (general) fiber bundle with typical fiber Q and bundle atlas $\{(U_j,\psi_j)\}$.

Using a vector bundle atlas one can define (fiberwise) linear combinations $\alpha\vec{\varphi}_1 + \beta\vec{\varphi}_2$ of any two sections $\vec{\varphi}_1, \vec{\varphi}_2$ $(\alpha,\beta \in \mathbb{R})$ by setting $\psi_j \circ (\alpha\vec{\varphi}_1 + \beta\vec{\varphi}_2)(p) = \alpha\psi_j \circ \vec{\varphi}_1(p) + \beta\psi_j \circ \vec{\varphi}_2(p)$, $p \in U_j$, $j \in J$. This definition is readily seen to be independent of the choice of vector bundle atlas with π-compatible local trivializations. In particular, every vector bundle π over $\mathscr{M}$ has a canonical section 0 (called the *zero section* of π), defined on every local trivialization ψ compatible with π by $\psi \circ 0(p) = (p,0)$, and with respect to which we can define the *support* of a section $\vec{\varphi}$ as $\operatorname{supp}\vec{\varphi} = \overline{\{p \in \mathscr{M} : \vec{\varphi}(p) \neq 0(p)\}} \subset \mathscr{M}$. It follows from the inverse function theorem that $\mathscr{M}$ is diffeomorphic to the range of the zero section in $\mathscr{E}$, which we also denote by 0. We denote by

$$\Gamma^\infty(\pi) = \Gamma^\infty(\mathscr{E} \to \mathscr{M}) = \{\vec{\varphi} : \mathscr{M} \to \mathscr{E} \text{ smooth } \mid \pi \circ \vec{\varphi} = \mathbb{1}_{\mathscr{M}}\}$$

the vector space of *smooth sections* of π, and by

$$\Gamma^\infty_c(\pi) = \Gamma^\infty_c(\mathscr{E} \to \mathscr{M}) = \{\vec{\varphi} \in \Gamma^\infty(\pi) \mid \operatorname{supp}\vec{\varphi} \text{ compact}\}$$

the vector space of smooth sections of π with compact support. Likewise, we denote by

$$\mathscr{D}'(\pi) = \mathscr{D}'(\mathscr{E} \to \mathscr{M}) = \Gamma^\infty_c(\mathscr{E}' \otimes \wedge^d T^*\mathscr{M} \to \mathscr{M})'$$

the space of $\mathscr{E}$-valued distributions, where $\pi' : \mathscr{E}' \to \mathscr{M}$ is the dual bundle of π. The fiberwise scalar multiplication turns $\Gamma^\infty(\pi)$, $\Gamma^\infty_c(\pi)$ and $\mathscr{D}'(\pi)$ into $\mathscr{C}^\infty(\mathscr{M})$-modules, so that multiplication of sections by $f \in \mathscr{C}^\infty_c(\mathscr{M})$ is even a $\mathscr{C}^\infty(\mathscr{M})$-linear map from $\Gamma^\infty(\pi)$ into $\Gamma^\infty_c(\pi)$, for $\operatorname{supp}(f\vec{\varphi}) \subset \operatorname{supp} f$ for all $f \in \mathscr{C}^\infty(\mathscr{M})$, $\vec{\varphi} \in \Gamma^\infty(\pi)$.

We also briefly recall the notion of *jets* of smooth maps between manifolds $\mathscr{M}, \mathscr{M}'$ of respective dimensions d, D, referring to [61] for a thorough exposition. Let $r \in \mathbb{N}$; we say that two smooth maps $\psi_1, \psi_2 : \mathscr{M} \to \mathscr{M}'$ *have the same r-th order jet* at $p \in \mathscr{M}$ if for some (hence, any) coordinate charts $x : U \supset p \to \mathbb{R}^d$, $y : V \supset \psi_1(p), \psi_2(p) \to \mathbb{R}^D$, the r-th order Taylor polynomials of $y \circ \psi_1 \circ x^{-1}$ and $y \circ \psi_2 \circ x^{-1}$ at $x(p)$ coincide. Having the same r-th order jet at $p \in \mathscr{M}$ is clearly an equivalence relation in the space $\mathscr{C}^\infty(\mathscr{M},\mathscr{M}')$ of all smooth maps from $\mathscr{M}$ into $\mathscr{M}'$, and the equivalence class of $\psi \in \mathscr{C}^\infty(\mathscr{M},\mathscr{M}')$ is called the *r-th order jet* of ψ at p, denoted by $j^r\psi(p)$. The *r-th order jet bundle* of $\mathscr{C}^\infty(\mathscr{M},\mathscr{M}')$, given by

$$\pi^r_0 : J^r(\mathscr{M},\mathscr{M}') \ni j^r\psi(p) \mapsto \pi^r_0(j^r\psi(p)) = (p,\psi(p)) \in \mathscr{M} \times \mathscr{M}' \ , \quad \psi \in \mathscr{C}^\infty(\mathscr{M},\mathscr{M}') \ ,$$

is an affine bundle over $\mathscr{M} \times \mathscr{M}'$, whose typical fiber is the space of r-th order, $\mathbb{R}^D$-valued polynomials vanishing at $0 \in \mathbb{R}^d$. Given $\psi \in \mathscr{C}^\infty(\mathscr{M},\mathscr{M}')$, the corresponding section $j^r\psi : p \mapsto j^r\psi(p)$ of π^r_0 is called the *r-th order jet prolongation* of ψ. Truncation of r-th order Taylor polynomials to order $1 \leq s < r$ induces surjective submersions $\pi^r_s : J^r(\mathscr{M}, \mathscr{M}') \to J^s(\mathscr{M}, \mathscr{M}')$ which satisfy $\pi^r_r = \mathbb{1}$ and $\pi^s_t \circ \pi^r_s = \pi^r_t$ for all $0 \leq t \leq s \leq r$, which allow one to define the projective limit $\pi^\infty_0 : J^\infty(\mathscr{M}, \mathscr{M}') \to \mathscr{M} \times \mathscr{M}'$, called the *infinite-order jet bundle* of $\mathscr{C}^\infty(\mathscr{M}, \mathscr{M}')$. One can then identify the sequence $(j^r\psi)_{r\geq 0}$ of jet prolongations with a section $j^\infty\psi$ of $J^\infty(\mathscr{M}, \mathscr{M}')$, called simply the *infinite-order jet prolongation* of ψ. $J^\infty(\mathscr{M}, \mathscr{M}')$, being a countable projective limit of second-countable, finite-dimensional manifolds, can be made into a second-countable, metrizable Fréchet manifold [63]. If $\pi : \mathscr{E} \to \mathscr{M}$ is a fiber bundle over $\mathscr{M}$, we can define the subspace $J^r(\pi) \subset J^r(\mathscr{M}, \mathscr{E})$ of r-jets $X = j^r\psi(p)$ of smooth *sections* ψ of π (i.e. smooth maps from $\mathscr{M}$ to $\mathscr{E}$ satisfying $\pi \circ \psi = \mathbb{1}_{\mathscr{M}}$), $1 \leq r \leq \infty$. Then we can identify $\pi^r_0|_{J^r(\pi)}$ with $\mathrm{pr}_2 \circ \pi^r_0$, and we call the affine bundle $\pi^r_0 : J^r(\pi) \to \mathscr{E}$ the *r-th order jet bundle* of π.

2.2. **Topology and geometry of the space of field configurations.** Let $(\mathscr{M}, g)$ be a globally hyperbolic space-time, and $\mathscr{C}^\infty(\mathscr{M}) \doteq \mathscr{C}^\infty(\mathscr{M}, \mathbb{R})$ be the space of real-valued smooth functions on $\mathscr{M}$. We call $\mathscr{C}^\infty(\mathscr{M})$ a(n *off-shell*) *space of (real scalar) field configurations*[2]. It can be topologized in two different ways by means of the infinite-order jet prolongation of its elements, as follows. Let $\mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$ be the space of continuous functions from $\mathscr{M}$ into $J^\infty(\mathscr{M}, \mathbb{R})$. The *compact-open* topology on $\mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$ is generated by the sub-basis

$$\mathscr{U}_{K,V} = \{X \in \mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R})) \mid X(K) \subset V\} ,$$

for all $K \subset \mathscr{M}$ compact, $V \subset J^\infty(\mathscr{M}, \mathbb{R})$ open. The initial topology on $\mathscr{C}^\infty(\mathscr{M}) \ni \varphi$ induced by the compact-open topology on $\mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$ through the map $\varphi \mapsto j^\infty\varphi$ is also called the *compact-open* topology on $\mathscr{C}^\infty(\mathscr{M})$. The *graph* (or *Whitney*) topology on $\mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$, on its turn, is given by taking

$$\mathscr{U}_W = \{X \in \mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R})) \mid (p, X(p)) \in W \text{ for all } p \in \mathscr{M}\} ,$$

for all $W \subset \mathscr{M} \times J^\infty(\mathscr{M}, \mathbb{R})$ open in the product topology, as a basis of open sets. Obviously, to have $\mathscr{U}_W \neq \varnothing$ one needs W to satisfy $\mathrm{pr}_1(W) = \mathscr{M}$. As $J^\infty(\mathscr{M}, \mathbb{R})$ is metrizable and $\mathscr{M}$ is paracompact, another basis for this topology is given around any $Y \in \mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$ by $\{X \in \mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R})) \mid d(X(p), Y(p)) < \epsilon(p)\}$, for all positive $\epsilon \in \mathscr{C}(\mathscr{M}, \mathbb{R})$. The initial topology on $\mathscr{C}^\infty(\mathscr{M}) \ni \varphi$ induced by the graph topology on $\mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$ through the single map $\varphi \mapsto j^\infty\varphi$ is called the *Whitney* topology on $\mathscr{C}^\infty(\mathscr{M})$. It is in general finer than the compact-open topology, and coincides with the latter if and only if $\mathscr{M}$ is compact, which is *not* our case. On the other hand, notice that since $\mathscr{M}$ is locally compact (for $\mathscr{M}$ is finite dimensional) and second countable, we have that $\mathscr{M}$ is *σ-compact*, that is, $\mathscr{M}$ admits a so-called *exhaustion* by a sequence $K_n \subset \mathring{K}_{n+1}$ of compact regions $K_n \subset \mathscr{M}$, which means that $\cup^\infty_{n=1} K_n = \mathscr{M}$. We can then use any exhaustion $(K_n)_{n\geq 1}$ of $\mathscr{M}$ to show that any set $\mathscr{U}_W$ as above must be a *G_δ set* (i.e. a countable intersection of open sets) in the compact-open topology of $\mathscr{C}(\mathscr{M}, J^\infty(\mathscr{M}, \mathbb{R}))$. Indeed, we have that

$$\mathscr{U}_W = \bigcap_{n=1}^\infty \mathscr{U}_{K_n, \mathrm{pr}_2(W)} ,$$

[2]Some physics texts, such as [30], call $\mathscr{C}^\infty(\mathscr{M})$ the *space of field histories* on $\mathscr{M}$.

where pr_2 is an open mapping. Therefore, the Whitney topology on $\mathscr{C}^\infty(\mathscr{M})$ admits a basis made of G_δ subsets of $\mathscr{C}^\infty(\mathscr{M})$ in the compact-open topology.

The compact-open topology on $\mathscr{C}^\infty(\mathscr{M}) \ni \varphi$ can be understood as the topology of uniform convergence of derivatives of all orders $k \geq 0$ on compact regions $K \subset \mathscr{M}$, as induced by the seminorms

$$\begin{aligned}\|\varphi\|_{\infty,k,K} &\doteq \sup_{p\in K}\sqrt{\sum_{j=0}^{k}|\nabla^j\varphi(p)|_e^2}\ , \\ |\nabla^j\varphi|_e^2 &\doteq \otimes^j e^{-1}(\nabla^j\varphi,\nabla^j\varphi)\ ,\end{aligned} \tag{1}$$

where $\otimes^j e^{-1}$ is the Riemannian metric induced on the bundle $\otimes^j T^*\mathscr{M}$ of covariant tensors of rank j on $\mathscr{M}$ by a Riemannian metric e on $T\mathscr{M}$, and $\nabla^j\varphi$ is the iterated covariant derivative of order j of φ with respect to a torsion-free connection ∇ on $T\mathscr{M}$, given recursively by

$$\begin{aligned}\nabla^1\varphi &= \nabla\varphi = \mathrm{d}\varphi\ , \\ \nabla^j\varphi(X_1,\ldots,X_j) &= \nabla_{X_1}\nabla^{j-1}\varphi(X_2,\ldots,X_j) \\ &\quad -\sum_{l=2}^{j}\nabla^{j-1}\varphi(X_2,\ldots,X_{l-1},\nabla_{X_1}X_l,X_{l+1},\ldots,X_j)\ .\end{aligned} \tag{2}$$

A countable family of seminorms is obtained by exploiting the σ-compactness of $\mathscr{M}$ and choosing an exhaustion $(K_n)_{n\geq 1}$ of $\mathscr{M}$ as above. The topology induced by the seminorms $\|\cdot\|_{\infty,k,K_n}$ is then independent of the choice of e, ∇ and the exhaustion $(K_n)_{n\in\mathbb{N}}$. It is clearly a vector space topology with respect to the standard vector space operations in a space of vector bundle sections, and gives rise to a Fréchet space structure on $\mathscr{C}^\infty(\mathscr{M})$. An equivalent, separating family of seminorms generating this topology is given by

$$\|\varphi\|_{\infty,k,f} \doteq \sup_{p\in\mathscr{M}}\sqrt{\sum_{j=0}^{k}|f(p)\nabla^j\varphi(p)|_e^2}\ , \tag{3}$$

where f runs over the space $\mathscr{C}_c^\infty(\mathscr{M}) \doteq \mathscr{C}_c^\infty(\mathscr{M},\mathbb{R})$ of real-valued smooth functions with compact support. To see the equivalence, let $(f_n)_{n\in\mathbb{N}}$ be a sequence in $\mathscr{C}_c^\infty(\mathscr{M})$ taking values in $[0,1]$ such that $f_n \equiv 1$ in K_n and $\operatorname{supp} f_n \subset \mathring{K}_{n+1}$, where $(K_n)_{n\in\mathbb{N}}$ is the exhaustion of $\mathscr{M}$ defined above. Then one clearly has $\|\varphi\|_{\infty,k,K_n} \leq \|\varphi\|_{\infty,k,f_n} \leq \|\varphi\|_{\infty,k,K_{n+1}}$ for all $\varphi \in \mathscr{C}^\infty(\mathscr{M})$. Finally, yet another equivalent, separating family of seminorms generating the compact-open topology which will play a major role in this work is given by the *local (L^2) Sobolev seminorms*

$$\|\varphi\|_{2,k,K} \doteq \sqrt{\sum_{j=0}^{k}\int_K|\nabla^j\varphi|_e^2\mathrm{d}\mu_e}\ , \quad K \subset \mathscr{M} \text{ compact}, \mathring{K} \neq \varnothing\ , \tag{4}$$

$$\|\varphi\|_{2,k,f} \doteq \sqrt{\sum_{j=0}^{k}\int_{\mathscr{M}}|f\nabla^j\varphi|_e^2\mathrm{d}\mu_e}\ , \quad f \in \mathscr{C}_c^\infty(\mathscr{M})\ , \tag{5}$$

where $\mathrm{d}\mu_e$ is the volume element associated to the Riemannian metric e on $\mathscr{M}$. The equivalence can be established by means of the sequence $(f_n)_{n\in\mathbb{N}}$ defined above together with the Sobolev inequalities, using a partition of unity subordinated to a finite covering of supp f_n by suitable domains of coordinate charts for each $n \in \mathbb{N}$.

2.2.1. Remark. Formulae (1)–(5) can be extended to the space $\Gamma^\infty(\pi)$ of smooth sections of a vector bundle $\pi : \mathscr{E} \to \mathscr{M}$ over $\mathscr{M}$: given a torsion-free connection $\bar{\nabla}$ on $\mathscr{E}$ and a torsion-free connection ∇ on $T\mathscr{M}$, we can combine them into a torsion-free connection on $\otimes^k T^*\mathscr{M} \otimes \mathscr{E}$ for all k by using Leibniz's rule. We denote such a connection by ∇ for all $k \geq 0$, since there will be no danger of confusion. Once we write $\nabla^1\vec{\varphi}(X) = \nabla_X\vec{\varphi}$ for all $\vec{\varphi} \in \Gamma^\infty(\pi)$, $X \in \Gamma^\infty(T\mathscr{M} \to \mathscr{M})$, we can define k-th order iterated covariant derivatives $\nabla^k\vec{\varphi}$ of $\vec{\varphi} \in \Gamma^\infty(\pi)$ for all $k \geq 2$ by means of (2). We can now endow $\mathscr{E}$ with a Riemannian fiber metric $\bar{e}$ and define

$$|\nabla^k\vec{\varphi}|^2_{\bar{e}} = ((\otimes^k\bar{e}^{-1}) \otimes \bar{e})(\nabla^k\vec{\varphi}, \nabla^k\vec{\varphi}) \; . \tag{6}$$

Substituting (6) into (1) and (3)–(5) allows us to define the seminorms $\|\vec{\varphi}\|_{p,k,f}$, $\|\vec{\varphi}\|_{p,k,K}$ of $\vec{\varphi} \in \Gamma^\infty(\pi)$ for all $f \in \mathscr{C}^\infty_c(\mathscr{M})$, $\varnothing \neq \mathring{K} \subset K \subset \mathscr{M}$ compact, $p = 2, \infty$.

The Whitney topology on $\mathscr{C}^\infty(\mathscr{M})$, unlike the compact-open topology, is *not* a vector space topology in general. Since a sequence $(\varphi_n)_{n\in\mathbb{N}}$ converges to $\psi \in \mathscr{C}^\infty(\mathscr{M})$ in this topology if and only if there is a compact subset $K \subset \mathscr{M}$ such that $\psi_n(p) = \psi(p)$ for all $p \in \mathscr{M} \smallsetminus K$ and ψ_n converges uniformly to ψ on K together with all its derivatives [63], we see that scalar multiplication is not Whitney-continuous at zero unless $\mathscr{M}$ is compact.

Nonetheless, the Whitney topology induces on $\mathscr{C}^\infty(\mathscr{M})$ the structure of a *flat affine manifold*, modelled over the subspace $\mathscr{C}^\infty_c(\mathscr{M})$. To wit, for every $\varphi \in \mathscr{C}^\infty(\mathscr{M})$ there is an open neighborhood basis on φ of the form $\mathscr{U} + \varphi = \{\varphi + \vec{\varphi} \mid \vec{\varphi} \in \mathscr{U}\}$, where $\mathscr{U}$ runs over a basis of open neighborhoods of zero in $\mathscr{C}^\infty_c(\mathscr{M})$ in the latter's usual inductive limit topology. In particular, the connected component of φ in the Whitney topology is exactly $\varphi + \mathscr{C}^\infty_c(\mathscr{M})$. The coordinate chart associated to $\mathscr{U} + \varphi$ is then given by $\kappa_\varphi(\varphi + \vec{\varphi}) = \vec{\varphi}$, and the coordinate change map from $\mathscr{U}_1$ to $\mathscr{U}_2$ is given by $\kappa_{\varphi_2} \circ \kappa^{-1}_{\varphi_1}(\vec{\varphi}_1) = \vec{\varphi}_1 + (\varphi_1 - \varphi_2)$, which is clearly affine. We remark that, due to the aforementioned connectedness property of the Whitney topology, the respective domains $\mathscr{U}_1 + \varphi_1$, $\mathscr{U}_2 + \varphi_2$ of κ_{φ_1} and κ_{φ_2} have nonvoid intersection if and only if $\varphi_1 - \varphi_2$ has compact support, in which case we conclude from the argument in the previous paragraph that $\kappa^{-1}_{\varphi_1} \circ \kappa_{\varphi_2}$ is even continuous with respect to the Whitney topology.

As argued in Appendix A, the notion of smooth curves in the modelling space $\mathscr{C}^\infty_c(\mathscr{M})$ allows one as well to use the atlas

$$\mathfrak{U} = \{(\mathscr{U} + \varphi, \kappa_\varphi) \mid \mathscr{U} \subset \mathscr{C}^\infty_c(\mathscr{M}) \ni 0 \text{ open}, \varphi \in \mathscr{C}^\infty(\mathscr{M})\} \; . \tag{7}$$

we have built in the previous paragraph to induce a *smooth* manifold structure on $\mathscr{C}^\infty(\mathscr{M})$. In particular, due to the affine structure of $\mathscr{C}^\infty(\mathscr{M})$, the tangent and cotangent bundles of $\mathscr{C}^\infty(\mathscr{M})$ are trivial, being respectively given by

$$\begin{aligned} T\mathscr{C}^\infty(\mathscr{M}) &= \mathscr{C}^\infty(\mathscr{M}) \times \mathscr{C}^\infty_c(\mathscr{M}) \; , \\ T^*\mathscr{C}^\infty(\mathscr{M}) &= \mathscr{C}^\infty(\mathscr{M}) \times \mathscr{D}'(\wedge^d T^*\mathscr{M} \to \mathscr{M}) \; , \end{aligned}$$

where $\mathscr{D}'(\wedge^d T^*\mathscr{M} \to \mathscr{M}) = \mathscr{C}^\infty_c(\mathscr{M})'$ is the space of d-form-valued distributions on $\mathscr{M}$. We endow $T\mathscr{C}^\infty(\mathscr{M})$ with a flat connection, to be defined as follows. The parallel transport operator

$P_\gamma^{\lambda_1,\lambda_2}(\gamma(\lambda_1),\vec{t}) = (\gamma(\lambda_2),\vec{t})$ on $T\mathbb{R} = \mathbb{R}\times\mathbb{R}$ along $\gamma \in \mathscr{C}^\infty(\mathbb{R},\mathbb{R})$ associated to the standard flat connection on the target space $\mathbb{R}$ of $\mathscr{C}^\infty(\mathscr{M})$ can be pulled back to $T\mathscr{C}^\infty(\mathscr{M})$ by setting

$$P_\alpha^{\lambda_1,\lambda_2}(\alpha(\lambda_1,\cdot),\vec{\varphi})(p) \doteq (\alpha(\lambda_2,p),\vec{\varphi}(p)) = P_{\alpha(\cdot,p)}^{\lambda_1,\lambda_2}(\alpha(\lambda_1,p),\vec{\varphi}(p)) \ ,$$

where $\alpha : \mathbb{R}\times\mathscr{M} \to \mathbb{R}$ defines a smooth curve in $\mathscr{C}^\infty(\mathscr{M})$ with respect to the Whitney topology (see Appendix A). Given sections X, Y of $T\mathscr{C}^\infty(\mathscr{M})$ taking smooth curves in $\mathscr{C}^\infty(\mathscr{M})$ with respect to the Whitney topology to smooth curves in $T\mathscr{C}^\infty(\mathscr{M})$, we may define at each $\varphi \in \mathscr{C}^\infty(\mathscr{M})$

$$D_Y X[\varphi] = \frac{\partial}{\partial\lambda}|_{\lambda=0}\left(P_\alpha^{\lambda,0}X[\alpha(\lambda,\cdot)]\right) \ , \tag{8}$$

where $\alpha : \mathbb{R}\times\mathscr{M} \to \mathbb{R}$ is a smooth curve in $\mathscr{C}^\infty(\mathscr{M})$ such that $\alpha(0,p) = \varphi(p)$ and $\frac{\partial}{\partial\lambda}|_{\lambda=0}\alpha(\lambda,p) = \mathrm{pr}_2(Y[\varphi])(p)$. An example of such a curve is

$$\alpha(\lambda,p) = \varphi(p) + \lambda\mathrm{pr}_2(Y[\varphi])(p) \ . \tag{9}$$

We say that D is the *ultralocal lift* of the standard flat connection on the target space[3] $\mathbb{R}$, for $D_Y X[\varphi](p)$ depends only on $\varphi(p)$. In what follows, we automatically extend D to all covariant and contravariant tensor fields on $\mathscr{C}^\infty(\mathscr{M})$ (see Appendix A for a precise definition) in the standard fashion, i.e. by tensoring and taking adjoint inverses of the parallel transport operator.

It is clear from the above definition that P_α defined above is the parallel transport operator along α associated to D. It is a consequence of the ultralocality of D, however, that much more is true:

(1) The geodesic α starting at $(\varphi,\vec{\varphi}) \in T\mathscr{C}^\infty(\mathscr{M})$ is given by (9). As a consequence, the exponential map $\exp_D : T\mathscr{C}^\infty(\mathscr{M}) \to \mathscr{C}^\infty(\mathscr{M})\times\mathscr{C}^\infty(\mathscr{M})$ of D is complete and given by

$$\exp_D(\varphi,\vec{\varphi}) = (\varphi,\varphi+\vec{\varphi}) = (\varphi,\kappa_\varphi(\vec{\varphi})) \ .$$

In other words, the chart κ_φ is precisely the normal coordinate chart around φ associated to D.

(2) The curvature tensor of D is given by

$$\mathrm{Riem}_D(X,Y)[\varphi](p) = \mathrm{Riem}_{\varphi(p)}(X[\varphi](p),Y[\varphi](p)) = 0 \ ,$$

where $\mathrm{Riem}_t \equiv 0$ is the Riemann curvature of the standard flat connection on the target space $\mathbb{R}$ at the point t. As a consequence, the k-th order iterated covariant derivative $D^k X(Y_1,\ldots,Y_k)$ of a tensor field X along vector fields $Y_1,\ldots,Y_k$ is *symmetric* in $Y_1,\ldots,Y_k$ for all k.

We close this Subsection with two technical Lemmata. The first is a simple but useful manifestation of the fact that the Whitney topology is finer than the compact-open topology:

[3] In the context of field theory, such connections were formally introduced in [30]. They allow one to extend to higher orders the notion of *fiber derivative* employed in the calculus of variations [11]. For a precise, general concept of ultralocal lifts of connections on target spaces, see for instance Example 4.5.3, pp. 94 of [45].

2.2.2. Lemma. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open with respect to the Whitney topology. Then for every $\varphi_0 \in \mathscr{U}$, $V \subset \mathscr{M}$ open, there is a $\varphi \in \mathscr{U}$ such that* $\operatorname{supp}(\varphi - \varphi_0) \neq \varnothing$ *is compact and contained in V, and $\lambda(\varphi - \varphi_0) \in \mathscr{U} - \varphi_0$ for all $\lambda \in [-1, 1]$.*

Proof. By the reasoning in the paragraphs preceding this Lemma, there is an absolutely convex open neighborhood $\mathscr{V}$ of zero in $\mathscr{C}^\infty_c(\mathscr{M})$ contained in $\mathscr{U} - \varphi_0$. Given any $\varphi_1 \in \mathscr{C}^\infty_c(\mathscr{M})$, there is a $t_1 > 0$ such that $t\psi_1 \in \mathscr{V}$ for all $t \in \mathbb{R}$ with $|t| \leq t_1$, since $\mathscr{V}$ is absorbent. Choose φ_1 with $\operatorname{supp}\varphi_1 \subset V$, set $\varphi = \varphi_0 + t_1\varphi_1$, and we are done. □

The second allows one to strengthen the conclusion of Lemma 2.2.2:

2.2.3. Lemma. *Let $\varphi_0 \in \mathscr{C}^\infty(\mathscr{M})$, $r \in \mathbb{N} \cup \{0\}$, $p \in \mathscr{M}$. Then there is $\varphi \in \mathscr{C}^\infty(\mathscr{M})$ satisfying $j^r\varphi(p) = j^r\varphi_0(p)$, such that* $\operatorname{supp}(\varphi - \varphi_0) \neq \varnothing$ *is contained in an arbitrarily small open neighborhood U of p with compact closure K, and $\|\varphi' - \varphi_0\|_{\infty,r,K} < \epsilon$ for $\epsilon > 0$ arbitrarily small.*

Proof. Since we are dealing with a local statement, we assume without loss of generality that $\mathscr{M} = \mathbb{R}^d$, $p = 0$, $\varphi_0 \equiv 0$, e is the standard Euclidean metric and $\nabla = \partial$ is the associated (flat) Levi-Civita connection. Let now $\varphi' \in \mathscr{C}^\infty(\mathscr{M})$ be such that $j^r\varphi'(p) = j^r\varphi_0(p)$; it follows from Taylor's formula with remainder that $\partial^\alpha\varphi'(x) = O(\|x\|^{r+1-|\alpha|})$ as $\|x\| \to 0$, for all multi-indices α such that $0 \leq |\alpha| \leq r$. Let $f \in \mathscr{C}^\infty_c(\mathbb{R}^d)$ such that $f(x) = 1$ for $\|x\| \leq \frac{1}{2}$ and $f(x) = 0$ for $\|x\| \geq 1$. Given $R > 0$, define $f_R(x) = f(R^{-1}x)$. It follows from the chain rule that $\partial^\alpha f_R(x) = R^{-|\alpha|}(\partial^\alpha f)(R^{-1}x)$. Define now $\varphi = f_R\varphi'$; Leibniz's rule gives us that

$$\|\varphi\|_{\infty,r,K} \leq C_{r,K}\|\varphi'\|_{\infty,r,\overline{B_R(0)}}\|f\|_{\infty,r,\overline{B_1(0)}}R$$

for all $K \subset \mathbb{R}^d$ such that $\mathring{K} \supset \overline{B_R(0)}$, where $B_\lambda(0) = \{x \in \mathbb{R}^d \mid \|x\| < \lambda\}$. Taking R sufficiently small yields the desired bound. □

2.3. **Functionals as observables.** Our observable quantities will be maps $F : \mathscr{U} \to \mathbb{C}$ which we call *functionals*, where $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ is usually some open set in the compact-open topology, though we may occasionally consider more general subsets. The need to localize the domain of definition of functionals comes from the fact that, in the study of nonlinear equations of motion, one is led to consider functionals which are not *a priori* defined for *all* field configurations due to the existence of solutions blowing up in finite time. We shall now introduce a concept which tells us in which sense functionals are localized in a certain region of space-time, following [15].

2.3.1. Definition (Space-time support). Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$. The *space-time support* $\operatorname{supp} F$ of a functional $F : \mathscr{U} \to \mathbb{C}$ is the (closed) subset composed by the points $p \in \mathscr{M}$ such that for any neighborhood U of p we can find $\psi \in \mathscr{U}, \varphi \in \mathscr{U} - \psi$ with $\operatorname{supp}\varphi \subset U$ for which $F(\varphi + \psi) \neq F(\psi)$. The space of functionals over $\mathscr{U}$ with *compact* space-time support in $\mathscr{M}$ will be denoted by $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$.

In other words, a functional F is insensitive to disturbances of its argument which are localized outside $\operatorname{supp} F$. As shown by Lemma 2.3.8 below, Definition 2.3.1 gives a nonlinear generalization of the notion of support of a distribution. It is important, on the one hand, to emphasize that Definition 2.3.1 depends on the domain of definition $\mathscr{U}$ of F. For instance, if we restrict F to a smaller domain of definition $\mathscr{V} \subset \mathscr{U}$, then $\operatorname{supp} F$ will in general be a *smaller* subset of $\mathscr{M}$ (see Remark 2.3.2 right below). On the other hand, the domain of definition of F will always be clear from the context, so we refrain from referring to it in the notation.

2.3.2. REMARK. Let us give some simple examples of functionals. Given a compact region $K \subset \mathscr{M}$ of the space-time manifold $\mathscr{M}$ and $0 \leq f \in \mathscr{C}^\infty_c(\mathscr{M})$ satisfying $\int_{\mathscr{M}} f \mathrm{d}\mu_g = 1$, we define the functionals $F, G, H : \mathscr{C}^\infty(\mathscr{M}) \to \mathbb{C}$ as

$$F(\varphi) = \|\varphi\|_{\infty,0,K} = \sup_K |\varphi| \ , \quad G(\varphi) = \int_{\mathscr{M}} f\varphi \mathrm{d}\mu_g \ , \quad H(\varphi) = \begin{cases} \frac{1}{1+\sup_{\mathscr{M}} |\varphi|} & \varphi \text{ bounded} \ , \\ 0 & \text{otherwise} \ . \end{cases} \tag{10}$$

One clearly sees that F and G have compact space-time support (indeed, we have that $\operatorname{supp} F = K$ and $\operatorname{supp} G = \operatorname{supp} f$), whereas H does not. Other examples are the local Sobolev seminorms $\|\varphi\|_{2,k,K}$ and $\|\varphi\|_{2,k,f}$ respectively defined in (4) and (5). We shall now give a slightly more complicated example which explicitly displays the dependence of the space-time support of a functional on the latter's domain. Let $\chi : \mathbb{R} \to [0, 1]$ be a smooth function such that $\chi^{-1}(1) = [-1, 1]$ and $\chi^{-1}(0) = \mathbb{R} \smallsetminus (-2, 2)$. Setting $\chi_R(t) = \chi(R^{-1}t)$ for $R > 0$, define

$$G_R(\varphi) = \exp\left(1 - \chi_R \circ G(\varphi)\right) \ , \tag{11}$$

with G as defined in (10). Let now $\mathscr{U}_{R'} = \{\varphi \in \mathscr{C}^\infty(\mathscr{M}) \mid \|\varphi\|_{\infty,0,\operatorname{supp} f} < R'\}$ for $R' > 0$; we have that

$$\operatorname{supp} G_R|_{\mathscr{U}_{R'}} = \begin{cases} \varnothing & R' \leq R \ , \\ \operatorname{supp} f & R' > R \ . \end{cases}$$

Indeed, in the first case, we have that $G_R|_{\mathscr{U}_{R'}} \equiv 1$.

We endow each $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$, for $\mathscr{U} \ni \varphi$ running over the compact-open topology of $\mathscr{C}^\infty(\mathscr{M})$, with the following pointwise algebraic operations:

- Sum $F, G \mapsto (F + G)(\varphi) \doteq F(\varphi) + G(\varphi)$;
- Product $F, G \mapsto (F \cdot G)(\varphi) \doteq F(\varphi)G(\varphi)$;
- Involution $F \mapsto F^*(\varphi) \doteq \overline{F(\varphi)}$;
- Multiplication by scalars $z \in \mathbb{C}$, $F \mapsto (z \cdot F)(\varphi) \doteq zF(\varphi)$;
- Unit $\mathbb{1} : \varphi \mapsto 1$.

Now we show that the algebraic operations of $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ preserve space-time supports. As a direct consequence, these operations turn $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ into a commutative unital *-algebra. Firstly, it is trivial to check that the scalar multiplication by any $0 \neq \lambda \in \mathbb{C}$ and the involution leave the support unchanged, whereas any scalar multiple of $\mathbb{1}$ has empty space-time support. The full assertion is then a consequence of the following

2.3.3. LEMMA. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$, F, G functionals over $\mathscr{U}$. Then:*

- *The sum $F + G$ satisfies*

$$\operatorname{supp}(F + G) \subset \operatorname{supp} F \cup \operatorname{supp} G \ ;$$

- *The product* $F \cdot G$ *satisfies*

$$\mathrm{supp}\,(F \cdot G) \subset \mathrm{supp}\, F \cup \mathrm{supp}\, G\ .$$

In particular, $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ *is a commutative unital *-algebra.*

Proof. Let us assume that $p \notin \mathrm{supp}\, F \cup \mathrm{supp}\, G$, that is,

$$p \in \complement(\mathrm{supp}\, F \cup \mathrm{supp}\, G) = \complement\mathrm{supp}\, F \cap \complement\mathrm{supp}\, G\ .$$

By the definition of space-time support, there is an open neighborhood V of p such that for all $\varphi_0 \in \mathscr{U}$, $\varphi \in \mathscr{U} - \varphi_0$ satisfying $\mathrm{supp}\,\varphi \subset V$, we have that $F(\varphi_0 + \varphi) = F(\varphi_0)$ and $G(\varphi_0 + \varphi) = G(\varphi_0)$, hence $(F + G)(\varphi_0 + \varphi) = (F + G)(\varphi_0)$ and $(F \cdot G)(\varphi_0 + \varphi) = (F \cdot G)(\varphi_0)$ for all such φ_0, φ. This entails that $p \notin \mathrm{supp}\,(F + G)$ and $p \notin \mathrm{supp}\,(F \cdot G)$, as desired. ☐

We emphasize that, unlike for supports of functions on $\mathscr{M}$, the stronger property $\mathrm{supp}(F \cdot G) \subset \mathrm{supp}\, F \cap \mathrm{supp}\, G$ *does not* hold for space-time supports of functionals. A counter-example is given by $F = G_{R_1}$ and $G = G_{R_2}$ with $R_1 < R_2$, where G_R is defined for all $R > 0$ in (11). The reason is that the notion of space-time support is a *relative* one; it is not necessarily true that $F(\varphi)$ vanishes if φ is supported outside $\mathrm{supp}\, F$. For instance, given $f \in \mathscr{C}^\infty(\mathscr{M})$ with $\int_{\mathscr{M}} f \mathrm{d}\mu_g = 1$, we have that the functional $F(\varphi) = \int_{\mathscr{M}} f \exp(\varphi) \mathrm{d}\mu_g$ satisfy $F(\varphi) = 1$ for all $\varphi \in \mathscr{C}^\infty(\mathscr{M})$ such that $\mathrm{supp}\,\varphi \cap \mathrm{supp}\, f = \varnothing$. In the above counter-example, we also have that G_R is nowhere vanishing for all $R > 0$.

The *raison d'être* of Definition 2.3.1 becomes evident if one assumes the following property:

2.3.4. Definition (Additivity). Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$. A functional $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ is said to be *additive* if for all $\varphi_1 \in \mathscr{U}, \varphi_2, \varphi_3 \in \mathscr{U} - \varphi_1$ such that $\varphi_2 + \varphi_3 \in \mathscr{U} - \varphi_1$ and $\mathrm{supp}\,\varphi_2 \cap \mathrm{supp}\,\varphi_3 = \varnothing$ we have

$$F(\varphi_1 + \varphi_2 + \varphi_3) = F(\varphi_1 + \varphi_2) - F(\varphi_1) + F(\varphi_1 + \varphi_3) \tag{12}$$

or, more concisely,

$$F_{\varphi_1}(\varphi_2 + \varphi_3) = F_{\varphi_1}(\varphi_2) + F_{\varphi_1}(\varphi_3) \tag{13}$$

where $F_\varphi(\psi) \doteq F(\varphi + \psi) - F(\varphi)$.

As it will be seen shortly, this notion essentially captures what it means for $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ to be *local* with respect to the space-time manifold $\mathscr{M}$. For instance, in the case that $\mathscr{U} = \mathscr{C}^\infty(\mathscr{M})$ we have[4] the following nonlinear analog of a partition of unity, introduced in Lemma 3.2 of [15]. Its simple proof is included here for the convenience of the reader.

2.3.5. Lemma. *Any additive functional* $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{C}^\infty(\mathscr{M}))$ *can be decomposed as a finite sum of additive functionals with arbitrarily small space-time support.*

[4]The restriction on $\mathscr{U}$ can be weakened in a certain sense. See Lemma 3.1.5.

Proof. First of all, let us endow $\mathscr{M}$ with a complete auxiliary Riemannian metric h, whose associated distance function is given by $d_h : \mathscr{M} \times \mathscr{M} \to [0, +\infty)$. In what follows, by "distance" between $p, q \in \mathscr{M}$ we mean $d_h(p, q)$, and a "ball of radius R", an open set $\{q \in \mathscr{M} : d_h(p, q) < R\}$ for some $p \in \mathscr{M}$.

Let $\epsilon > 0$ be arbitrary, and $(B_i)_{i=1,\ldots,n}$ a finite covering of $\operatorname{supp} F$ by balls of radius $\epsilon/4$. Associate to this covering a subordinate partition of unity $(\chi_i)_{i=1,\ldots,n}$. By a repeated use of the additivity of F we arrive at a decomposition of the form

$$F = \sum_I s_I F_I \ , \tag{14}$$

with $s_I \in \{\pm 1\}$, $F_I(\varphi) = F(\varphi \sum_{i \in I} \chi_i)$, where $\varphi \in \mathscr{C}^\infty(\mathscr{M})$ and I runs over all subsets of $\{1, \ldots, n\}$ such that $B_i \cap B_j \neq \varnothing$ for all $i, j \in I$. It is obvious that F_I is again an additive functional, and from the definition of space-time support we immediately find that $\operatorname{supp} F_I \subset \bigcup_{i \in I} B_i \doteq B_I$. Since any two points in B_I have distance less than ϵ, then each B_I is contained in a ball of radius ϵ. $\square$

2.3.6. Remark. The concept of an additive functional, although not exactly mainstream, is by no means new in the mathematical literature (consider [77] as a starting point). In the present case, it was motivated by the study of the set of possible counterterms generated by all choices of renormalization prescription in perturbative algebraic quantum field theory [35, 15]. We have already seen examples of additive functionals, such as the square of the local Sobolev seminorm (5). Counter-examples include the functional F defined in (10) and the functional G_R defined in (11).

A further property we will demand from our functionals concerns their differentiability. We will just spell the complete definition we need for convenience, which builds on the discussion in Appendix A.

2.3.7. Definition. Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology. We say that a functional $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ is *differentiable of order* m if for all $k = 1, \ldots, m$ the k-th order directional (Gâteaux) derivatives (henceforth called *functional derivatives*)

$$F^{(k)}[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k) = \left\langle F^{(k)}[\varphi], \vec{\varphi}_1 \otimes \cdots \otimes \vec{\varphi}_k \right\rangle \doteq \frac{\partial^k}{\partial \lambda_1 \cdots \partial \lambda_k}\Big|_{\lambda_1 = \cdots = \lambda_k = 0} F\left(\varphi + \sum_{j=1}^k \lambda_j \vec{\varphi}_j\right) \tag{15}$$

exist as jointly continuous maps from $\mathscr{U} \times \mathscr{C}^\infty(\mathscr{M})^k$ to $\mathbb{R}$, where $\langle \cdot, \cdot \rangle$ denotes dual pairing. In particular, for each φ fixed, $F^{(k)}[\varphi]$ is a distribution *density* of compact support on $\mathscr{M}^k$. If F is differentiable of order m for all $m \in \mathbb{N}$, we say that F is *smooth*.

In certain cases, we can extend Definition 2.3.7 to the case when $\mathscr{U}$ is no longer open (see Appendix A).

The relation of the notion of space-time support of a functional to the notion of support of a distribution can be made more transparent for *differentiable* elements of $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$:

2.3.8. LEMMA. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology and convex. If $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ is a differentiable functional of order one, then*

$$\operatorname{supp} F = \overline{\bigcup_{\varphi \in \mathscr{U}} \operatorname{supp} F^{(1)}[\varphi]} \ . \tag{16}$$

Proof. If $p \in \operatorname{supp} F$, then by definition there are $\varphi \in \mathscr{U}$, $\vec{\varphi} \in \mathscr{U} - \varphi$ with $\vec{\varphi}$ supported in a neighborhood of p such that $F(\varphi + \vec{\varphi}) \neq F(\varphi)$. By the fundamental theorem of Calculus (A.2), there is a $\lambda_0 \in (0,1)$ such that $F^{(1)}[\varphi + \lambda_0 \vec{\varphi}](\vec{\varphi}) \neq 0$ (this is the only place where convexity of $\mathscr{U}$ is used). This implies the inclusion $\operatorname{supp} F \subset \overline{\bigcup_{\varphi \in \mathscr{U}} \operatorname{supp} F^{(1)}[\varphi]}$.

For the opposite one we argue as follows. Let us suppose that $p \in \operatorname{supp} F^{(1)}[\varphi]$, then this means that there is a $\vec{\varphi} \in \mathscr{C}^\infty(\mathscr{M})$ supported in a neighborhood of p such that $F^{(1)}[\varphi](\vec{\varphi}) \neq 0$, whence it follows that $F(\varphi + \lambda \vec{\varphi}) \neq F(\varphi)$ for all λ chosen sufficiently small (depending on $\vec{\varphi}$) so that $\varphi + \lambda \vec{\varphi} \in \mathscr{U}$. We then conclude that $p \in \operatorname{supp} F$, i.e.

$$\operatorname{supp} F^{(1)}[\varphi] \subset \operatorname{supp} F \ .$$

Taking the union of the left-hand side with respect to all $\varphi \in \mathscr{U}$ and closing implies the thesis. □

We remark that the same argument used in Lemma 2.3.8 to prove the inclusion $\operatorname{supp} F^{(1)}[\varphi] \subset \operatorname{supp} F$ can be used to show that if F is differentiable of order $m \geq 1$, then $\operatorname{supp} F^{(k)}[\varphi] \subset (\operatorname{supp} F)^k$ for all $1 \leq k \leq m$.

We shall now display formula (16) in action using a specific example. Let $G_R = G_R|_{\mathscr{U}_{R'}} \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U}_{R'})$ be the functional defined as in (11). By Faà di Bruno's formula (A.7), one sees that G_R is smooth for all $R, R' > 0$. In particular, by the chain rule (A.3),

$$G_R^{(1)}[\varphi](\vec{\varphi}) = -\frac{1}{R} G_R(\varphi)(\chi')_R \circ G(\varphi) G(\vec{\varphi}) \ .$$

When $R' \leq R$, we have that $(\chi')_R \circ G(\varphi) = 0$ for all $\varphi \in \mathscr{U}_{R'}$, whence $G_R^{(1)}[\varphi] = 0$ for all such φ. If $R' > R$, then we have that $\operatorname{supp} G_R^{(1)}[\varphi] = \varnothing$ if $\|\varphi\|_{\infty,0,\operatorname{supp} f} \leq R$, and $\operatorname{supp} G_R^{(1)}[\varphi] = \operatorname{supp} f$ if $R < \|\varphi\|_{\infty,0,\operatorname{supp} f} < R'$.

2.3.9. REMARK. A natural question that arises at this point, whose answer is in general evaded in the literature, is how Definition 2.3.7 fits into the manifold structure of $\mathscr{C}^\infty(\mathscr{M})$ induced by the Whitney topology. This question is answered by means of the following fact: given any compact region $K \subset \mathscr{M}$ and any nonvoid subset $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$, one can uniquely extend any $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ with $\operatorname{supp} F \subset \mathring{K}$ to the subset $i_\chi^{-1}(\mathscr{U})$, where $i_\chi : \mathscr{C}^\infty(\mathscr{M}) \to \varphi_0 + \mathscr{C}_c^\infty(\mathscr{M})$ is defined by $i_\chi(\varphi) = \varphi_0 + \chi(\varphi - \varphi_0)$, $\varphi_0 \in \mathscr{U}$ is fixed and $\chi \in \mathscr{C}_c^\infty(\mathscr{M})$ satisfies $\chi(p) = 1$ for all $p \in K$. It is clear that i_χ is a continuous (in fact, even smooth) map from $\mathscr{C}^\infty(\mathscr{M})$ into itself, if the domain is endowed with the *compact-open* topology and the codomain is endowed with the *Whitney* topology. In particular, if $\mathscr{U}$ is a connected, Whitney-open neighborhood of φ_0, then $i_\chi^{-1}(\mathscr{U})$ is open in the compact-open topology, where $F^{(k)}$ becomes uniquely defined whenever it exists, for all $k \geq 1$. Moreover, since $\operatorname{supp} F^{(k)}[\varphi] \subset (\operatorname{supp} F)^k$, one also concludes that

$$F^{(k)}[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k) = F^{(k)}[\varphi](\chi\vec{\varphi}_1, \ldots, \chi\vec{\varphi}_k) = D^k F[\varphi](\chi\vec{\varphi}_1, \ldots, \chi\vec{\varphi}_k) \ , \tag{17}$$

where $\chi\vec{\varphi}_j$ is understood as the covariantly constant vector field $\varphi \mapsto (\varphi, \chi\vec{\varphi})$, $1 \leq j \leq k$. Since the left hand side of the above formula is independent of χ, we just write

$$F^{(k)}[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k) = D^k F[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k)\ . \tag{18}$$

In particular, D^kF defines a smooth tensor field on $\mathscr{C}^\infty(\mathscr{M})$ when the latter is endowed with the smooth manifold structure induced from $\mathscr{C}^\infty_c(\mathscr{M})$ (see Remark A.2 and the discussion preceding it).

Throughout the paper, our functionals F of interest will always be smooth functionals with compact space-time support. Thanks to Remark 2.3.9, if F is only defined in an open subset $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ in the Whitney topology, we can uniquely extend such a F to an open subset $\mathscr{C}^\infty(\mathscr{M}) \supset \tilde{\mathscr{U}} \supset \mathscr{U}$ in the compact-open topology and unambiguously define $F^{(k)}$ therein for all $k \geq 1$. Three very important spaces of such functionals are the following:

2.3.10. Definition. Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open with respect to the compact-open topology. The vector subspaces of $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ given by

$$\mathscr{F}_0(\mathscr{M}, \mathscr{U}) = \{F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U}) \text{ smooth } \mid F^{(k)}[\varphi] \in \Gamma^\infty_c(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k), \forall \varphi \in \mathscr{U},\ k \geq 1\}\ , \tag{19}$$

$$\mathscr{F}_{\mathrm{loc}}(\mathscr{M}, \mathscr{U}) = \{F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U}) \text{ smooth } \mid \operatorname{supp} F^{(2)}[\varphi] \subset \Delta_2(\mathscr{M}), \forall \varphi \in \mathscr{U}\} \text{ and} \tag{20}$$

$$\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U}) = \{F \in \mathscr{F}_{\mathrm{loc}}(\mathscr{M}, \mathscr{U}) \mid F^{(1)}[\varphi] \in \Gamma^\infty_c(\wedge^d T^*\mathscr{M} \to \mathscr{M}), \forall \varphi \in \mathscr{U}\}\ , \tag{21}$$

where $\Delta_k(\mathscr{M}) = \{(p, \ldots, p) \in \mathscr{M}^k : p \in \mathscr{M}\}$ is the small diagonal of $\mathscr{M}$ in $\mathscr{M}^k$, are said to be respectively the spaces of *regular*, *local* and *microlocal* functionals over $\mathscr{U}$.

Criterion (20) for locality of a functional was put forward in [35] in the case of functionals depending polynomially on the field configuration. We stress that $\mathscr{F}_0(\mathscr{M}, \mathscr{U})$ is even a *-subalgebra of $\mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$.

Microlocal functionals comprise many functionals of physical interest. For instance, let $\omega \in \Gamma^\infty(\wedge^d T^* J^r(\mathscr{M}, \mathbb{R}) \to J^r(\mathscr{M}, \mathbb{R}))$; given any $f \in \mathscr{C}^\infty_c(\mathscr{M})$, the functional

$$F(\varphi) = \int_{\mathscr{M}} f (j^r\varphi)^*\omega \tag{22}$$

is clearly seen to be microlocal over any $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ open in the compact-open topology. Conversely, it will be shown in Proposition 2.3.13 below that all microlocal functionals are essentially of this form. The above example becomes somewhat trivial if we take instead a closed p-form ω on $J^r(\mathscr{M}, \mathbb{R})$ with $p < d$, and define

$$G(\varphi) = \int_{\mathscr{N}} (j^r\varphi)^*\omega\ , \tag{23}$$

where $\mathscr{N} \subset \mathscr{M}$ is a compact, p-dimensional submanifold without boundary. More precisely, it can be shown [88] that $DG[\varphi](\vec{\varphi})$ for G as in (23) is represented by the integral over $\mathscr{N}$ of an *exact* p-form on $\mathscr{M}$, hence $DG[\varphi] = 0$ for all $\varphi \in \mathscr{U}$. In particular, $\operatorname{supp} G = \varnothing$, that is,

G is locally constant. If ω is not closed or $\mathscr{N}$ has a nonvoid boundary, then G is still a local functional, but *not* microlocal (see also example (25) below).

It is easy to display examples of smooth functionals with compact space-time support which are *not* local. If $F, G \in \mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$, Leibniz's rule (A.4) applied twice to $(F \cdot G)^{(2)}[\varphi](\vec{\varphi}_1, \vec{\varphi}_2)$ gives rise to a term of the form $F^{(1)}[\varphi](\vec{\varphi}_1)G^{(1)}[\varphi](\vec{\varphi}_2) + G^{(1)}[\varphi](\vec{\varphi}_1)F^{(1)}[\varphi](\vec{\varphi}_2)$, whose kernel for fixed φ is represented by a smooth, compactly supported density on $\mathscr{M}^2$ and hence *not* supported on $\Delta_2(\mathscr{M})$ unless it is identically zero, in which case either F or G must be constant. Hence, we conclude that $F \cdot G$ cannot be local if $\operatorname{supp} F, \operatorname{supp} G \neq \varnothing$. It follows from the same argument (using Faà di Bruno's formula (A.7) instead of Leibniz's rule) that if, for instance, $\psi : \mathbb{C} \to \mathbb{C}$ is entire analytic and not affine, and G is microlocal with $\operatorname{supp} G \neq \varnothing$, then $F = \psi \circ G$ cannot be local. A typical such example is

$$F(\varphi) = \exp\left(\int_{\mathscr{M}} \varphi\omega\right) \ , \quad \omega \in \Gamma^\infty_c(\wedge^d T^*\mathscr{M} \to \mathscr{M}) \ , \tag{24}$$

which even happens to be regular. In fact, one immediately sees that a regular functional is local if and only if it is affine, in which case it is also microlocal.

Finally, to display the difference between local and microlocal functionals, consider a closed, smooth timelike submanifold without boundary $\mathscr{N} \subset \mathscr{M}$ and with codimension $p > 0$ (e.g. a smooth timelike curve parametrized over $\mathbb{R}$). If $\iota : \mathscr{N} \hookrightarrow \mathscr{M}$ is the natural inclusion, X is a normal unit p-vector field on $\mathscr{N}$ with respect to g (suitably extended to an open neighborhood of $\mathscr{N}$ in $\mathscr{M}$) and $f \in \mathscr{C}^\infty_c(\mathscr{M})$, set

$$F(\varphi) = \int_{\mathscr{N}} \iota^*(\varphi f i_X \mathrm{d}\mu_g) \ . \tag{25}$$

F is clearly local, for $F^{(2)} \equiv 0$. However, $F^{(1)}[\varphi]$ is f times the submanifold measure induced by $\mathrm{d}\mu_g$ on $\mathscr{N}$, hence it is *not* a smooth density on $\mathscr{M}$ and thus F is not microlocal.

Returning to the general development of our framework, now we are in a position to make more precise the claim preceding Lemma 2.3.5, sharpening Lemma 3.1 of [15].

2.3.11. PROPOSITION. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open with respect to the compact-open topology, and $F \in \mathscr{F}_{00}(\mathscr{M}, \mathscr{U})$ be smooth. Then F belongs to $\mathscr{F}_{\mathrm{loc}}(\mathscr{M}, \mathscr{U})$ if and only if it is additive. Moreover, in this case we have that* $\operatorname{supp} F^{(k)}[\varphi] \subset \Delta_k(\mathscr{M})$ *for all $k \geq 2$, $\varphi \in \mathscr{U}$.*

Proof. ($\Leftarrow$) for any $k \geq 2$, assume that in the support of $F^{(k)}[\varphi]$ there are two points $x_i \neq x_j$. Then, there exist two smooth functions φ_i, φ_j such that $x_i \in \operatorname{supp} \varphi_i$, $x_j \in \operatorname{supp} \varphi_j$ and $\operatorname{supp} \varphi_i \cap \operatorname{supp} \varphi_j = \varnothing$. By additivity we split the right-hand side of the formula for $F^{(k)}$ in Definition 2.3.7 according to the supports of φ_i and φ_j, but the derivatives act always on all λ_j's, hence we get zero. In particular, the last assertion holds.
($\Rightarrow$) Assume that $\varphi_1, \varphi_2 \in \mathscr{V} \subset \mathscr{U} - \varphi$ are such that $\operatorname{supp} \varphi_1 \cap \operatorname{supp} \varphi_2 = \varnothing$, where $\mathscr{V}$ is an absolutely convex open neighborhood of zero. Using the fundamental theorem of Calculus (A.2), we write

$$F_\varphi(\varphi_1 + \varphi_2) = F_\varphi(\varphi_1) + \int_0^1 \mathrm{d}\lambda \, \frac{\mathrm{d}}{\mathrm{d}\lambda} \, F_\varphi(\varphi_1 + \lambda\varphi_2) \ .$$

The integral in the right hand side can be rewritten as

$$\int_0^1 \mathrm{d}\lambda\, \frac{\mathrm{d}}{\mathrm{d}\lambda}\, F_\varphi(\varphi_1+\lambda\varphi_2) = F_\varphi(\varphi_2) + \int_0^1 \mathrm{d}\lambda \int_0^1 \mathrm{d}\mu\, F^{(2)}[\mu\varphi_1+\lambda\varphi_2+\varphi](\varphi_1,\varphi_2)\ .$$

By locality, $F^{(2)}[\mu\varphi_1+\lambda\varphi_2+\varphi]$ is supported in $\Delta_2(\mathscr{M})$, but by our initial assumption $\operatorname{supp}\varphi_1\cap\operatorname{supp}\varphi_2=\varnothing$, hence (13) and the last assertion of the Proposition holds. □

For *microlocal* functionals there is a refinement of Proposition 2.3.11 which identifies this class of functionals with the kind of local functionals usually employed by physicists, such as (22) and (23). We build over the argument sketched in the proof of Theorem 2, pp. 139 of [17], with a few changes (see also Theorem I.2 of [14]). The only missing ingredient is the following mild technical condition:

2.3.12. Definition. Let $\mathscr{F}_1,\mathscr{F}_2$ be locally convex vector spaces, $\varnothing\neq\mathscr{U}\subset\mathscr{F}_1$ open. A map $T:\mathscr{U}\to\mathscr{F}_2$ is said to be *locally bornological* (into $\mathscr{F}_2$) if for all $\varphi\in\mathscr{U}$ there is $\mathscr{V}\ni\varphi$, $\mathscr{V}\subset\mathscr{U}$ open such that $T|_{\mathscr{V}}$ maps bounded subsets of $\mathscr{V}$ into bounded subsets of $\mathscr{F}_2$.

If $\mathscr{F}_1$ is normable, then locally bornological maps are just the same as locally bounded maps. If $\mathscr{F}_1$ is semi-Montel (that is, any bounded subset of $\mathscr{F}_1$ is relatively compact), then any continuous map $T:\mathscr{U}\to\mathscr{F}_2$ is locally bornological: given any $\varphi\in\mathscr{U}$, take an open neighborhood $\mathscr{V}$ of φ such that $\overline{\mathscr{V}}$ is contained in $\mathscr{U}$, so that $\overline{\mathscr{W}}$ is contained in $\mathscr{U}$ and therefore T is defined in $\overline{\mathscr{W}}$ for all bounded subsets $\mathscr{W}\subset\mathscr{V}$. By the semi-Montel property of $\mathscr{F}_1$ and the continuity of T, we have that $\overline{\mathscr{W}}$ and therefore $T(\overline{\mathscr{W}})$ are compact, hence the latter is bounded and thus $T(\mathscr{W})$ is bounded as well.

2.3.13. Proposition. *Let $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ be convex and open in the compact-open topology, $\varphi_0\in\mathscr{U}$, and $F\in\mathscr{F}_{00}(\mathscr{M},\mathscr{U})$ be smooth. Assume in addition that $F^{(1)}$ is locally bornological into $\Gamma^\infty_c(\wedge^d T^*\mathscr{M}\to\mathscr{M})$ (Definition 2.3.12). Then F is microlocal if and only if there is a smooth d-form ω_{F,φ_0} on $J^\infty(\mathscr{M},\mathbb{R})$ such that its pullback $(j^\infty\varphi)^*\omega_{F,\varphi_0}$ by the infinite jet prolongation $j^\infty\varphi$ of any $\varphi\in\mathscr{U}$ is a smooth d-form of compact support on $\mathscr{M}$, and*

$$F(\varphi)=F(\varphi_0)+\int_{\mathscr{M}}(j^\infty\varphi)^*\omega_{F,\varphi_0}\ . \tag{26}$$

Moreover, ω_{F,φ_0} depends on infinite-order jets in the sense that for each $p\in\mathscr{M}$ there is a $r\in\mathbb{N}$ such that if $\varphi_1,\varphi_2\in\mathscr{U}$ are such that $j^r\varphi_1(p)=j^r\varphi_2(p)$, then $((j^\infty\varphi_1)^*\omega_{F,\varphi_0})(p)=((j^\infty\varphi_2)^*\omega_{F,\varphi_0})(p)$.

In order to prove Proposition 2.3.13, we need first a preparatory lemma which is of independent interest.

2.3.14. Lemma. *Let $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology, $F\in\mathscr{F}_{00}(\mathscr{M},\mathscr{U})$ smooth. Then $F^{(1)}$ is a (MB-)smooth map from $\mathscr{U}$ into $\Gamma^\infty_c(\wedge^d T^*\mathscr{M}\to\mathscr{M})$ if and only if $F^{(1)}$ is locally bornological into $\Gamma^\infty_c(\wedge^d T^*\mathscr{M}\to\mathscr{M})$.*

Proof. Let $*_g$ be the Hodge star operator associated to the metric g (see formula (54) below). It is clear from Lemma 2.3.8 that $T=*_gF^{(1)}$ takes values in $\mathscr{D}(K)$ for any $K\subset\mathscr{M}$ compact such that $\operatorname{supp} F \subset \mathring{K}$.[5] Moreover, it follows from the MB-smoothness of F that T is a MB-smooth map from $\mathscr{U}$ into $\mathscr{E}'(K)$, as argued e.g. in the discussion following Definition A.3 below. Therefore, the thesis will follow if we can show that T is MB-smooth into $\mathscr{D}(K)$ if and only if T is locally bornological into $\mathscr{D}(K)$.

Due to the discussion right after Definition 2.3.12, necessity of local bornology into $\mathscr{D}(K)$ follows from the fact that any MB-smooth map is continuous and $\mathscr{C}^\infty(\mathscr{M})$ is nuclear and complete, hence semi-Montel by Proposition 4.4.7, pp. 81–82 of [76] and Theorem 3.5.1, pp. 64 of [54]. To get sufficiency, consider a finite open cover $\{U_1, \ldots, U_q\}$ of K by domains of coordinate charts $\psi_i : U_i \to \mathbb{R}^d$ such that $\psi_i(U_i)$ is an open neighborhood of the standard unit d-cube $Q = [0,1]^d$ for all $i = 1, \ldots, q$ and such that $\cup_{i=1}^q \psi_i^{-1}(\mathring{Q}) \supset K$. Given a partition of unity $\{f_1, \ldots, f_q\}$ subordinate to the open covering $\{\psi_1^{-1}(\mathring{Q}), \ldots, \psi_q^{-1}(\mathring{Q})\}$ of K, define for each $i = 1, \ldots, q$ the map $T_i : \mathscr{U} \to \mathscr{D}(Q)$ given by

$$T_i(\varphi) = (\psi_i)_*(f_i T(\varphi)) \ , \quad \varphi \in \mathscr{U} \ .$$

It is clear that T_i is a smooth map into $\mathscr{E}'(Q)$ which is locally bornological into $\mathscr{D}(Q)$ and $\operatorname{supp} T_i(\varphi) \subset \mathring{Q}$ for all $i = 1, \ldots, q$, $\varphi \in \mathscr{U}$. Moreover, thanks to the latter, we have that

$$T(\varphi) = \sum_{i=1}^q (\psi_i^{-1})_* T_i(\varphi) \ , \quad \varphi \in \mathscr{U} \ .$$

Finally, it suffices to prove that each T_i maps smooth curves in $\mathscr{U}$ to smooth curves in $\mathscr{D}(Q)$ (i.e. T_i is conveniently smooth from $\mathscr{U}$ into $\mathscr{D}(Q)$), since the above formula then clearly implies that T maps smooth curves in $\mathscr{U}$ to smooth curves in $\mathscr{D}(K)$. The sufficiency claim will follow since $\mathscr{C}^\infty(\mathscr{M}) \ni \mathscr{U}$ is metrizable and $\mathscr{D}(K)$ is complete [39] (see Remark A.4 below). Convenient smoothness of T_i from $\mathscr{U}$ into $\mathscr{D}(Q)$ ensues from the following two facts:

(i) Given $u \in \mathscr{E}'(Q)$, $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{Z}^d$, define the α-th Fourier coefficient of u as

$$\hat{u}_\alpha = u(e^{2\pi i \langle \alpha, \cdot \rangle}) \ .$$

It immediately follows that there are $k \in \mathbb{N}$, $C' > 0$ such that for all $\alpha \in \mathbb{Z}^d$ we have

$$|\hat{u}_\alpha| \leq C'(1 + |\alpha|)^k \ , \text{ where } |\alpha| = \sum_{i=1}^d |\alpha_i| \ .$$

Moreover, if it happens that $u \in \mathscr{D}(Q)$ then for all $k \in \mathbb{N}$ there is a $C_k > 0$ such that for all $\alpha \in \mathbb{Z}^d$ we have

$$|\hat{u}_\alpha| \leq C_k(1 + |\alpha|)^{-k} \ .$$

Conversely, if the sequence $\hat{u} = (\hat{u}_\alpha)_{\alpha \in \mathbb{Z}^d}$ of Fourier coefficients of $u \in \mathscr{E}'(Q)$ satisfies the last family of estimates above, then we must have $u \in \mathscr{D}(Q)$. For a proof of this

[5] For simplicity, here we allow ourselves a slight abuse of notation – strictly speaking, the smooth density supported in $\operatorname{supp} F$ representing $F^{(1)}[\varphi]$ for each $\varphi \in \mathscr{U}$ is only defined up to an exact d-form, so when we write $*_g F^{(1)}$ we apply $*_g$ simultaneously to *all* representatives of $F^{(1)}[\varphi]$ for each $\varphi \in \mathscr{U}$. In other words, we are dealing with all d-forms representing $F^{(1)}[\varphi]$ simultaneously. We shall be more precise with this from the proof of Proposition 2.3.13 onwards.

(well known) Fourier-analytic characterization of $\mathscr{D}(Q)$, see e.g. Corollary 3.2.10 and Proposition 3.2.12, pp. 181–182 of [43].

(ii) Let $\gamma : I = [a,b] \to \mathbb{C}^{\mathbb{Z}^d}$, $\gamma(t) = (\gamma_\alpha(t))_{\alpha\in\mathbb{Z}^d}$ be a smooth curve (that is, $\gamma_\alpha : I \to \mathbb{C}$ is smooth for all $\alpha \in \mathbb{Z}^d$) such that for all $k \in \mathbb{N}$ there is a $C_k > 0$ such that

$$\|\gamma_\alpha\|_{\infty,0,I} \leq C_k(1+|\alpha|)^{-k} \text{ for all } \alpha \in \mathbb{Z}^d$$

and for all $j \in \mathbb{N}$ there are $k' \in \mathbb{N}$, $C'_j > 0$ such that

$$\|\gamma_\alpha^{(j)}\|_{\infty,0,I} \leq C'_j(1+|\alpha|)^{k'} \text{ for all } \alpha \in \mathbb{Z}^d \ .$$

Then for all $j,k \in \mathbb{N}$ there is a $C''_{j,k} > 0$ such that

$$\|\gamma_\alpha^{(j)}\|_{\infty,0,I} \leq C''_{j,k}(1+|\alpha|)^{-k} \text{ for all } \alpha \in \mathbb{Z}^d \ .$$

This is a consequence of the following special case of the Gagliardo-Nirenberg interpolation inequality (see e.g. Theorem 5.2, pp. 135–139 of [2]): if $f : I \to \mathbb{C}$ is smooth, then for all $0 < j < m \in \mathbb{N}$ we have a constant $C = C_{j,m,I} > 0$ independent of f such that

$$\|f^{(j)}\|_{\infty,0,I} \leq C\|f^{(m)}\|_{\infty,0,I}^{\frac{j}{m}}\|f\|_{\infty,0,I}^{1-\frac{j}{m}} \ .$$

Indeed, given $j,k \in \mathbb{N}$, let $m,k' \in \mathbb{N}$, $C'_j > 0$ so that $j < m$ and $(1+|\alpha|)^{-k'}\|\gamma_\alpha^{(j)}\|_{\infty,0,I} \leq C'_j$ for all $\alpha \in \mathbb{Z}^d$. The Gagliardo-Nirenberg interpolation inequality entails that for all $\alpha \in \mathbb{Z}^d$

$$\begin{aligned}(1+|\alpha|)^k\|\gamma_\alpha^{(j)}\|_{\infty,0,I} &\leq \left((1+|\alpha|)^{-k'}\|\gamma_\alpha^{(m)}\|_{\infty,0,I}\right)^{\frac{j}{m}} \\ &\quad \cdot \left((1+|\alpha|)^{\frac{mk+jk'}{m-j}}\|\gamma_\alpha\|_{\infty,0,I}\right)^{1-\frac{j}{m}} \\ &\leq C_j'^{\frac{j}{m}}C_{\frac{mk+jk'}{m-j}}^{1-\frac{j}{m}} \doteq C''_{j,k} \ .\end{aligned}$$

Since j,k were arbitrary, the conclusion follows.

If $\gamma : \mathbb{R} \to \mathscr{U}$ is a smooth curve, then $\widehat{T_i \circ \gamma}|_{[a,b]}$ clearly satisfies the assumptions of (ii) for all $a < b \in \mathbb{R}$, $i = 1,\ldots,q$, therefore by (i) $T_j \circ \gamma : \mathbb{R} \to \mathscr{D}(K)$ is smooth for all $i = 1,\ldots,q$ as desired. □ □

We note that, unlike Proposition 2.3.13, the analogous Theorem I.2 of [14] assumes MB-smoothness of $F^{(1)}$ into $\Gamma_c^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$. This condition has been considered before in similar contexts, see for instance Appendix A of [19]. Local bornology into $\Gamma_c^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$, on its turn, does not seem to follow from microlocality alone. As a rather indirect evidence of this (in view of the proof of Lemma 2.3.14), let us display an example of a smooth curve γ from $[0,1]$ into the space s' of polynomially bounded sequences which takes values in the space s of rapidly decaying sequences but fails to be bounded therein. Consider the sequence $\gamma = (\gamma_n)_{n\in\mathbb{N}}$ of smooth curves from $[0,1]$ into $\mathbb{R}$ given by

$$\gamma_n(t) = n^2t^n(1-t) \ .$$

Since $\gamma_n(0) = \gamma_n(1) = 0$ for all n and $(n^k\gamma_n(t))_{n\in\mathbb{N}}$ is bounded for all $k \in \mathbb{N}$, $t \in (0,1)$, we see that $(\gamma_n(t))_{n\in\mathbb{N}} \in s$ for all $t \in [0,1]$. However, it is *not* true that $(n^k\|\gamma_n\|_{\infty,0,[0,1]})_{n\in\mathbb{N}}$ is bounded for all $k \in \mathbb{N}$: to see this, notice that the maximum of γ_n takes place at the unique positive zero $t_n = 1 - \frac{1}{n+1}$ of $\gamma_n'(t) = n^3 t^{n-1}(1 - \frac{n+1}{n}t)$ and equals $\gamma_n(t_n) = \frac{n^2}{n+1}(1 - \frac{1}{n+1})^n$. From this formula one gets that asymptotically $\gamma_n(t_n) \sim \frac{n}{e}$ for large n and therefore $(n^k \|\gamma_n\|_{\infty,0,[0,1]})_{n\in\mathbb{N}}$ is unbounded for all $k \in \mathbb{N}$, as claimed. A similar argument shows, on the other hand, that $(n^{-k-1}\|\gamma_n^{(k)}\|_{\infty,0,[0,1]})_{n\in\mathbb{N}}$ is bounded for all $k \in \mathbb{N} \cup \{0\}$ and therefore $(\gamma_n)_{n\in\mathbb{N}}$ is a smooth curve into s'.

Proof (of Proposition 2.3.13). Smooth functionals F with compact space-time support that satisfy the representation formula (26) with ω_{F,φ_0} as above are obviously microlocal. Moreover, by Lemma 2.3.14 $F^{(1)}$ is locally bornological into $\Gamma_c^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$ since it is smooth therein, so we are only left with proving the opposite implication. By Lemma 2.3.14, $F^{(1)}$ is a (MB-)smooth map from $\mathscr{U}$ into $\Gamma_c^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$. Since $\mathscr{U}$ is assumed convex, the fundamental theorem of Calculus (A.2) yields

$$F(\varphi) = F(\varphi_0) + \int_0^1 \mathrm{d}\lambda F^{(1)}[\varphi_0 + \lambda\varphi'](\varphi') = F(\varphi_0) + \int_0^1 \mathrm{d}\lambda \int_{\mathscr{M}} \varphi' E(F)[\varphi_0 + \lambda\varphi'] \ ,$$

where $\varphi' = \varphi - \varphi_0$ and $E(F)[\psi]$ is the smooth density of compact support that represents $F^{(1)}[\psi]$. Therefore,

$$p \mapsto F_p(\varphi) \doteq \int_0^1 \mathrm{d}\lambda (\varphi(p) - \varphi_0(p)) E(F)[\varphi_0 + \lambda(\varphi - \varphi_0)](p)$$

is our candidate for the density $(j^\infty\varphi)^*\omega_{F,\varphi_0}$, which we will identify with a smooth function by a choice of a volume element on a neighborhood of $\operatorname{supp} F$, when needed. Take now $\varphi_1, \varphi_2 \in \mathscr{V} \subset \mathscr{U} - \varphi$ such that $\varphi_1 + \varphi_2 \in \mathscr{V}$ and $\varphi_1 - \varphi_2$ vanishes together with all its partial derivatives in some (hence, any) coordinate chart at some $p \in \mathscr{M}$, where $\mathscr{V}$ is an absolutely convex open neighborhood of zero. The first condition can always be achieved by multiplying $\varphi_1, \varphi_2 \in \mathscr{V}$ by a suitably small constant – this operation does not modify the second condition. Applying the fundamental theorem of Calculus (A.2) once more, together with the Fubini-Tonelli theorem, we get

$$\begin{aligned} &F_p(\varphi_0 + \varphi_2) - F_p(\varphi_0 + \varphi_1) = \\ &\quad = \varphi_1(p) \int_0^1 \mathrm{d}\lambda \left(E(F)[\varphi_0 + \lambda\varphi_2](p) - E(F)[\varphi_0 + \lambda\varphi_1](p) \right) \\ &\quad = \varphi_1(p) \int_0^1 \lambda \mathrm{d}\lambda \int_0^1 \mathrm{d}\mu E(F)^{(1)}[\varphi_0 + \lambda(\varphi_1 + \mu(\varphi_2 - \varphi_1))](\varphi_2 - \varphi_1)(p) \ , \end{aligned}$$

where we have also made use of the fact that $\varphi_1(p) = \varphi_2(p)$. However, for each $\psi_1, \psi_2 \in \mathscr{V}$ such that $\psi_1 + \psi_2 \in \mathscr{V}$, the linear map

$$\mathscr{C}^\infty(\mathscr{M}) \ni \vec{\varphi} \mapsto \int_0^1 \mathrm{d}\lambda \int_0^1 \mathrm{d}\mu E(F)^{(1)}[\varphi_0 + \lambda(\psi_1 + \mu\psi_2)](\vec{\varphi}) \in \mathscr{C}^\infty(\mathscr{M})$$

decreases supports, for the integrand in the right hand side coincides with $F^{(2)}[\varphi_0 + \lambda(\psi_1 + \mu\psi_2)](\vec{\varphi}, \cdot)$ in the sense of distributions and F is local. By Peetre's theorem [74], the above linear map must be a linear differential operator of order r' with smooth coefficients supported in $\operatorname{supp} F$ for some $r' \in \mathbb{N}$. Due to the joint continuity of $F^{(2)}$, one may take the same r' for all $\psi_1, \psi_2 \in \mathscr{V}$ (possibly after suitably shrinking $\mathscr{V}$). Since we have assumed that φ_1 and φ_2 coincide up to infinite order at p, it turns out that

$$\int_0^1 \mathrm{d}\lambda \varphi_1(p) E(F)[\varphi_0 + \lambda\varphi_1](p) = \int_0^1 \mathrm{d}\lambda \varphi_2(p) E(F)[\varphi_0 + \lambda\varphi_2](p) \ ,$$

hence proving the first assertion. Moreover, since $F^{(2)}[\varphi_0 + \lambda(\psi_1 + \mu\psi_2)](\varphi, \cdot)$ is a distribution supported in $\operatorname{supp} F$, it must be of finite order $r \in \mathbb{N}$ (say) for all $\psi_1, \psi_2 \in \mathscr{V}$, hence we may require that φ_1 and φ_2 coincide only up to order r at p, thus proving the second assertion. Finally, since infinite-order jet prolongations are conveniently smooth and the infinite jet bundle is metrizable, it also follows from the same reasoning employed in the proof of Lemma 2.3.14 that ω_{F,φ_0} is MB-smooth. □ □

2.3.15. Remark. A consequence of Proposition 2.3.13 is that a microlocal functional F depends on derivatives of its argument φ at each $p \in \operatorname{supp} F$ only up to some *finite* order $r \geq 0$, which can be taken to be constant on some neighborhood of φ but otherwise depending on φ, thanks e.g. to Proposition 2, pp. 355 of [91]. A natural question at this point is whether the density determined by a microlocal functional F is of *finite* order r, that is, r is actually *φ-independent*, so that (26) reduces to the form (22). Obviously, this is equivalent to the same question posed for the smooth density $E(F)[\varphi]$ representing $F^{(1)}[\varphi]$. It follows from Lemma 2.3.5 and the fundamental theorem of Calculus (A.2) that a necessary condition for $E(F)[\varphi]$ to be of globally finite order (say) $r \in \mathbb{N}$ is that for every $R \geq 0$, $k \in \mathbb{N}$ there is a $C > 0$ such that the Lipschitz estimates

$$\|*_g E(F)[\varphi_2] - *_g E(F)[\varphi_1]\|_{\infty,k,\operatorname{supp} F} \leq C\|\varphi_2 - \varphi_1\|_{\infty,k+r,\operatorname{supp} F} \tag{27}$$

hold for every $\varphi_1, \varphi_2 \in \mathscr{U}$ such that $\|\varphi_1 - \varphi_2\|_{\infty,k+r,\operatorname{supp} F} < R$, where $*_g$ is the Hodge star operator associated to the metric g (see (54) below). On the other hand, (27) implies that $F^{(1)}$ is locally bornological. Moreover, it follows from Lemma 2.2.3 that if $\mathscr{U}$ is such that for every $\varphi_0 \in \mathscr{U}$ there is a $\delta > 0$ such that $\{\varphi \in \mathscr{C}^\infty(\mathscr{M}) \mid \|\varphi - \varphi_0\|_{\infty,r,\operatorname{supp} F} < \delta\} \subset \mathscr{U}$, then these estimates are also sufficient to yield finite order (see Proposition 5 and Theorem 1 in [91] for details). Slovák proposed in [80] a different condition on the domain $\mathscr{U}$, related to the applicability of Whitney's extension theorem, which allows one to get finite order from microlocality and convenient smoothness of $F^{(1)}$ into $\Gamma^\infty_c(\wedge^d T^*\mathscr{M} \to \mathscr{M})$ without the need of assuming (27). This was shown in the particular case $\mathscr{U} = \mathscr{C}^\infty(\mathscr{M})$ in [14]. However, as argued in [91], Slovák's criterion seems unnatural for domains $\mathscr{U}$ coming e.g. from the study of differential equations and flows.

We close this Section with a few comments on the algebraic structure of the spaces of local and microlocal functionals. As we have seen, in spite of the nice structure of its elements, $\mathscr{F}_{\mathrm{loc}}(\mathscr{M}, \mathscr{U})$ and $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$ are not closed under pointwise products. However, the dynamical developments in the next Section will lead, for each $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ open in the compact-open topology, to a space of functionals which includes both $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$ and $\mathscr{F}_0(\mathscr{M}, \mathscr{U})$ and is not only closed under products, but will also be shown later to possess good topological properties (see Section 4).

3. Off-shell linearized dynamics

Unlike the standard approaches to classical field theory, we will not attempt to impose equations of motion directly on field configurations, but instead we do this algebraically by studying the effect of dynamics on observable quantities. More precisely, in this Section we want to describe how *perturbing* a given dynamics affects observables. On an infinitesimal level, this corresponds to endowing a sufficiently large space of observables with a Poisson structure associated to this dynamics, which will be introduced in Subsection 3.2.

3.1. **Preliminaries. Generalized Lagrangians and the Euler-Lagrange derivative.** Our approach to dynamics is based on a local variational principle of Euler-Lagrange type. In order to formulate it in our context, first we need to make the representation formula for microlocal functionals provided by Proposition 2.3.13 more flexible by allowing the support of the functional to be prescribed at will. This is accomplished by the following concept, introduced in a slightly different form by Definition 6.1 of [15] (see also the footnote preceding Lemma 3.1.3 below).

3.1.1. Definition. Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$. A *generalized Lagrangian* $\mathscr{L}$ on $\mathscr{U}$ is a map

$$\mathscr{L} : \mathscr{C}_c^\infty(\mathscr{M}) \to \mathscr{F}_{00}(\mathscr{M}, \mathscr{U}) ,$$

such that the following properties hold:

(1) $\operatorname{supp}(\mathscr{L}(f)) \subset \operatorname{supp} f$;
(2) $\mathscr{L}(f_1 + f_2 + f_3) = \mathscr{L}(f_1 + f_2) - \mathscr{L}(f_2) + \mathscr{L}(f_2 + f_3)$, if $\operatorname{supp} f_1 \cap \operatorname{supp} f_3 = \varnothing$.

We call the argument f of $\mathscr{L}(f)$ its *support function*. We say that $\mathscr{L}$ is *smooth* if $\mathscr{L}(f)$ is smooth for all $f \in \mathscr{C}_c^\infty(\mathscr{M})$.

In other words, a generalized Lagrangian is additive *with respect to support functions*. As with the case with additive functionals, one can work instead with *relative* generalized Lagrangians $\mathscr{L}_{f_0}$ with respect to $f_0 \in \mathscr{C}_c^\infty(\mathscr{M})$, given by

$$\mathscr{L}_{f_0}(f) \doteq \mathscr{L}(f_0 + f) - \mathscr{L}(f_0) ,$$

in terms of which the additivity property with respect to support functions reads, for all $f_1, f_2, f_3 \in \mathscr{C}_c^\infty(\mathscr{M})$ such that $\operatorname{supp} f_1 \cap \operatorname{supp} f_3 = \varnothing$,

$$\mathscr{L}_{f_2}(f_1 + f_3) = \mathscr{L}_{f_2}(f_1) + \mathscr{L}_{f_2}(f_3) .$$

Moreover, one has the following result, extracted from the proof of Proposition 6.2 of [15].

3.1.2. Lemma. *Let $\mathscr{L}$ be a generalized Lagrangian. Then* $\operatorname{supp} \mathscr{L}_{f_0}(f) \subset \operatorname{supp} f$, *for all* $f, f_0 \in \mathscr{C}^\infty(\mathscr{M})$.

Proof. Let $p \notin \operatorname{supp} f$, and choose $f_0' \in \mathscr{C}_c^\infty(\mathscr{M})$ such that $f_0' \equiv f_0$ in a neighborhood of p and $\operatorname{supp} f \cap \operatorname{supp} f_0' = \varnothing$. By additivity of $\mathscr{L}$ with respect to support functions, we have that $\mathscr{L}_{f_0}(f) = \mathscr{L}_{f_0 - f_0'}(f)$, which implies that $\operatorname{supp} \mathscr{L}_{f_0}(f) \subset \operatorname{supp}(f + f_0 - f_0') \cup \operatorname{supp}(f_0 - f_0')$. Therefore, $p \notin \operatorname{supp} \mathscr{L}_{f_0}(f)$, as asserted. □

Additivity with respect to support functions is a weak substitute for linearity, but is strong enough to yield useful consequences. One of them is that the argument involving field configurations inherits this property[6]:

3.1.3. LEMMA. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$, and $\mathscr{L}$ a generalized Lagrangian on $\mathscr{U}$. Then, for all $f \in \mathscr{C}^\infty_c(\mathscr{M})$, $\mathscr{L}(f)$ is additive.*

Proof. Fix an arbitrary $f \in \mathscr{C}^\infty(\mathscr{M})$, and let $\varphi_2 \in \mathscr{U}$, $\varphi_1, \varphi_3 \in \mathscr{U} - \varphi_2$ be such that $\operatorname{supp}\varphi_1 \cap \operatorname{supp}\varphi_3 = \varnothing$. Let $\chi_1, \chi_3 \in \mathscr{C}^\infty(\mathscr{M})$ be such that $\chi_j \equiv 1$ in a neighborhood of $\operatorname{supp}\varphi_j$, $j = 1, 3$, and $\operatorname{supp}\chi_1 \cap \operatorname{supp}\chi_3 = \varnothing$. Define $f_1 \doteq \chi_1 f$, $f_3 \doteq \chi_3 f$, and $f_2 \doteq f - f_1 - f_3$. Then, by properties (1) and (2) in Definition 3.1.1,

$$\mathscr{L}(f)(\varphi_1 + \varphi_2 + \varphi_3) = \mathscr{L}(f_1 + f_2)(\varphi_1 + \varphi_2) - \mathscr{L}(f_2)(\varphi_2) + \mathscr{L}(f_2 + f_3)(\varphi_2 + \varphi_3)\ .$$

However, we also have that

$$\begin{aligned}
\mathscr{L}(f)(\varphi_1 + \varphi_2) &= \mathscr{L}(f_1 + f_2)(\varphi_1 + \varphi_2) - \mathscr{L}(f_2)(\varphi_2) + \mathscr{L}(f_2 + f_3)(\varphi_2)\ ,\\
\mathscr{L}(f)(\varphi_2) &= \mathscr{L}(f_1 + f_2)(\varphi_2) - \mathscr{L}(f_2)(\varphi_2) + \mathscr{L}(f_2 + f_3)(\varphi_2)\ ,\\
\mathscr{L}(f)(\varphi_2 + \varphi_3) &= \mathscr{L}(f_1 + f_2)(\varphi_2) - \mathscr{L}(f_2)(\varphi_2) + \mathscr{L}(f_2 + f_3)(\varphi_2 + \varphi_3)\ ,
\end{aligned}$$

whence it follows that

$$\begin{aligned}
&\mathscr{L}(f)(\varphi_1 + \varphi_2) - \mathscr{L}(f)(\varphi_2) + \mathscr{L}(f)(\varphi_2 + \varphi_3)\\
&\qquad = \mathscr{L}(f_1 + f_2)(\varphi_1 + \varphi_2) - \mathscr{L}(f_2)(\varphi_2) + \mathscr{L}(f_2 + f_3)(\varphi_2 + \varphi_3)\\
&\qquad = \mathscr{L}(f)(\varphi_1 + \varphi_2 + \varphi_3)\ ,
\end{aligned}$$

which proves our assertion. □

3.1.4. COROLLARY. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open with respect to the compact-open topology, and $\mathscr{L}$ be a* smooth *generalized Lagrangian on $\mathscr{U}$. Then $\mathscr{L}(f) \in \mathscr{F}_{\mathrm{loc}}(\mathscr{M}, \mathscr{U})$ for all $f \in \mathscr{C}^\infty_c(\mathscr{M})$.*

Proof. Apply Proposition 2.3.11 to the outcome of Lemma 3.1.3. □

Another consequence is the following generalization of Lemma 2.3.5 to *any* open subset of $\mathscr{C}^\infty(\mathscr{M})$:

3.1.5. LEMMA. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$, and $\mathscr{L}$ be a generalized Lagrangian on $\mathscr{U}$. Then, for any $f \in \mathscr{C}^\infty_c(\mathscr{M})$ fixed, $\mathscr{L}(f)$ can be written as a finite sum of additive functionals of arbitrarily small space-time support.*

Proof. Let $(\chi_i)_{i=1,\dots,n}$ a the partition of unity subordinated to the finite open covering of $\operatorname{supp} f$ constructed in the proof of Lemma 2.3.5. Then

$$\mathscr{L}(f) = \mathscr{L}\left(\sum_{i=1}^n \chi_i f\right)\ .$$

Applying additivity of $\mathscr{L}$ with respect to support functions just as we did in the proof of Lemma 2.3.5 yields the desired result. □

[6]This property is assumed *a priori* in Definition 6.1 of [15].

Motivated by Corollary 3.1.4, we say that a generalized Lagrangian $\mathscr{L}$ is *microlocal* if $\mathscr{L}(f) \in \mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M},\mathscr{U})$ for all $f \in \mathscr{C}^\infty_c(\mathscr{M})$, and *of (finite) order* $r \geq 0$ if, in addition, $\mathscr{L}(f)$ is of finite order $r \in \mathbb{N}$ for all such f. A simple but important example of microlocal generalized Lagrangians of order r are the squares of the local Sobolev seminorms (5) at order $k = r$

$$\mathscr{L}(f)(\varphi) = \|\varphi\|^2_{2,r,f} \ . \tag{28}$$

With the concept of microlocal generalized Lagrangian at hand, we can write down the Euler-Lagrange variational principle in the form we will use.

3.1.6. Definition. Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology, $\mathscr{L}$ a smooth generalized Lagrangian, $k \geq 1$. The k-th order *Euler-Lagrange derivative* of $\mathscr{L}$ at $\varphi \in \mathscr{U}$ along $\vec{\varphi}_1, \ldots, \vec{\varphi}_k \in \mathscr{C}^\infty(\mathscr{M})$ is given by

$$D^k\mathscr{L}(1)[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k) = D^k\mathscr{L}(f)[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k) \ ,$$

where $f \in \mathscr{C}^\infty_c(\mathscr{M})$ satisfies $f \equiv 1$ on $\operatorname{supp}\vec{\varphi}_j$ for at least one $j = 1, \ldots, k$ (due to Proposition 2.3.11 and Lemma 3.1.2, the above definition is independent of the choice of f). If $\mathscr{L}$ is microlocal of finite order and $\operatorname{supp}\vec{\varphi}_1$ is compact, we have that for $k = 1$,

$$D\mathscr{L}(1)[\varphi](\vec{\varphi}_1) = \langle E(\mathscr{L})[\varphi], \vec{\varphi}_1\rangle$$

defines a partial differential operator $E(\mathscr{L}) : \mathscr{U} \to \Gamma^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$, called the *Euler-Lagrange operator* associated to $\mathscr{L}$. The map $E(\mathscr{L})$ is clearly smooth, with derivatives of order $k \geq 1$ at $\varphi \in \mathscr{U}$ along $\vec{\varphi}_2, \ldots, \vec{\varphi}_{k+1} \in \mathscr{C}^\infty(\mathscr{M})$ given by the identity

$$\int_{\mathscr{M}} \vec{\varphi}_1 D^k E(\mathscr{L})[\varphi](\vec{\varphi}_2, \ldots, \vec{\varphi}_{k+1}) = D^{k+1}\mathscr{L}(1)[\varphi](\vec{\varphi}_1, \vec{\varphi}_2, \ldots, \vec{\varphi}_{k+1}) \ .$$

For $\varphi \in \mathscr{U}$ fixed, the maps $D^kE(\mathscr{L})[\varphi] : \otimes^k\mathscr{C}^\infty(\mathscr{M}) \to \Gamma^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$ are (symmetric) k-linear k-differential operators (i.e. for each $j = 2, \ldots, k+1$, $D^kE(\mathscr{L})[\varphi](\vec{\varphi}_2, \ldots, \vec{\varphi}_j, \ldots, \vec{\varphi}_{k+1})$ is a linear partial differential operator acting on $\vec{\varphi}_j$ with all other arguments fixed). We call

$$E'(\mathscr{L})[\varphi] = DE(\mathscr{L})[\varphi]$$

the *linearized Euler-Lagrange operator* around $\varphi \in \mathscr{U}$.

For notational convenience, we occasionally write

$$E'(\mathscr{L})[\varphi](\vec{\varphi}) = E'(\mathscr{L})[\varphi]\vec{\varphi} \ ,$$
$$D^kE(\mathscr{L})[\varphi](\vec{\varphi}_1, \ldots, \vec{\varphi}_k) = D^kE(\mathscr{L})[\varphi](\vec{\varphi}_2, \ldots, \vec{\varphi}_k)\vec{\varphi}_1 \ , \quad k > 1 \ .$$

Definition 3.1.6 prompts us to compare it with the standard formulation of the Euler-Lagrange variational principle in field theory [60]. We sketch this comparison below. Our definition of Euler-Lagrange derivatives is tailored to get rid of boundary terms automatically; to make them appear, let $\mathscr{L}(f)$ be a microlocal generalized Lagrangian which depends *linearly* on the supporting function f. It follows from Peetre's theorem [74] that $D\mathscr{L}(f)[\varphi]$ is a linear partial differential operator acting on f for each fixed φ, taking values on $\Gamma^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$. Let now

f converge to the characteristic function χ_K of a compact region K of $\mathscr{M}$ with smooth boundary ∂K – the part of $D\mathscr{L}(f)[\varphi](\vec{\varphi})$ proportional to the term of zeroth order in f yields

$$\int_K \vec{\varphi}_1 E(\mathscr{L})[\varphi] \ ,$$

and the remaining terms become the integral over ∂K of the Poincaré-Cartan $(d-1)$-form $\Theta[\varphi]$ associated to the action integral $\mathscr{L}(\chi_K)$ over K. If $\mathscr{L}$ is of order r, one can show [60] that $E(\mathscr{L})$ has order at most $2r$. Therefore, Definition 3.1.6 does provide a generalization of the Euler-Lagrange variational principle. If $E(\mathscr{L})[\varphi] = 0$, then one recovers the usual formula for the on-shell variation of the action functional in terms of the integral of $\Theta[\varphi]$ over ∂K, which is of importance in the so-called *covariant phase space formalism* for field theory (see e.g. formulae (94), pp. 398 of [37] and (6.24), pp. 114 of [47]).

The role in our setup of Lagrangians which are total divergences (also called *null Lagrangians* in the literature, see e.g. Section 3.2 of [24]) is played by the following

3.1.7. Definition. Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$. A generalized Lagrangian $\mathscr{L}$ on $\mathscr{U}$ is said to be *trivial* if $\operatorname{supp}\mathscr{L}(f) \subset \operatorname{supp}(\mathrm{d}f)$ for all $f \in \mathscr{C}^\infty_c(\mathscr{M})$. Two generalized Lagrangians $\mathscr{L}_1, \mathscr{L}_2$ are said to be *equivalent* if $(\mathscr{L}_1 - \mathscr{L}_2)(f) \doteq \mathscr{L}_1(f) - \mathscr{L}_2(f)$ is trivial. This is clearly an equivalence relation in the space of all generalized Lagrangians. If $\mathscr{U}$ is open in the compact-open topology and $\mathscr{L}$ is a microlocal generalized Lagrangian of order r, its equivalence class $S_{\mathscr{L}}$ in the space of all microlocal generalized Lagrangians of order r is called an *action functional of order* r.

Trivial generalized Lagrangians are thus called because they obviously have vanishing Euler-Lagrange derivatives of all orders whenever they are defined. Therefore, two equivalent generalized Lagrangians have the same Euler-Lagrange derivatives. In particular, the action functional $S_{\mathscr{L}}$ associated to a microlocal generalized Lagrangian $\mathscr{L}$ of finite order uniquely determines the Euler-Lagrange operator $E(\mathscr{L})$. As a typical class of examples of trivial generalized Lagrangians, we may take

$$\mathscr{L}(f)[\varphi] = \int_{\mathscr{M}} \mathrm{d}f \wedge (j^r\varphi)^*\omega$$

with $\omega \in \Gamma^\infty(\wedge^{d-1}T^*J^r(\mathscr{M},\mathbb{R}) \to J^r(\mathscr{M},\mathbb{R}))$.

To briefly illustrate the relation of trivial generalized Lagrangians with the more standard notion of null lagrangians, consider once more a microlocal generalized Lagrangian $\mathscr{L}(f)$ which depends linearly on the supporting function f. The reasoning preceding Definition 3.1.7 shows that $D\mathscr{L}(f)[\varphi]$ can be written as

$$D\mathscr{L}(f)[\varphi] = \Theta[\varphi] \wedge \mathrm{d}f + \mathrm{d}\Xi(f)[\varphi] \ ,$$

where $\Xi(f)[\varphi]$ is a smooth $(d-1)$-form supported in $\operatorname{supp} f$. If $\mathscr{L}(f)$ is of finite order (say, r) and *trivial* (e.g. the example written in the previous paragraph), making f converge to χ_K as before shows that $D\mathscr{L}(f)[\varphi](\vec{\varphi})$ converges to the integral of $\Theta[\varphi]$ over ∂K alone.

3.2. **Normally hyperbolic Euler-Lagrange operators. Infinitesimal solvability and the Peierls bracket.** As discussed in the Introduction, we are mainly interested in relativistic classical field theories. This means that the action functional determining the dynamics must give rise to Euler-Lagrange equations of motion which are *hyperbolic*. There are several different concepts of hyperbolicity for partial differential operators (see for instance [24]); the one we use is the notion of *normal hyperbolicity*, as defined for instance in [4] for linear partial differential operators. For future convenience, the discussion in the linear case takes place in the wider context of smooth sections of vector bundles.

3.2.1. Definition. Let $\pi : \mathscr{E} \to \mathscr{M}$ be a real vector bundle of rank D over the space-time manifold $\mathscr{M}$. A linear partial differential operator of second order $P : \Gamma^\infty(\pi) \to \Gamma^\infty(\pi)$ acting on $\Gamma^\infty(\pi)$ is said to be *normally hyperbolic* if its principal symbol $\hat{p} \in \Gamma^\infty(\vee^2 T\mathscr{M} \otimes \mathscr{E}' \otimes \mathscr{E} \to \mathscr{M})$, given by

$$\frac{1}{2} P((f - f(x))^2 \vec{\varphi})(x) \doteq \hat{p}(x, \mathrm{d}f(x)) \vec{\varphi}(x) ,$$

$(f \in \mathscr{C}^\infty(\mathscr{M}), \vec{\varphi} \in \Gamma^\infty(\pi))$ is of the form

$$\hat{p}(x, \xi) = \hat{g}^{-1}(x)(\xi, \xi) \otimes \mathbb{1}_{\pi^{-1}(x)} , \quad x \in \mathscr{M} , \xi \in T^*_x\mathscr{M} ,$$

where $\hat{g}$ is a Lorentzian metric on $\mathscr{M}$.

We remark that a linear partial differential operator P is normally hyperbolic if and only if P is regularly hyperbolic in the sense of Christodoulou [24] and has a scalar principal symbol.

Any second-order linear partial differential operator $P : \Gamma^\infty(\pi) \to \Gamma^\infty(\pi)$ can be written in a coordinate-invariant fashion as follows. If we define iterated covariant derivatives of smooth sections of π with respect to some connection ∇ (see Remark 2.2.1), P assumes the form

$$P\vec{\varphi} = \hat{p}\nabla^2\vec{\varphi} + A\nabla\vec{\varphi} + B\vec{\varphi} , \tag{29}$$

where $A \in \Gamma^\infty(T\mathscr{M} \otimes \mathscr{E}' \otimes \mathscr{E} \to \mathscr{M})$, $B \in \Gamma^\infty(\mathscr{E}' \times \mathscr{E} \to \mathscr{M})$ and $\hat{p} \in \Gamma^\infty(\vee^2 T\mathscr{M} \otimes \mathscr{E}' \otimes \mathscr{E} \to \mathscr{M})$ is the principal symbol. We remark that, unlike A and B, $\hat{p}$ is independent of the choice of ∇.

Before we continue, we introduce a strict partial order $<$ and a partial order $\lesssim$ in the space $\mathrm{Lor}^0(\mathscr{M})$ of continuous Lorentzian metrics on $\mathscr{M}$. Let $g_1, g_2 \in \mathrm{Lor}^0(\mathscr{M})$; we say that

$$\begin{aligned} g_1 < g_2 \quad &\text{if} \quad g_1(X,X) \leq 0 \quad \text{implies} \quad g_2(X,X) < 0 ; \\ g_1 \lesssim g_2 \quad &\text{if} \quad g_1(X,X) < 0 \quad \text{implies} \quad g_2(X,X) < 0 , \end{aligned} \tag{30}$$

for all $X \in T\mathscr{M}$. As usual, we write $g_1 > g_2$ (resp. $g_1 \gtrsim g_2$) if $g_2 < g_1$ (resp. $g_2 \lesssim g_1$). By continuity, $g_1 \lesssim g_2$ implies that $g_2(X,X) \leq 0$ for all X such that $g_1(X,X) \leq 0$ (the converse is not necessarily true). Both partial orders clearly enjoy the property that if $g_1 < g_2$ (resp. $g_1 \lesssim g_2$), then $\Omega_1 g_1 < \Omega_2 g_2$ (resp. $\Omega_1 g_1 \lesssim \Omega_2 g_2$) for all positive, real-valued continuous functions Ω_1, Ω_2 on $\mathscr{M}$. In other words, $<$ and $\lesssim$ depend only on the conformal classes (hence, only on the causal structures) of g_1 and g_2. As shown by Lerner [64], the order topology on $\mathrm{Lor}^0(\mathscr{M})$ associated to $<$ (i.e. the topology generated by the open intervals $\{g \mid g_1 < g < g_2\}$ as g_1, g_2 run through $\mathrm{Lor}^0(\mathscr{M})$), called the *interval topology* on $\mathrm{Lor}^0(\mathscr{M})$, coincides with the latter's relative graph (Whitney) topology. Moreover, Benavides Navarro and Minguzzi have shown [6] (building on earlier results by Geroch [40]) that, given g globally hyperbolic, there is $g_2 > g$ such that g_2 is also globally hyperbolic. We shall use this fact to prove the following useful result:

3.2.2. LEMMA. *The space of continuous, time-oriented and globally hyperbolic Lorentzian metrics on $\mathscr{M}$ is an open subset of* $\mathrm{Lor}^0(\mathscr{M})$ *in the interval topology (hence also in the Whitney topology). Moreover, given any such metric g_2, all $g_1 \in \mathrm{Lor}^0(\mathscr{M})$ such that $g_1 \lesssim g_2$ are also globally hyperbolic and have the same time orientation as g_2, and any Cauchy time function with respect to g_2 is also a Cauchy time function with respect to g_1.*

Proof. Notice that if $g_1 \lesssim g_2$ and g_2 is globally hyperbolic, then any Cauchy hypersurface in $\mathscr{M}$ with respect to g_2 is also a Cauchy hypersurface with respect to g_1, therefore g_1 is globally hyperbolic as well. The results of Lerner, Benavides Navarro and Minguzzi quoted above then imply that any globally hyperbolic g is contained in the open interval $\{g' \mid g_1 < g' < g_2\}$ for some pair $g_1, g_2 \in \mathrm{Lor}^0(\mathscr{M})$ such that g_2 is also globally hyperbolic. By the above reasoning, any g' in this set is globally hyperbolic as well. In particular, if τ is a Cauchy time function on $\mathscr{M}$ with respect to g_2, then τ is also a Cauchy time function with respect to any $g_1 \lesssim g_2$ – notice that (30) implies that if the tangent vector X is spacelike with respect to g_2, then it is also spacelike with respect to g_1; therefore $\mathrm{d}\tau$ is a timelike covector field with respect to g_1, since it is normal to the tangent bundle of all level sets of τ, whose elements must be all spacelike with respect to g_1. Finally, if $T_1 = g_1^\sharp(\mathrm{d}\tau)$ and $T_2 = g_2^\sharp(\mathrm{d}\tau)$, where $g_1 \lesssim g_2$ are time oriented and τ is a Cauchy time function with respect to g_2, then $g_1(T_1, T_2) = \mathrm{d}\tau(T_2) = g_2(T_2, T_2) < 0$ and $g_2(T_1, T_2) = \mathrm{d}\tau(T_1) = g_1(T_1, T_1) < 0$. In particular, if T_1 is future directed with respect to g_1, then it is also future directed with respect to g_2. □

Lemma 3.2.2 and its proof obviously extend to smooth metrics. Let now P be a normally hyperbolic linear partial differential operator on $\Gamma^\infty(\pi)$. We assume the *working hypothesis* (NH_g) on P, given as follows:

(NH_g) The Lorentzian metric $\hat{g}$ on $\mathscr{M}$ associated to the principal symbol $\hat{p}$ of P satisfies $\hat{g} \lesssim g$.

By the above discussion, all such $\hat{g}$'s are globally hyperbolic and have the same time orientation as g. Moreover, by Lemma 3.2.2 these implications of (NH_g) are stable under perturbations of $\hat{g}$ in the interval topology, a fact that is also useful when dealing with nonlinear dynamics.

For P normally hyperbolic and satisfying (NH_g), one can prove the following fact, which is a restatement of results in [4] (related partial results for the scalar case may be found e.g. in [48]).

3.2.3. THEOREM. *Let $(\mathscr{M}, g)$ be a globally hyperbolic space-time, and $\mathscr{E} \to \mathscr{M}$ be a real vector bundle of rank D over the space-time manifold $\mathscr{M}$, endowed with a connection ∇. We assume that $T\mathscr{M}$ is endowed with the Levi-Civita connection associated to the space-time metric g. Let P be a normally hyperbolic linear partial differential operator on $\Gamma^\infty(\pi)$ satisftying (NH_g). Let Σ be a Cauchy hypersurface for $(\mathscr{M}, g)$, with future directed timelike normal $n \in \Gamma^\infty(T_\Sigma\mathscr{M} \to \mathscr{M})$ (i.e. $g(n,n) = -1$ and $g(n,X) = 0$ for all $X \in T\Sigma$), suitably extended to an open neighborhood of Σ in $\mathscr{M}$ (the exact form of the extension is irrelevant for what follows). Given $\vec{\varphi} \in \Gamma^\infty(\pi)$, define*

$$\rho_0^\Sigma(\vec{\varphi}) = \vec{\varphi}|_\Sigma \ , \tag{31}$$

$$\rho_1^\Sigma(\vec{\varphi}) = (\nabla_n \vec{\varphi})|_\Sigma \ . \tag{32}$$

Then for every $\vec{\varphi}_0, \vec{\varphi}_1 \in \Gamma^\infty(\pi|_\Sigma)$*,* $\psi \in \Gamma^\infty(\pi)$*, there is a unique* $\vec{\varphi} \in \Gamma^\infty(\pi)$ *such that*

$$\begin{aligned} P\vec{\varphi} &= \vec{\psi}\ , \\ \rho^\Sigma_j(\vec{\varphi}) &= \vec{\varphi}_j\ , \quad j = 0, 1\ . \end{aligned} \tag{33}$$

In other words, the map $\Phi : \Gamma^\infty(\pi) \to \Gamma^\infty(\pi) \oplus \Gamma^\infty(\pi|_\Sigma) \oplus \Gamma^\infty(\pi|_\Sigma)$ *given by*

$$\Phi(\vec{\varphi}) = (P\vec{\varphi}, \rho^\Sigma_0(\vec{\varphi}), \rho^\Sigma_1(\vec{\varphi})) \tag{34}$$

is a linear isomorphism. □

We stress that Φ is even a *topological* linear isomorphism with respect to the standard Fréchet space topology on spaces of smooth sections of vector bundles.

Let Ψ be the inverse of Φ. By the principle of superposition, one can write

$$\Psi(\vec{\psi}, \vec{\varphi}_0, \vec{\varphi}_1) = K^{\Sigma,0}_P \vec{\varphi}_0 + K^{\Sigma,1}_P \vec{\varphi}_1 + \Delta^\Sigma_P \vec{\psi}\ , \tag{35}$$

where $K^{\Sigma,j}_P \vec{\varphi}_j$, $j = 0, 1$ is the unique solution of the initial value problem

$$\begin{cases} P\vec{\varphi} &= 0\ , \\ \rho^\Sigma_{1-j}(\vec{\varphi}) &= 0\ , \\ \rho^\Sigma_j(\vec{\varphi}) &= \vec{\varphi}_j\ , \end{cases} \tag{36}$$

and $\Delta^\Sigma_P \vec{\psi}$ is the unique solution of the initial value problem

$$\begin{cases} P\vec{\varphi} &= \vec{\psi}\ , \\ \rho^\Sigma_0(\vec{\varphi}) &= 0\ , \\ \rho^\Sigma_1(\vec{\varphi}) &= 0\ . \end{cases} \tag{37}$$

In the scalar case, there is the following refinement of Theorem 3.2.3, which is a restatement of Theorem 5.1.6 of [33] that, on its turn, tells us in great detail how supports and singularities propagate under the dynamics associated to P.

3.2.4. THEOREM. *Assume the hypotheses and definitions of Theorem 3.2.3. Suppose that* $\mathscr{E} = \mathscr{M} \times \mathbb{R}$ *and* $\pi(p, \lambda) = \mathrm{pr}_1(p, \lambda) = p$ *for* $p \in \mathscr{M}$*,* $\lambda \in \mathbb{R}$*, identifying* $\Gamma^\infty(\pi)$ *with* $\mathscr{C}^\infty(\mathscr{M})$*. Then* $\Delta^\Sigma_P : \mathscr{C}^\infty(\mathscr{M}) \to \mathscr{C}^\infty(\mathscr{M})$*,* $K^{\Sigma,0}_P : \mathscr{C}^\infty(\Sigma) \to \mathscr{C}^\infty(\mathscr{M})$ *and* $K^{\Sigma,1}_P : \mathscr{C}^\infty(\Sigma) \to \mathscr{C}^\infty(\mathscr{M})$ *satisfy the following properties:*

(a) *Continuity:* $K^{\Sigma,j}_P$ *is a (continuous) linear map which admits a continuous linear extension to the space* $\mathscr{D}'(\Sigma)$ *of distributions on* Σ *for* $j = 0, 1$*, and* Δ^Σ_P *is a (continuous) linear map which admits a continuous*[7] *linear extension to*

$$\mathscr{D}'_\Sigma(\mathscr{M}) = \{v \in \mathscr{D}'(\mathscr{M}) \mid \mathrm{WF}(v) \cap N^*\Sigma = \varnothing\}\ , \tag{38}$$

[7]Here "continuous" means *sequentially* continuous with respect to the (weak) Hörmander topology on the extended domain (see Subsection 4.1 below), as shown e.g. by Theorem 8.2.13, pp. 268–269 of [50] and, more precisely, by Theorems 8.2.9. (iii) and 8.2.10, pp. 515–520 of [23]. One can see indirectly from the arguments in [13] that one *cannot* hope to upgrade this result to full continuity, unless one uses instead the *strong* Hörmander topology (see also Remark 4.2.3 below).

where $\mathrm{WF}(v)$ *denotes the wave front set of* v *and* $N^*\Sigma = \{\xi \in T^*_\Sigma\mathscr{M} \mid \xi(X) = 0$ *for all* $X \in T\Sigma\}$ *denotes the conormal bundle of* Σ*. We remark that the continuous linear maps* $\rho^\Sigma_j : \mathscr{C}^\infty(\mathscr{M}) \to \mathscr{C}^\infty(\Sigma)$ *also admit a continuous*[7] *linear extension to* $\mathscr{D}'_\Sigma(\mathscr{M}) \ni v$*, satisfying for* $j = 0, 1$ [50]

$$\mathrm{WF}(\rho^\Sigma_j(v)) = \{(x, \xi|_{T\Sigma}) \in T^*\Sigma \mid (x, \xi) \in \mathrm{WF}(v)\}\ . \tag{39}$$

(b) *Propagation of supports:*

$$\mathrm{supp}\,(K^{\Sigma,j}_P u_j) \subset J^+(\mathrm{supp}\,u_j, \hat{g}) \cup J^-(\mathrm{supp}\,u_j, \hat{g}) \subset J^+(\mathrm{supp}\,u_j, g) \cup J^-(\mathrm{supp}\,u_j, g) \tag{40}$$

and

$$\mathrm{supp}\,(\Delta^\Sigma_P v) \subset J^+(\mathrm{supp}\,v \cap J^+(\Sigma, \hat{g}), \hat{g}) \cup J^-(\mathrm{supp}\,v \cap J^-(\Sigma, \hat{g}), \hat{g})\ , \tag{41}$$

for all $u_j \in \mathscr{D}'(\Sigma)$*,* $v \in \mathscr{D}'_\Sigma(\mathscr{M})$*,* $j = 0, 1$*.*

(c) *Propagation of singularities: given any* $u_j \in \mathscr{D}'(\Sigma)$*,* $j = 0, 1$*, we have that* $(x, \xi) \in \mathrm{WF}(K^{\Sigma,j}_P u_j)$ only if *there is* $\lambda > 0$ *and a null geodesic segment* $\gamma : [0, \Lambda] \to \mathscr{M}$ *with respect to* $\hat{g}$ *(i.e.* $\hat{g}(\dot\gamma(\lambda), \dot\gamma(\lambda)) = 0$ *for all* $\lambda \in [0, \Lambda]$*) such that if*

$$E^{\hat{g}}_\gamma = \{(\gamma(0), \hat{g}^\flat(\dot\gamma(0))), (\gamma(\Lambda), \hat{g}^\flat(\dot\gamma(\Lambda)))\} \subset T^*\mathscr{M}$$

is the set of endpoints of the bicharacterstic strip $\{(\gamma(\lambda), \hat{g}^\flat(\dot\gamma(\lambda))) \in T^*\mathscr{M} \mid \lambda \in [0, \Lambda]\}$*, then* $(x', \xi'|_{T\Sigma}) \in \mathrm{WF}(u_j)$ *for some* $(x', \xi') \in E^{\hat{g}}_\gamma$ *and* $(x, \xi) \in E^{\hat{g}}_\gamma$*. Given any* $v \in \mathscr{D}'_\Sigma(\mathscr{M})$*, we have that* $(x, \xi) \in \mathrm{WF}(\Delta^\Sigma_P v)$ only if *either* $(x, \xi) \in \mathrm{WF}(v)$ *or there is* $\Lambda > 0$ *and a null geodesic segment* $\gamma : [0, \Lambda] \to \mathscr{M}$ *with respect to* $\hat{g}$ *such that* $\gamma((0, \Lambda)) \cap \Sigma = \varnothing$ *and* $\mathrm{WF}(v) \cap E^{\hat{g}}_\gamma \neq \varnothing$*,* $(x, \xi) \in E^{\hat{g}}_\gamma$*.*

In particular, given any $u_0, u_1 \in \mathscr{D}'(\Sigma)$*,* $v \in \mathscr{D}'_\Sigma(\mathscr{M})$*, we have that* $K^{\Sigma,j}_P u_j$ *and* $\Delta^\Sigma_P v$ *belong to* $\mathscr{D}'_\Sigma(\mathscr{M})$*. We have that* $u = K^{\Sigma,j}_P u_j$*,* $j = 0, 1$ *is the unique solution in* $\mathscr{D}'_\Sigma(\mathscr{M})$ *of the initial value problem*

$$\begin{cases} Pu &= 0\ , \\ \rho^\Sigma_{1-j}(u) &= 0\ , \\ \rho^\Sigma_j(u) &= u_j\ , \end{cases} \tag{42}$$

and $u = \Delta^\Sigma_P v$ *is the unique solution in* $\mathscr{D}'_\Sigma(\mathscr{M})$ *of the initial value problem*

$$\begin{cases} Pu &= v\ , \\ \rho^\Sigma_0(u) &= 0\ , \\ \rho^\Sigma_1(u) &= 0\ . \end{cases} \tag{43}$$

□

We note that part (b) of Theorem 3.2.4 is actually stronger than that provided by Theorem 5.1.6 of [33] but it can be derived from energy estimates for P. There are two particular cases of the initial value problem (37) that deserve special attention:

(R) $\operatorname{supp}\vec{\psi} \subset I^+(\Sigma, g)$ – The restriction of Δ_P^Σ to the space of smooth sections of $\mathscr{E}$ with *past compact* support with respect to g

$$
\begin{aligned}
\Gamma^\infty_+(\pi, g) &= \{\vec{\psi} \in \Gamma^\infty(\pi) \mid \forall p \in \mathscr{M}, \\
&\qquad J^-(p, g) \cap \operatorname{supp}\vec{\psi} \text{ is compact}\} \\
&= \{\vec{\psi} \in \Gamma^\infty(\pi) \mid \forall K \subset \mathscr{M} \text{ compact}, \\
&\qquad J^-(K, g) \cap \operatorname{supp}\vec{\psi} \text{ is compact}\}
\end{aligned}
\tag{44}
$$

no longer depends on Σ, as long as condition (R) is satisfied. In this case we write $\Delta_P^\Sigma = \Delta_P^{\mathrm{ret}}$, calling it the *retarded fundamental solution* of P.

(A) $\operatorname{supp}\vec{\psi} \subset I^-(\Sigma, g)$ – The restriction of Δ_P^Σ to the space of smooth sections of $\mathscr{E}$ with *future compact* support with respect to g

$$
\begin{aligned}
\Gamma^\infty_-(\pi, g) &= \{\vec{\psi} \in \Gamma^\infty(\pi) \mid \forall p \in \mathscr{M}, \\
&\qquad J^+(p, g) \cap \operatorname{supp}\vec{\psi} \text{ is compact}\} \\
&= \{\vec{\psi} \in \Gamma^\infty(\pi) \mid \forall K \subset \mathscr{M} \text{ compact}, \\
&\qquad J^+(K, g) \cap \operatorname{supp}\vec{\psi} \text{ is compact}\}
\end{aligned}
\tag{45}
$$

no longer depends on Σ either, as long as condition (A) is satisfied. In this case we write $\Delta_P^\Sigma = \Delta_P^{\mathrm{adv}}$, calling it the *advanced fundamental solution* of P.

The difference $\Delta_P = \Delta_P^{\mathrm{ret}} - \Delta_P^{\mathrm{adv}} : \Gamma^\infty_+(\pi, g) \cap \Gamma^\infty_-(\pi, g) \to \Gamma^\infty(\pi)$ is called the *causal propagator* of P. We obviously have the identity $P \circ \Delta_P = \Delta_P \circ P = 0$ wherever it is defined.

In the scalar case discussed in Theorem 3.2.4, Δ_P^{ret} (resp. Δ_P^{adv}) is defined on the space of smooth functions on $\mathscr{M}$ with past (resp. future) compact support with respect to g

$$
\begin{aligned}
\mathscr{C}^\infty_{+/-}(\mathscr{M}, g) &= \{\psi \in \mathscr{C}^\infty(\mathscr{M}) \mid \forall p \in \mathscr{M}, J^{-/+}(p, g) \cap \operatorname{supp}\psi \text{ is compact}\} \\
&= \{\psi \in \mathscr{C}^\infty(\mathscr{M}) \mid \forall K \subset \mathscr{M} \text{ compact}, J^{-/+}(K, g) \cap \operatorname{supp}\psi \text{ is compact}\}\ .
\end{aligned}
\tag{46}
$$

Specializing Theorem 3.2.4 to these two cases yields the

3.2.5. COROLLARY. *Let the hypotheses and notation of Theorem 3.2.4 be satisfied. Then Δ_P^{ret} and Δ_P^{adv} satisfy the following properties:*

(a) *Continuity: Δ_P^{ret} (resp. Δ_P^{adv}) admits a continuous extension to the space of distributions on $\mathscr{M}$ with past (resp. future) compact support with respect to g*

$$
\begin{aligned}
\mathscr{D}'_{+/-}(\mathscr{M}, g) &= \{v \in \mathscr{D}'(\mathscr{M}) \mid \forall p \in \mathscr{M}\ ,\ J^{-/+}(p, g) \cap \operatorname{supp} v \textit{ is compact}\} \\
&= \{v \in \mathscr{D}'(\mathscr{M}) \mid \forall K \subset \mathscr{M} \textit{ compact}, J^{-/+}(K, g) \cap \operatorname{supp} v \textit{ is compact}\}\ .
\end{aligned}
\tag{47}
$$

(b) *Propagation of supports:*

$$
\operatorname{supp}(\Delta_P^{\mathrm{ret/adv}} v) \subset J^{+/-}(\operatorname{supp} v, \hat{g}) \subset J^{+/-}(\operatorname{supp} v, g)
\tag{48}
$$

for all $v \in \mathscr{D}'_{+/-}(\mathscr{M}, g)$.

(c) *Propagation of singularities: Given any $v \in \mathscr{D}'_{+/-}(\mathscr{M}, g)$, we have that* $(x, \xi) \in \mathrm{WF}(\Delta_P^{\mathrm{ret/adv}} v)$ only if *either $(x, \xi) \in \mathrm{WF}(v)$ or there is $\Lambda > 0$ and a null geodesic segment $\gamma : [0, \Lambda] \to \mathscr{M}$ with respect to $\hat{g}$ such that* $\mathrm{WF}(v) \cap E^{\hat{g}}_\gamma \neq \varnothing$, $(x, \xi) \in E^{\hat{g}}_\gamma$.

We have that for all $v \in \mathscr{D}'_{+/-}(\mathscr{M}, g)$, $u = \Delta_P^{\mathrm{ret/adv}} v$ is the unique solution of $Pu = v$ on $\mathscr{M}$ belonging to $\mathscr{D}'_{+/-}(\mathscr{M}, g)$. □

Corollary 3.2.5 implies that the causal propagator Δ_P propagates singularities in the following fashion: since $\mathrm{WF}(u) \subset \mathrm{WF}(Pu) \cup \{(x,\xi) \in T^*\mathscr{M} \smallsetminus 0 \mid g^{-1}(x)(\xi,\xi) = 0\}$ for all $u \in \mathscr{D}'(\mathscr{M})$ (see for instance Proposition 5.1.1, page 113 of [33]), we conclude that, for all $v \in \mathscr{D}'_+(\mathscr{M}, g) \cap \mathscr{D}'_-(\mathscr{M}, g)$, $(x,\xi) \in \mathrm{WF}(\Delta_P v)$ only if there is $\Lambda > 0$ and a null geodesic segment $\gamma : [0, \Lambda] \to \mathscr{M}$ with respect to $\hat{g}$ such that $\mathrm{WF}(v) \cap E^{\hat{g}}_\gamma \neq \varnothing$, $(x,\xi) \in E^{\hat{g}}_\gamma$, for we have that $P\Delta_P v = 0$.

3.2.6. Remark. It is easy to see that $\mathscr{D}'_\pm(\mathscr{M}, g)$ is the topological dual of the space

$$\mathscr{D}_\mp(\wedge^d T^*\mathscr{M} \to \mathscr{M}) = \{\omega \in \Gamma^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M}) \mid \exists K \subset \mathscr{M} \text{ compact: } \operatorname{supp}\omega \subset J^\mp(K, g)\}\ . \tag{49}$$

The causal propagator Δ_P allows a covariant description of the space of solutions of $Pu = 0$, which is a strengthening of Lemma A.3, page 227 of [32]. We state and prove the result only for scalar fields, but it actually holds for arbitrary vector bundles [4]:

3.2.7. Lemma. *Let $u \in \mathscr{D}'(\mathscr{M})$. Then $Pu = 0$ if and only if $u = \Delta_P v$ for some $v \in \mathscr{D}'(\mathscr{M})$ such that* $\operatorname{supp} v$ *is both past and future compact. If* $\operatorname{supp} u \cap \Sigma$ *is compact for some (hence, any) Cauchy hypersurface, we can choose v such that* $\operatorname{supp} v$ *is compact. In both cases, we can choose v such that* $\operatorname{supp} v$ *is contained in a neighborhood of any prescribed Cauchy hypersurface Σ for $(\mathscr{M}, g)$. Moreover, $\Delta_P v = 0$ if and only if $v = Pw$ for some $w \in \mathscr{D}'(\mathscr{M})$ such that* $\operatorname{supp} w$ *is both past and future compact; if* $\operatorname{supp} u \cap \Sigma$ *is compact for some (hence, any) Cauchy hypersurface, then* $\operatorname{supp} w$ *is compact.*

Proof. Let Σ be any Cauchy hypersurface for $(\mathscr{M}, g)$. By the results in [9], there is a Cauchy time function τ in $(\mathscr{M}, g)$ such that $\Sigma = \tau^{-1}(t_0)$ for some $t_0 \in \mathbb{R}$. We consider the following separate cases:

(a) $\operatorname{supp} u \cap \Sigma$ non-compact: $U_1, U_2 \subset \mathscr{M}$ open such that $U_1 = \tau^{-1}((-\infty, t_0 + \epsilon))$ and $U_2 = \tau^{-1}((t_0 - \epsilon, +\infty))$ for some $\epsilon > 0$. Let $\{\chi_1, \chi_2\}$ be a partition of unity subordinated to $\{U_1, U_2\}$. We have that $u = \chi_1 u + \chi_2 u$, and hence $P(\chi_1 u) = -P(\chi_2 u) = v$ is supported inside $\tau^{-1}((t_0 - \epsilon, t_0 + \epsilon))$, whose closure is past and future compact. Since $\chi_1 u$ has past compact support and $\chi_2 u$ has future compact support, we have that $\chi_1 u = \Delta_P^{\mathrm{ret}}(P(\chi_1 u)$ and $\chi_2 u = \Delta_P^{\mathrm{adv}}(P(\chi_2 u)) = -\Delta_P^{\mathrm{adv}}(P(\chi_1 u))$, whence it follows that $u = \Delta_P(P(\chi_1 u)) = -\Delta_P(P(\chi_2 u)) = \Delta_P v$.

(b) $\operatorname{supp} u \cap \Sigma$ compact: $V_1, V_2, V_3 \subset \mathscr{M}$ open such that $U_1 = I^-(K \cap \Sigma, g)$, $U_2 = I^+(K \cap \Sigma, g)$ and $V_3 = \mathscr{M} \smallsetminus (J^+(\operatorname{supp} u \cap \Sigma, g) \cup J^-(\operatorname{supp} u \cap \Sigma, g))$, where $K \subset \Sigma$ is a compact subset whose interior in Σ contains $\operatorname{supp} u \cap \Sigma$, so that $\overline{U_1 \cap U_2}$ is compact. Let $\{\chi'_1, \chi'_2, \chi'_3\}$ be a partition of unity subordinated to $\{V_1, V_2, V_3\}$. We have by Theorem 3.2.4 that $u = \chi'_1 u + \chi'_2 u$ and hence $P(\chi'_1 u) = -P(\chi'_2 u) = v$ is supported in the compact subset $J^-(K, g) \cap J^+(K, g)$. Since $\chi'_1 u$ has past compact support and $\chi_2 u$ has future compact support, we have that $\chi'_1 u = \Delta_P^{\mathrm{ret}}(P(\chi'_1 u)$ and $\chi'_2 u = \Delta_P^{\mathrm{adv}}(P(\chi'_2 u)) = -\Delta_P^{\mathrm{adv}}(P(\chi'_1 u))$, whence it follows that $u = \Delta_P(P(\chi'_1 u)) = -\Delta_P(P(\chi'_2 u)) = \Delta_P v$.

Finally, if v has past and future compact support, and $\Delta_P v = 0$, we clearly have that $\Delta^{\mathrm{ret}}_P v = \Delta^{\mathrm{adv}}_P v = w$ has past and future compact support as well, whence $v = Pw$ by Corollary 3.2.5. If in addition $\operatorname{supp} v$ is compact, then w has compact support as well. □

We conclude with the following result:

3.2.8. PROPOSITION. *Let $\lambda \mapsto P_\lambda$, $\lambda \in (a,b)$, $a < b \in \mathbb{R}$ be a smooth curve of normally hyperbolic linear partial differential operators on $\Gamma^\infty(\pi)$ satisfying (NH_g), in the sense that P_λ is such an operator for every $\lambda \in (a,b)$ and $\lambda \mapsto (P_\lambda u)(\omega)$ is smooth for all $u \in \mathscr{D}'(\pi\omega \in \Gamma^\infty_c(\mathscr{E}' \otimes \wedge^d T^*\mathscr{M} \to \mathscr{M})$. Then $\lambda \mapsto K^{\Sigma,j}_{P_\lambda}$ $(j = 0,1)$, $\lambda \mapsto \Delta^\Sigma_{P_\lambda}$, $\lambda \mapsto \Delta^{\mathrm{ret}}_{P_\lambda}$ and $\lambda \mapsto \Delta^{\mathrm{adv}}_{P_\lambda}$ are smooth in the sense that $\lambda \mapsto (K^{\Sigma,j}_{P_\lambda} u_j)(\omega)$, $\lambda \mapsto (\Delta^\Sigma_{P_\lambda} v)(\omega)$, $\lambda \mapsto (\Delta^{\mathrm{ret}}_{P_\lambda} v^+)(\omega)$ and $\lambda \mapsto (\Delta^{\mathrm{adv}}_{P_\lambda} v^-)(\omega)$ are smooth for all $u_j \in \mathscr{D}'(\Sigma)$, $j = 0,1$, $v \in \mathscr{D}'_\Sigma(\mathscr{M})$, $v^\pm \in \mathscr{D}'_\pm(\mathscr{M}, g)$. Moreover, one has the following* resolvent formulae*:*

$$\frac{\partial}{\partial\lambda} K^{\Sigma,j}_{P_\lambda} = -\Delta^\Sigma_{P_\lambda} \dot{P}_\lambda K^{\Sigma,j}_{P_\lambda} \ , \tag{50}$$

$$\frac{\partial}{\partial\lambda} \Delta^\Sigma_{P_\lambda} = -\Delta^\Sigma_{P_\lambda} \dot{P}_\lambda \Delta^\Sigma_{P_\lambda} \ , \tag{51}$$

$$\frac{\partial}{\partial\lambda} \Delta^{\mathrm{ret}}_{P_\lambda} = -\Delta^{\mathrm{ret}}_{P_\lambda} \dot{P}_\lambda \Delta^{\mathrm{ret}}_{P_\lambda} \ , \tag{52}$$

$$\frac{\partial}{\partial\lambda} \Delta^{\mathrm{adv}}_{P_\lambda} = -\Delta^{\mathrm{adv}}_{P_\lambda} \dot{P}_\lambda \Delta^{\mathrm{adv}}_{P_\lambda} \ , \tag{53}$$

where $\dot{P}_\lambda u = \frac{\partial}{\partial\lambda}(P_\lambda u)$ for all $u \in \mathscr{D}'(\mathscr{M})$. In particular, for all $u_j \in \mathscr{D}'(\Sigma)$, $j = 0,1$, $v \in \mathscr{D}'_\Sigma(\mathscr{M})$, $v^\pm \in \mathscr{D}'_\pm(\mathscr{M}, g)$, we have that $\mathrm{WF}(\frac{\partial}{\partial\lambda} K^{\Sigma,j}_{P_\lambda} u_j) \subset \mathrm{WF}(K^{\Sigma,j}_{P_\lambda} u_j)$, $\mathrm{WF}(\frac{\partial}{\partial\lambda} \Delta^\Sigma_{P_\lambda} v) \subset \mathrm{WF}(\Delta^\Sigma_{P_\lambda} v)$, $\mathrm{WF}(\frac{\partial}{\partial\lambda} \Delta^{\mathrm{ret}}_{P_\lambda} v^+) \subset \mathrm{WF}(\Delta^{\mathrm{ret}}_{P_\lambda} v^+)$ and $\mathrm{WF}(\frac{\partial}{\partial\lambda} \Delta^{\mathrm{adv}}_{P_\lambda} v^-) \subset \mathrm{WF}(\Delta^{\mathrm{adv}}_{P_\lambda} v^-)$.

Proof. We shall restrict our discussion to $u_j, v, v^\pm$ smooth, $j = 0,1$. The general case then follows from Theorem 3.2.4 and Corollary 3.2.5.

It is straightforward to show that P_λ is smooth in λ in the above sense if and only if the coefficients of P_λ with respect to some (hence, any) choice of connections on π and $T\mathscr{M}$ are jointly smooth on $(a,b) \times \mathscr{M}$. Likewise, since $\dot{P}_\lambda$ is a differential operator with smooth coefficients and hence preserves wave front sets, the above statements on the latter also follow from Theorem 3.2.4 and Corollary 3.2.5.

First we prove (50). Notice that for every $h \in \mathbb{R}$ with $0 < |h| < \min\{\lambda - a, b - \lambda\}$ we have that

$$P_{\lambda+h}\left(\frac{1}{h}(K^{\Sigma,j}_{P_{\lambda+h}} u_j - K^{\Sigma,j}_{P_\lambda} u_j)\right) = -\frac{1}{h}(P_{\lambda+h} - P_\lambda) K^{\Sigma,j}_{P_\lambda} u_j$$

and

$$\rho^\Sigma_0\left(\frac{1}{h}(K^{\Sigma,j}_{P_{\lambda+h}} u_j - K^{\Sigma,j}_{P_\lambda} u_j)\right) = \rho^\Sigma_1\left(\frac{1}{h}(K^{\Sigma,j}_{P_{\lambda+h}} u_j - K^{\Sigma,j}_{P_\lambda} u_j)\right) = 0 \ .$$

This implies that $\lim_{h\to 0} \frac{1}{h}(K^{\Sigma,j}_{P_{\lambda+h}} u_j - K^{\Sigma,j}_{P_\lambda} u_j) \doteq u$ exists in the sense of distributions and solves the initial-value problem

$$\begin{cases} Pu &= \dot{P}_\lambda K^{\Sigma,j}_{P_\lambda} u_j \ , \\ \rho^\Sigma_0(u) &= 0 \ , \\ \rho^\Sigma_1(u) &= 0 \ , \end{cases}$$

since

$$\frac{1}{h}\left\langle (K^{\Sigma,j}_{P_{\lambda+h}}u_j - K^{\Sigma,j}_{P_\lambda}u_j), P'_{\lambda+h}\omega\right\rangle = -\frac{1}{h}\left\langle (P_{\lambda+h}-P_\lambda)K^{\Sigma,j}_{P_\lambda}u_j, \omega\right\rangle$$

for all $\omega\in\Gamma^\infty_c(\mathscr{E}'\otimes\wedge^dT^*\mathscr{M}\to\mathscr{M})$ and all $h\in\mathbb{R}$ with $0<|h|<\min\{\lambda-a,b-\lambda\}$, where $P'_{\lambda+h}$ is the formal adjoint of $P_{\lambda+h}$. Hence, u must be smooth and is given by the right-hand side of (50) applied to u_j. Finally, by Corollary 1.9, pp. 14 of [63], u must coincide with the left-hand side of (50) applied to u_j.

The reasoning for proving (51) is similar, since for every $h\in\mathbb{R}$ with $0<|h|<\min\{\lambda-a,b-\lambda\}$ we have that

$$\begin{aligned} P_{\lambda+h}\left(\frac{1}{h}(\Delta^\Sigma_{P_{\lambda+h}}v-\Delta^\Sigma_{P_\lambda}v)\right) &= \frac{1}{h}v-\frac{1}{h}(P_{\lambda+h}-P_\lambda)\Delta^\Sigma_{P_\lambda}v-\frac{1}{h}v \\ &= -\frac{1}{h}(P_{\lambda+h}-P_\lambda)\Delta^\Sigma_{P_\lambda}v \end{aligned}$$

and

$$\rho^\Sigma_0\left(\frac{1}{h}(\Delta^\Sigma_{P_{\lambda+h}}v-\Delta^\Sigma_{P_\lambda}v)\right) = \rho^\Sigma_1\left(\frac{1}{h}(\Delta^\Sigma_{P_{\lambda+h}}v-\Delta^\Sigma_{P_\lambda}v)\right) = 0\ .$$

The same goes for (52) and (53), once we choose a Cauchy hypersurface Σ contained in $I^-(\mathrm{supp}\,v^+)\smallsetminus\mathrm{supp}\,v^+$ (resp. $I^+(\mathrm{supp}\,v^-)\smallsetminus\mathrm{supp}\,v^-$), which can always be done since $\mathrm{supp}\,v^+$ (resp. $\mathrm{supp}\,v^-$) is past (resp. future) compact – we omit the remaining details. □

In the same way one derives the k-th order resolvent formula (A.12) from the first-order case (A.11), the same can be done from (50)–(53).

Let g' be a Lorentzian metric on $\mathscr{M}$, *a priori* unrelated to either the space-time metric g or the metric $\hat{g}$ associated to the principal symbol of a normally hyperbolic linear partial differential operator P. Recall now the definition of the Hodge star operator $*_{g'}$ acting on d-forms on $\mathscr{M}$: Given $\omega\in\Gamma^\infty(\wedge^dT^*\mathscr{M}\to\mathscr{M})$, we define $*_{g'}\omega\in\mathscr{C}^\infty(\mathscr{M})$ as the unique smooth function on $\mathscr{M}$ such that

$$\omega = (*_{g'}\omega)\mathrm{d}\mu_{g'}\ . \tag{54}$$

Conversely, if $\vec{\varphi}\in\mathscr{C}^\infty(\mathscr{M})$, we have that

$$\vec{\varphi} = *_{g'}(\vec{\varphi}\mathrm{d}\mu_{g'})\ . \tag{55}$$

The following result follows immediately from Theorem 3.2.4.

3.2.9. LEMMA. *Let g' be a Lorentzian metric on $\mathscr{M}$ and $P:\mathscr{C}^\infty(\mathscr{M})\to\mathscr{C}^\infty(\mathscr{M})$ be a linear partial differential operator. Then P is formally self-adjoint with respect to the L^2 scalar product associated to $\mathrm{d}\mu_{g'}$ if and only if the map $\mathscr{C}^\infty(\mathscr{M})\ni\vec{\varphi}\mapsto(P\vec{\varphi})\mathrm{d}\mu_{g'}\in\Gamma^\infty(\wedge^dT^*\mathscr{M}\to\mathscr{M})$ has a symmetric distribution kernel. If either fact holds (hence both), the distribution kernel of $\Delta^{\mathrm{adv}}_P\circ *_{g'}$ is the adjoint of the distribution kernel of $\Delta^{\mathrm{ret}}_P\circ *_{g'}$.* □

The situation we have in mind is, of course, when $P\vec{\varphi} = *_{g'}E'(\mathscr{L})[\varphi_0]\vec{\varphi}$, where $\mathscr{L}$ is a *real-valued*, microlocal generalized Lagrangian of first order on $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ open in the compact-open topology. Generally, given a microlocal generalized Lagrangian $\mathscr{L}$ of order r on $\mathscr{U}$, $E(\mathscr{L})$ is a *quasi-linear* partial differential operator, that is, $E(\mathscr{L})[\varphi]$ is linear in the highest order derivatives of φ. Therefore, we say that the partial differential operator of second order $E(\mathscr{L})$ is *normally hyperbolic* on $\mathscr{U}$ if, for all $\varphi_0 \in \mathscr{U}$, $P = *_{g'} E'(\mathscr{L})[\varphi_0]$ is normally hyperbolic for some (hence any) Lorentzian metric g' on $\mathscr{M}$. In this case, we denote the metric associated to the principal symbol of P defined as above by $\hat{g}_{\mathscr{L}} = \hat{g}_{\mathscr{L}}[\varphi_0]$, and write

$$K^{\Sigma,j}_{\mathscr{L}}[\varphi_0] \doteq K^{\Sigma,j}_P \quad (j = 0,1) \ , \tag{56}$$

$$\Delta^{\Sigma}_{\mathscr{L}}[\varphi_0] \doteq \Delta^{\Sigma}_P \circ *_{g'} \ , \tag{57}$$

$$\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0] \doteq \Delta^{\mathrm{ret}}_P \circ *_{g'} \ , \tag{58}$$

$$\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0] \doteq \Delta^{\mathrm{adv}}_P \circ *_{g'} \ , \tag{59}$$

$$\Delta_{\mathscr{L}}[\varphi_0] \doteq \Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0] - \Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0] \ . \tag{60}$$

We remark that different choices of g' affect $\hat{g}_{\mathscr{L}}$ only by a φ_0-independent conformal factor – in particular, the causal structure of $\hat{g}_{\mathscr{L}}$ is independent of g'. For future convenience, we summarize the estimates on the wave front sets of the distribution kernels of the linear operators (56)–(59) derived from Theorem 3.2.4 and Corollary 3.2.5. To wit, if $\gamma : [0,1] \to \mathscr{M}$ is a null geodesic segment with respect to $\hat{g}_{\mathscr{L}}[\varphi]$ and

$$E^{\hat{g}_{\mathscr{L}}[\varphi]}_\gamma = \{(\gamma(0), \hat{g}_{\mathscr{L}}[\varphi]^\flat(\dot{\gamma}(0))),\, (\gamma(1), \hat{g}_{\mathscr{L}}[\varphi]^\flat(\dot{\gamma}(1)))\}$$

is the set of endpoints of the corresponding bicharacteristic strip, then

$$\begin{aligned}\mathrm{WF}(K^{\Sigma,j}_{\mathscr{L}}[\varphi]) \subset \{(x_0, y; \xi_0, \eta) \in T^*(\Sigma \times \mathscr{M}) \mid \exists \gamma : [0,1] \to \mathscr{M} \text{ null geodesic}\\ \text{such that } E^{\hat{g}_{\mathscr{L}}[\varphi]}_\gamma = \{(x_0,\xi_0),(y,-\eta)\}\},\end{aligned} \tag{61}$$

$$\begin{aligned}\mathrm{WF}(\Delta^{\Sigma}_{\mathscr{L}}[\varphi]) \subset \{(x, y; \xi, \eta) \in T^*(\mathscr{M} \times \mathscr{M}) \mid x = y,\, \xi = \eta \text{ or } \exists \gamma : [0,1] \to \mathscr{M} \text{ null geodesic}\\ \text{such that either } x \leq_g y \leq_g \Sigma \text{ or } \Sigma \leq_g y \leq_g x \text{ and } E^{\hat{g}_{\mathscr{L}}[\varphi]}_\gamma = \{(x,\xi),(y,-\eta)\}\} \ ,\end{aligned} \tag{62}$$

$$\begin{aligned}\mathrm{WF}(\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]) \subset \{(x, y; \xi, \eta) \in T^*(\mathscr{M} \times \mathscr{M}) \mid x = y,\, \xi = \eta \text{ or } \exists \gamma : [0,1] \to \mathscr{M}\\ \text{null geodesic such that } x \geq_g y \text{ and } E^{\hat{g}_{\mathscr{L}}[\varphi]}_\gamma = \{(x,\xi),(y,-\eta)\}\} \ ,\end{aligned} \tag{63}$$

$$\begin{aligned}\mathrm{WF}(\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]) \subset \{(x, y; \xi, \eta) \in T^*(\mathscr{M} \times \mathscr{M}) \mid x = y,\, \xi = \eta \text{ or } \exists \gamma : [0,1] \to \mathscr{M}\\ \text{null geodesic such that } x \leq_g y \text{ and } E^{\hat{g}_{\mathscr{L}}[\varphi]}_\gamma = \{(x,\xi),(y,-\eta)\}\} \ ,\end{aligned} \tag{64}$$

$$\begin{aligned}\mathrm{WF}(\Delta_{\mathscr{L}}[\varphi]) \subset \{(x, y; \xi, \eta) \in T^*(\mathscr{M} \times \mathscr{M}) \mid \exists \gamma : [0,1] \to \mathscr{M} \text{ null geodesic}\\ \text{such that } E^{\hat{g}_{\mathscr{L}}[\varphi]}_\gamma = \{(x,\xi),(y,-\eta)\}\} \ ,\end{aligned} \tag{65}$$

where we identify each of the propagators above with the corresponding distribution kernels. We stress once more that, due to the identity $E'(\mathscr{L})[\varphi]\Delta_{\mathscr{L}}[\varphi] = 0$, $\mathrm{WF}(\Delta_{\mathscr{L}}[\varphi])$ has only pairs of *null* covectors, even over the diagonal $\Delta_2(\mathscr{M})$ of $\mathscr{M}^2$. This is no longer the case for $\mathrm{WF}(\Delta^{\Sigma}_{\mathscr{L}}[\varphi])$, $\mathrm{WF}(\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi])$ or $\mathrm{WF}(\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi])$, which may have conormal covectors over $\Delta_2(\mathscr{M})$ which consist of pairs of covectors of arbitrary causal character.

3.2.10. REMARK. Let us display a sufficiently nontrivial example of a microlocal generalized Lagrangian with normally hyperbolic Euler-Lagrange operator. For instance,

$$\mathscr{L}(f)(\varphi) = -\frac{1}{2}\int_{\mathscr{M}} f\left[g^{-1}(\mathrm{d}\varphi,\mathrm{d}\varphi) + \frac{\epsilon}{2}(1+\varphi^2)g^{-1}(\mathrm{d}\varphi,\mathrm{d}\varphi)^2\right]\mathrm{d}\mu_g\ ,\quad \epsilon \geq 0\ . \tag{66}$$

The Euler-Lagrange operator of $\mathscr{L}$ is given by

$$\begin{aligned} E(\mathscr{L})[\varphi] &= \left[(1+\epsilon(1+\varphi^2)g^{-1}(\mathrm{d}\varphi,\mathrm{d}\varphi))\Box_g\varphi + \epsilon(2\nabla^2\varphi(g^\sharp(\mathrm{d}\varphi),g^\sharp(\mathrm{d}\varphi)) - \frac{1}{2}g^{-1}(\mathrm{d}\varphi,\mathrm{d}\varphi)\varphi)\right]\mathrm{d}\mu_g\ ,\\ \Box_g\varphi &= g^{-1}(\nabla^2\varphi)\ , \end{aligned} \tag{67}$$

whose linearization around φ_0 is given by

$$\begin{aligned} E'(\mathscr{L})[\varphi_0]\vec{\varphi} &= \big[(1+\epsilon(1+\varphi_0^2)g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0))\Box_g\vec{\varphi} + 2\epsilon\nabla^2\vec{\varphi}(g^\sharp(\mathrm{d}\varphi_0),g^\sharp(\mathrm{d}\varphi_0))\\ &\quad + 2\epsilon\left[\left((1+\varphi_0^2)\Box_g\varphi_0 - \frac{1}{2}\varphi_0\right)g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\vec{\varphi}) + 2\nabla^2\varphi_0(g^\sharp(\mathrm{d}\varphi_0),g^\sharp(\mathrm{d}\vec{\varphi}))\right.\\ &\quad \left.+\epsilon g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0)\left(2\Box_g\varphi_0 - \frac{1}{2}\right)\vec{\varphi}\right]\mathrm{d}\mu_g\\ &= \big[\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](\nabla^2\vec{\varphi}) + \nabla_A\vec{\varphi} + B\vec{\varphi}\big]\,\mathrm{d}\mu_g\ , \end{aligned} \tag{68}$$

where $A(p) = A(g(p),\varphi_0(p),\nabla\varphi_0(p),\nabla^2\varphi_0(p))$ and $B = B(g(p),\varphi_0(p),\nabla\varphi_0(p),\nabla^2\varphi_0(p))$ for all $p \in \mathscr{M}$. The principal symbol of $P = *_g E'(\mathscr{L})[\varphi_0]$ reads

$$\begin{aligned} \hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X_1),g^\flat(X_2)) &= (1+\epsilon(1+\varphi_0^2)g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0))g(X_1,X_2)\\ &\quad + 2\epsilon(\nabla_{X_1}\varphi_0)(\nabla_{X_2}\varphi_0)\ , \end{aligned} \tag{69}$$

whence we conclude that

$$\begin{aligned} \hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) > 0 &\Leftrightarrow (1+\epsilon(1+\varphi_0^2)g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0))g(X,X) > -2\epsilon(\nabla_X\varphi_0)^2\ ,\\ \hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) = 0 &\Leftrightarrow (1+\epsilon(1+\varphi_0^2)g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0))g(X,X) = -2\epsilon(\nabla_X\varphi_0)^2\ ,\\ \hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) < 0 &\Leftrightarrow (1+\epsilon(1+\varphi_0^2)g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0))g(X,X) < -2\epsilon(\nabla_X\varphi_0)^2\ . \end{aligned} \tag{70}$$

We consider the following three possibilities:

$$g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0) > -\frac{1}{2\epsilon(1+\varphi_0^2)}\ , \tag{71}$$

$$g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0) = -\frac{1}{2\epsilon(1+\varphi_0^2)}\ , \tag{72}$$

$$g^{-1}(\mathrm{d}\varphi_0,\mathrm{d}\varphi_0) < -\frac{1}{2\epsilon(1+\varphi_0^2)}\ . \tag{73}$$

Inequalities (71) and (73) define open subsets of $\mathscr{C}^\infty(\mathscr{M})$ in the Whitney topology. In case (71) holds, we have that $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) < 0$ implies $g(X,X) < 0$ and $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) = 0$ implies $g(X,X) \leq 0$, whereas $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) > 0$ does not constrain the causal character of X with respect to g. In case (72) holds, we have that $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(Y)) = 0$ for all tangent vectors Y if X satisfies $\nabla_X\varphi_0 = 0$ (hence $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0]$ becomes degenerate); moreover, $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0]$ cannot have any timelike covectors. In case (73) holds, we have that $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X),g^\flat(X)) < 0$ implies

$g(X,X) > 0$ and $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X), g^\flat(X)) = 0$ implies $g(X,X) \geq 0$, whereas $\hat{g}^{-1}_{\mathscr{L}}[\varphi_0](g^\flat(X), g^\flat(X)) > 0$ does not constrain the causal character of X with respect to g. To summarize,

$$g^{-1}(\mathrm{d}\varphi_0, \mathrm{d}\varphi_0) > -\frac{1}{2\epsilon(1+\varphi_0^2)} \Rightarrow \hat{g}_{\mathscr{L}}[\varphi_0] \lesssim g \ , \tag{74}$$

$$g^{-1}(\mathrm{d}\varphi_0, \mathrm{d}\varphi_0) = -\frac{1}{2\epsilon(1+\varphi_0^2)} \Rightarrow \hat{g}^{-1}_{\mathscr{L}}[\varphi_0] \text{ degenerate} \ , \tag{75}$$

$$g^{-1}(\mathrm{d}\varphi_0, \mathrm{d}\varphi_0) < -\frac{1}{2\epsilon(1+\varphi_0^2)} \Rightarrow -\hat{g}_{\mathscr{L}}[\varphi_0] \lesssim g \ . \tag{76}$$

In other words, crossing the boundary $g^{-1}(\mathrm{d}\varphi_0, \mathrm{d}\varphi_0) = -\frac{1}{2\epsilon(1+\varphi_0^2)}$ causes $\hat{g}_{\mathscr{L}}[\varphi_0]$'s signature to change sign, partitioning $\mathscr{C}^\infty(\mathscr{M})$ into two Whitney-open, disjoint "domains of hyperbolicity" separated by the boundary $g^{-1}(\mathrm{d}\varphi_0, \mathrm{d}\varphi_0) = -\frac{1}{2\epsilon(1+\varphi_0^2)}$. The presence of this boundary is linked to the lifespan of solutions of $E(\mathscr{L})[\varphi] = 0$; indeed, the "sharp continuation principle" of Majda (Theorem 2.2, pp. 31–32 in [67]) implies that, at least when $(\mathscr{M}, g)$ is the Minkowski space-time, if a solution φ to $E(\mathscr{L})[\varphi] = 0$ with given Cauchy data at $\Sigma = \tau^{-1}(0)$ blows up in $\mathscr{C}^\infty(\mathscr{M})$ as $\tau(p) \to t^* > 0$ but the second-order jet prolongation of φ is bounded in $K \cap \tau^{-1}([0, t^*))$ for any compact subset $K \subset \mathscr{M}$, then we must have that $g^{-1}(\mathrm{d}\varphi(p), \mathrm{d}\varphi(p)) + \frac{1}{2\epsilon(1+\varphi^2(p))} \overset{\tau(p)\to t^*}{\longrightarrow} 0$, where τ is a Cauchy time function on $(\mathscr{M}, g)$. We stress that it is not hard to provide examples of φ_0 which fall into either (74) or (76) – for (74) to hold, it suffices to choose φ_0 with everywhere spacelike gradient; as for (76), any Cauchy time function $\varphi_0 = \tau$ on $(\mathscr{M}, g)$ satisfying $g^{-1}(\mathrm{d}\tau, \mathrm{d}\tau) < -(2\epsilon)^{-1}$ does the trick, and any globally hyperbolic space-time admits such Cauchy time functions [73]. On the other hand, this is a typical "large data" phenomenon, specially if ϵ is small. Since the nonlinear terms of $E(\mathscr{L})[\varphi]$ vanish to third order at $\varphi = 0$, one can show, at least when $(\mathscr{M}, g)$ is the Minkowski space-time, that $E(\mathscr{L})[\varphi] = 0$ has unique, global smooth solutions for sufficiently small Cauchy data [52, 81].

Motivated by formula (17) in Remark 2.3.9, we write for each $\vec{\psi}_j \in \mathscr{C}^\infty(\Sigma)$, $j = 0, 1$, $\omega \in \Gamma^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$, $\omega^\pm \in \Gamma^\infty_\mp(\wedge^d T^*\mathscr{M} \to \mathscr{M}, g)$

$$D^k K^{\Sigma;j}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1, \ldots, \vec{\varphi}_k)\vec{\psi}_j \doteq \frac{\partial^k}{\partial\lambda_1 \cdots \partial\lambda_k}\Big|_{\lambda_1 = \cdots = \lambda_k = 0} K^{\Sigma;j}_{\mathscr{L}}\left[\varphi_0 + \sum_{l=1}^k \lambda_l \vec{\varphi}_l\right]\vec{\psi}_j \ , \tag{77}$$

$$D^k \Delta^{\Sigma}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1, \ldots, \vec{\varphi}_k)\omega \doteq \frac{\partial^k}{\partial\lambda_1 \cdots \partial\lambda_k}\Big|_{\lambda_1 = \cdots = \lambda_k = 0} \Delta^{\Sigma}_{\mathscr{L}}\left[\varphi_0 + \sum_{l=1}^k \lambda_l \vec{\varphi}_l\right]\omega \ , \tag{78}$$

$$D^k \Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1, \ldots, \vec{\varphi}_k)\omega^+ \doteq \frac{\partial^k}{\partial\lambda_1 \cdots \partial\lambda_k}\Big|_{\lambda_1 = \cdots = \lambda_k = 0} \Delta^{\mathrm{ret}}_{\mathscr{L}}\left[\varphi_0 + \sum_{l=1}^k \lambda_l \vec{\varphi}_l\right]\omega^+ \ , \tag{79}$$

$$D^k \Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1, \ldots, \vec{\varphi}_k)\omega^- \doteq \frac{\partial^k}{\partial\lambda_1 \cdots \partial\lambda_k}\Big|_{\lambda_1 = \cdots = \lambda_k = 0} \Delta^{\mathrm{adv}}_{\mathscr{L}}\left[\varphi_0 + \sum_{l=1}^k \lambda_l \vec{\varphi}_l\right]\omega^- \ . \tag{80}$$

Combining Proposition 3.2.3 with the chain rule (A.3) yields for each $\vec{\psi}_j \in \mathscr{C}^\infty(\Sigma)$, $j = 0,1$, $\omega \in \Gamma^\infty(\wedge^d T^*\mathscr{M} \to \mathscr{M})$, $\omega^\pm \in \Gamma^\infty_\pm(\wedge^d T^*\mathscr{M} \to \mathscr{M}, g)$ that

$$DK^{\Sigma,j}_{\mathscr{L}}[\varphi_0](\vec{\varphi})\vec{\psi}_j = -\Delta^\Sigma_{\mathscr{L}}[\varphi_0]D^2E(\mathscr{L})[\varphi_0](\vec{\varphi})K^{\Sigma,j}_{\mathscr{L}}\vec{\psi}_j \ , \tag{81}$$

$$D\Delta^\Sigma_{\mathscr{L}}[\varphi_0](\vec{\varphi})\omega = -\Delta^\Sigma_{\mathscr{L}}[\varphi_0]D^2E(\mathscr{L})[\varphi_0](\vec{\varphi})\Delta^\Sigma_{\mathscr{L}}\omega \ , \tag{82}$$

$$D\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0](\vec{\varphi})\omega^+ = -\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0]D^2E(\mathscr{L})[\varphi_0](\vec{\varphi})\Delta^{\mathrm{ret}}_{\mathscr{L}}\omega^+ \ , \tag{83}$$

$$D\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0](\vec{\varphi})\omega^- = -\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0]D^2E(\mathscr{L})[\varphi_0](\vec{\varphi})\Delta^{\mathrm{adv}}_{\mathscr{L}}\omega^- \ , \tag{84}$$

whence it follows from the same reasoning leading from the first-order resolvent formula (A.11) to the k-th order resolvent formula (A.12) that

(85)
$$\begin{aligned}&D^kK^{\Sigma,j}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\vec{\psi}_j\\ &\quad=\sum_{l=1}^k(-1)^l\sum_{\{I_1,\ldots,I_l\}\in P_k}\sum_{\sigma\in S_l}\left(\prod_{j=1}^l\Delta^\Sigma_{\mathscr{L}}[\varphi_0]D^{|I_{\sigma(j)}|+1}E(\mathscr{L})[\varphi_0](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\right)K^{\Sigma,j}_{\mathscr{L}}[\varphi_0]\vec{\psi}_j \ ,\end{aligned}$$

(86)
$$\begin{aligned}&D^k\Delta^\Sigma_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\omega\\ &\quad=\sum_{l=1}^k(-1)^l\sum_{\{I_1,\ldots,I_l\}\in P_k}\sum_{\sigma\in S_l}\left(\prod_{j=1}^l\Delta^\Sigma_{\mathscr{L}}[\varphi_0]D^{|I_{\sigma(j)}|+1}E(\mathscr{L})[\varphi_0](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\right)\Delta^\Sigma_{\mathscr{L}}[\varphi_0]\omega \ ,\end{aligned}$$

(87)
$$\begin{aligned}&D^k\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\omega^+\\ &\quad=\sum_{l=1}^k(-1)^l\sum_{\{I_1,\ldots,I_l\}\in P_k}\sum_{\sigma\in S_l}\left(\prod_{j=1}^l\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0]D^{|I_{\sigma(j)}|+1}E(\mathscr{L})[\varphi_0](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\right)\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0]\omega^+ \ ,\end{aligned}$$

(88)
$$\begin{aligned}&D^k\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\omega^-\\ &\quad=\sum_{l=1}^k(-1)^l\sum_{\{I_1,\ldots,I_l\}\in P_k}\sum_{\sigma\in S_l}\left(\prod_{j=1}^l\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0]D^{|I_{\sigma(j)}|+1}E(\mathscr{L})[\varphi_0](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\right)\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0]\omega^- \ .\end{aligned}$$

and therefore

$$\begin{aligned}D^kK^{\Sigma,j}_{\mathscr{L}}&:\mathscr{U}\times(\mathscr{C}^\infty(\mathscr{M}))^k\times\mathscr{D}(\Sigma)\to\mathscr{D}'_\Sigma(\mathscr{M})\quad j=0,1\ ,\\ D^k\Delta^\Sigma_{\mathscr{L}}&:\mathscr{U}\times(\mathscr{C}^\infty(\mathscr{M}))^k\times\mathscr{D}'_\Sigma(\wedge^dT^*\mathscr{M}\to\mathscr{M})\to\mathscr{D}'_\Sigma(\mathscr{M})\ ,\\ D^k\Delta^{\mathrm{ret}}_{\mathscr{L}}&:\mathscr{U}\times(\mathscr{C}^\infty(\mathscr{M}))^k\times\mathscr{D}'_+(\wedge^dT^*\mathscr{M}\to\mathscr{M},g)\to\mathscr{D}'_\Sigma(\mathscr{M})\text{ and}\\ D^k\Delta^{\mathrm{adv}}_{\mathscr{L}}&:\mathscr{U}\times(\mathscr{C}^\infty(\mathscr{M}))^k\times\mathscr{D}'_-(\wedge^dT^*\mathscr{M}\to\mathscr{M},g)\to\mathscr{D}'_\Sigma(\mathscr{M})\end{aligned}\tag{89}$$

exist and are jointly continuous for all $k \geq 1$, where

$$\mathscr{D}'_\Sigma(\wedge^d T^*\mathscr{M} \to \mathscr{M}) \doteq \{u \in \mathscr{D}'(\wedge^d T^*\mathscr{M} \to \mathscr{M}) \mid \mathrm{WF}(u) \cap N^*\Sigma = \varnothing\} \ ,$$
$$\mathscr{D}'_\pm(\wedge^d T^*\mathscr{M} \to \mathscr{M}, g) \doteq \{u \in \mathscr{D}'(\wedge^d T^*\mathscr{M} \to \mathscr{M}) \mid \exists K \subset \mathscr{M} \text{ compact such that } J^\mp(K) \cap \operatorname{supp} u \text{ is compact}\} \ .$$

3.2.11. Definition. Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology, and $F, G \in \mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$. The *retarded* and *advanced products* $\mathsf{R}_\mathscr{L}(F,G)$, $\mathsf{A}_\mathscr{L}(F,G)$ with respect to $\mathscr{L}$ are functionals respectively given by

$$\mathsf{R}_\mathscr{L}(F,G)(\varphi) \doteq \left\langle F^{(1)}[\varphi], \Delta^{\mathrm{ret}}_\mathscr{L}[\varphi] G^{(1)}[\varphi] \right\rangle \tag{90}$$

and

$$\begin{aligned} \mathsf{A}_\mathscr{L}(F,G)(\varphi) &\doteq \left\langle F^{(1)}[\varphi], \Delta^{\mathrm{adv}}_\mathscr{L}[\varphi] G^{(1)}[\varphi] \right\rangle \\ &= \mathsf{R}_\mathscr{L}(G,F)(\varphi) \ . \end{aligned} \tag{91}$$

Their difference

$$\{F,G\}_\mathscr{L} \doteq \mathsf{R}_\mathscr{L}(F,G) - \mathsf{A}_\mathscr{L}(F,G) = \mathsf{R}_\mathscr{L}(F,G) - \mathsf{R}_\mathscr{L}(G,F) \tag{92}$$

is called the *Peierls bracket* of F with G with respect to $\mathscr{L}$.

By Lemma 3.2.9, the Peierls bracket is antisymmetric in its entries, becoming an obvious candidate for a Poisson bracket. Let us prove some basic properties of $\mathsf{R}_\mathscr{L}(\cdot,\cdot)$, $\mathsf{A}_\mathscr{L}(\cdot,\cdot)$ and $\{\cdot,\cdot\}_\mathscr{L}$. For later convenience, given $\varnothing \neq K, L \subset \mathscr{M}$ we define

$$\mathscr{O}^{\mathrm{ret}}_{K,L} = J^+(K,g) \cap J^-(L,g) \ , \ \mathscr{O}^{\mathrm{adv}}_{K,L} = \mathscr{O}^{\mathrm{ret}}_{L,K} \ , \ \mathscr{O}_{K,L} = \mathscr{O}^{\mathrm{ret}}_{K,L} \cup \mathscr{O}^{\mathrm{adv}}_{K,L} \ . \tag{93}$$

By global hyperbolicity of $(\mathscr{M}, g)$, we have that $\mathscr{O}^{\mathrm{ret}}_{K,L}$, $\mathscr{O}^{\mathrm{adv}}_{K,L}$ and $\mathscr{O}_{K,L}$ are compact if K, L also are.

3.2.12. Proposition. *Let $\mathscr{U}, F, G$ as in Definition 3.2.11. Then $\mathsf{R}_\mathscr{L}(F,G)$, $\mathsf{A}_\mathscr{L}(F,G)$ and $\{F,G\}_\mathscr{L}$ are smooth and satisfy the support properties*

$$\operatorname{supp} \mathsf{R}_\mathscr{L}(F,G) \subset \mathscr{O}^{\mathrm{ret}}_{\operatorname{supp} F, \operatorname{supp} G} \ , \tag{94}$$

$$\operatorname{supp} \mathsf{A}_\mathscr{L}(F,G) \subset \mathscr{O}^{\mathrm{adv}}_{\operatorname{supp} F, \operatorname{supp} G} \ , \tag{95}$$

$$\operatorname{supp} \{F,G\}_\mathscr{L} \subset \mathscr{O}_{\operatorname{supp} F, \operatorname{supp} G} \ . \tag{96}$$

Proof. Notice that $\Delta^{\mathrm{ret}}_\mathscr{L}[\varphi]$ and $\Delta^{\mathrm{adv}}_\mathscr{L}[\varphi]$ depend on the background field configuration φ only so far as the coefficients of $E'(\mathscr{L})[\varphi]$ depend on φ. Therefore, by part (b) of Theorem 3.2.4, for all $\omega \in \Gamma^\infty_c(\wedge^d T^*\mathscr{M} \to \mathscr{M})$ any modification of φ outside $J^+(\operatorname{supp} f, g)$ (resp. $J^-(\operatorname{supp} f, g)$) leaves $\Delta^{\mathrm{ret}}_\mathscr{L}[\varphi] f$ (resp. $\Delta^{\mathrm{adv}}_\mathscr{L}[\varphi] f$) unaltered. Since $\Delta^{\mathrm{ret}}_\mathscr{L}[\varphi]$ is the formal adjoint of $\Delta^{\mathrm{adv}}_\mathscr{L}[\varphi]$, the above reasoning together with part (b) of Theorem 3.2.4 imply that $\Delta^{\mathrm{ret}}_\mathscr{L}[\varphi]$ and $\Delta^{\mathrm{adv}}_\mathscr{L}[\varphi]$ have the desired support properties. Now we are only left with proving that $\mathsf{R}_\mathscr{L}(F,G)$ and $\mathsf{A}_\mathscr{L}(F,G)$ are smooth functionals, since this implies the corresponding result for $\{F,G\}_\mathscr{L}$. This, however, follows from formulae (87) and (88) together with the trilinear Leibniz rule (A.8) (i.e. with $l = 3$ therein), which give us that

$$
\begin{aligned}
D^k\mathsf{R}_{\mathscr{L}}(F,G)[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k) = & \sum_{\{J_1,J_2,J_3\}\subset P_k} F^{(|J_1|+1)}[\varphi]((\otimes_{j_1\in J_1}\vec{\varphi}_{j_1}) \\
& \otimes D^{|J_2|}\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]((\otimes_{j_2\in J_2}\vec{\varphi}_{j_2})\otimes G^{(|J_3|+1)}[\varphi](\otimes_{j_3\in J_3}\vec{\varphi}_{j_3}))) \ , \\
D^k\mathsf{A}_{\mathscr{L}}(F,G)[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k) = & \sum_{\{J_1,J_2,J_3\}\subset P_k} F^{(|J_1|+1)}[\varphi]((\otimes_{j_1\in J_1}\vec{\varphi}_{j_1}) \\
& \otimes D^{|J_2|}\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]((\otimes_{j_2\in J_2}\vec{\varphi}_{j_2})\otimes G^{(|J_3|+1)}[\varphi](\otimes_{j_3\in J_3}\vec{\varphi}_{j_3}))) \ .
\end{aligned}
\tag{97}
$$

where P_k is set of all partitions of the set $\{1,\ldots,k\}$. We notice that due to (87) and (88), each term in the right-hand side of (97) before smearing with $\vec{\varphi}_1,\ldots,\vec{\varphi}_k$ can be seen as a string of compositions of:

(i) $l+1$ propagators of the form $\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]$ (for the retarded product) or $\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]$ (for the advanced product); and
(ii) $l+2$ k_i-linear *differential* operators, $i = 0,\ldots,l+1$ whose distribution kernels are either of the form $F^{(k_0+1)}[\varphi]$, $D^{k_i+2}\mathscr{L}(1)[\varphi]$ for $1\leq i\leq l$ or $G^{(k_{l+1}+1)}[\varphi]$,

for each $l = 1,\ldots,k$ with $k_0+\cdots+k_{l+1} = k$, followed by an integration over $\mathscr{M}$ = smearing with the test function $f(x)\equiv 1$. The pairing of variables in such a composition for each term in the right-hand side of (87) and (88) is of the following form:

- The first variable of the kernel of the first propagator pairs with the first variable of $F^{(k_1+1)}[\varphi]$;
- The first variable of $D^{k_i+2}\mathscr{L}(1)[\varphi]$ pairs with the second variable of the kernel of the i-th propagator;
- The second variable of $D^{k_i+2}\mathscr{L}(1)[\varphi]$ pairs with the first variable of the kernel of the $(i+1)$-th propagator;
- The second variable of the kernel of the last propagator pairs with the first variable of $G^{(k_{l+1}+1)}[\varphi]$.

It is clear that such a string of compositions is well defined. Finally, the smearing with $\vec{\varphi}_1,\ldots,\vec{\varphi}_k$ is allowed since the distribution obtained is compactly supported. The proof is complete. □

By (65), $\{F,G\}_{\mathscr{L}}$ is actually defined for any pair of smooth functionals F,G with compact space-time support such that $\mathrm{WF}(F^{(1)}[\varphi])$ and $\mathrm{WF}(G^{(1)}[\varphi])$ do not contain any causal covectors with respect to g for all $\varphi\in\mathscr{U}$, provided that $\hat{g}_{\mathscr{L}}[\varphi]\lesssim g$ for all such φ. This motivates the following

3.2.13. DEFINITION. Let $(\mathscr{M}, g)$ be a globally hyperbolic space-time. Define for all $k \geq 1$ the open subsets $\Upsilon_{k,g} \subset T^*\mathscr{M}^k \smallsetminus 0$ as follows:

$$\begin{aligned}
\Upsilon_{k,g} &= \{(x_1, \ldots, x_k; \xi_1, \ldots, \xi_k) \in T^*\mathscr{M}^k \smallsetminus 0 \mid \\
&\qquad (\xi_1, \ldots, \xi_k) \notin \overline{V}^k_{+,g}(x_1, \ldots, x_k) \cup \overline{V}^k_{-,g}(x_1, \ldots, x_k)\} , \\
\overline{V}^k_{\pm,g}(x_1, \ldots, x_k) &= \prod_{j=1}^k \overline{V}_{\pm,g}(x_j) , \\
V_{\pm,g}(x) &= I^{\pm}(0, g^{-1}(x)) \subset T^*_x\mathscr{M} , \; x \in \mathscr{M} .
\end{aligned} \tag{98}$$

Let now $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology. We say that a smooth functional F with compact space-time support is *microcausal* with respect to g if $\mathrm{WF}(F^{(k)}[\varphi]) \subset \Upsilon_{k,g}$ for all $\varphi \in \mathscr{U}$, $k \geq 1$. The space of all microcausal functionals in $\mathscr{U}$ with respect to g is denoted by $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$.

We obviously have that $\mathscr{F}_0(\mathscr{M}, \mathscr{U}) \subset \mathscr{F}((\mathscr{M}, g), \mathscr{U})$. A much more interesting inclusion is given by the following

3.2.14. PROPOSITION. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology, $F \in \mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$. Then $\mathrm{WF}(F^{(k)}[\varphi]) \perp T\Delta_k(\mathscr{M})$ for all $\varphi \in \mathscr{U}$, $k \geq 2$. In particular, $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U}) \subset \mathscr{F}((\mathscr{M}, g), \mathscr{U})$.*

Proof. Let $\varphi \in \mathscr{U}$. For all $k \geq 2$, $F^{(k)}[\varphi]$ is the kernel of a $(k-1)$-linear, $(k-1)$-differential operator taking values in the vector bundle of $\mathbb{C}$-valued d-forms, as shown by Propositions 2.3.11 and 2.3.13. That is, if $\vec{\varphi}_1, \ldots, \vec{\varphi}_{k-1} \in \mathscr{C}^\infty(\mathscr{M})$, then $F^{(k)}[\varphi](\cdot, \vec{\varphi}_1, \ldots, \vec{\varphi}_{k-1})$ can be thought of locally in $\mathscr{M}$ as a sum of products of d-form-valued linear partial differential operators acting on $\vec{\varphi}_1$ multiplied by a product of derivatives of $\vec{\varphi}_j$ for all $2 \leq j \leq k-1$. This means that $F^{(k)}[\varphi]$ can be written locally as a finite sum of derivatives of the Dirac kernel δ_k in $\mathscr{M}^k$, defined by

$$\delta_k(\omega \otimes \vec{\varphi}_1 \otimes \cdots \otimes \vec{\varphi}_{k-1}) \doteq \int_{\mathscr{M}} \prod_{j=1}^{k-1} \vec{\varphi}_j \omega , \quad \omega \in \Gamma^\infty_c(\wedge^d T^*\mathscr{M} \to \mathscr{M}) ,$$

with each term of the sum evaluated at a possibly different, φ-dependent ω. Since δ_k is simply the pullback of the constant function $u \equiv 1$ (seen as a distribution in $\mathscr{M}^k$) by the inclusion $\Delta_k(\mathscr{M}) \hookrightarrow \mathscr{M}^k$, the assertion follows from Theorem 8.2.4, pp. 263–265 of [50]. $\square$

Proposition 3.2.14 justifies the term "microlocal" for designating the elements of $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$, establishing the link with the notion of local functional employed in [15]. One may wonder whether locality in the sense of Definition 2.3.10 (i.e. through formula (20)) and microcausality together entail microlocality, as claimed e.g. in Section 2 of [35] (more precisely, see formula (2.8), pp. 1296). This happens to be *false*, as example (25) shows – there $F^{(k)} \equiv 0$ for $k > 1$ but $\mathrm{WF}(F^{(1)}[\varphi])$ is conormal to $\mathscr{N}$, hence it consists of spacelike covectors only. This shows that such an F is microcausal. However, we have seen that F is local but not microlocal, thus establishing our claim.

It is of paramount importance that the Peierls bracket can actually be extended from microlocal to arbitrary microcausal functionals.

3.2.15. THEOREM. *Let $\mathscr{U}, \mathscr{L}$ be as in Proposition 3.2.12. The Peierls bracket associated with any such $\mathscr{L}$ extends to the whole of $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$, possesses the support property* (96) *and depends* only locally on $\mathscr{L}$ – *that is, for all $F, G \in \mathscr{F}((\mathscr{M}, g), \mathscr{U})$ we have that $\{F, G\}_{\mathscr{L}}$ is* unaffected *by perturbations of $\mathscr{L}$ outside $\mathscr{O}_{\mathrm{supp}\,F, \mathrm{supp}\,G}$. Likewise, for all $F, G \in \mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M}, \mathscr{U})$ we have that $\mathsf{R}_{\mathscr{L}}(F, G)$ (resp. $\mathsf{A}_{\mathscr{L}}(F, G)$) is unaffected by perturbations of $\mathscr{L}$ outside $\mathscr{O}^{\mathrm{ret}}_{\mathrm{supp}\,F, \mathrm{supp}\,F}$ (resp. $\mathscr{O}^{\mathrm{adv}}_{\mathrm{supp}\,F, \mathrm{supp}\,F}$).*

Proof. We first check whether the Peierls bracket is well defined when extended to $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$. As argued right after the proof of Proposition 3.2.12, since the wave front set of the first derivative of a microcausal functional contains only spacelike covectors and, by (65), the wave front set of $\Delta_{\mathscr{L}}[\varphi]$ contains only pairs of null covectors, which after parallel transport along a null geodesic add to zero, the term $\Delta_{\mathscr{L}}[\varphi]G^{(1)}[\varphi]$ is smooth and can therefore be integrated with the compactly supported distributional density $F^{(1)}[\varphi]$. The proof of (96) then carries through *ipsis literis* as in the case that F and G are microlocal (Proposition 3.2.12).

Concerning the dependence of the Peierls bracket on local data of $\mathscr{L}$, let us first pick two arbitrary microcausal functionals F, G. Now, let two Lagrangians $\mathscr{L}_1, \mathscr{L}_2$ satisfy the hypotheses of Proposition 3.2.12 and such that we have for any $\varphi \in \mathscr{U}$ $E'(\mathscr{L}_1)[\varphi]$ and $E'(\mathscr{L}_2)[\varphi]$ differ only outside $\mathscr{O}_{\mathrm{supp}\,F, \mathrm{supp}\,G}$. More precisely, we suppose that

$$\mathrm{supp}\,(E'(\mathscr{L}_1)[\varphi] - E'(\mathscr{L}_2)[\varphi]) \cap \mathscr{O}_{\mathrm{supp}\,F, \mathrm{supp}\,G} = \varnothing \tag{99}$$

for all $\varphi \in \mathscr{U}$. We see that

$$\begin{aligned} \Big\langle \Delta^{\mathrm{adv}}_{\mathscr{L}_1}[\varphi]F^{(1)}[\varphi], (E'(\mathscr{L}_2)[\varphi] &- E'(\mathscr{L}_1)[\varphi])\Delta^{\mathrm{ret}}_{\mathscr{L}_2}[\varphi]G^{(1)}[\varphi] \Big\rangle \\ &= \Big\langle F^{(1)}[\varphi], (\Delta^{\mathrm{ret}}_{\mathscr{L}_1}[\varphi] - \Delta^{\mathrm{ret}}_{\mathscr{L}_2}[\varphi])G^{(1)}[\varphi] \Big\rangle = 0\ , \end{aligned} \tag{100}$$

$$\begin{aligned} \Big\langle \Delta^{\mathrm{ret}}_{\mathscr{L}_1}[\varphi]F^{(1)}[\varphi], (E'(\mathscr{L}_2)[\varphi] &- E'(\mathscr{L}_1)[\varphi])\Delta^{\mathrm{adv}}_{\mathscr{L}_2}[\varphi]G^{(1)}[\varphi] \Big\rangle \\ &= \Big\langle F^{(1)}[\varphi], (\Delta^{\mathrm{adv}}_{\mathscr{L}_1}[\varphi] - \Delta^{\mathrm{adv}}_{\mathscr{L}_2}[\varphi])G^{(1)}[\varphi] \Big\rangle = 0 \end{aligned} \tag{101}$$

for all $\varphi \in \mathscr{U}$ thanks to (99), which also guarantees that the left-hand sides of (100) and (101) are well defined since there are no common base points in the wave front sets of either side for any of the dual pairings involved therein. This already entails the desired properties for $\mathsf{R}_{\mathscr{L}}(F, G)$ and $\mathsf{A}_{\mathscr{L}}(F, G)$ if F, G are microlocal, since (100) (resp. (101)) remain valid if we allow $E'(\mathscr{L}_1)[\varphi]$ and $E'(\mathscr{L}_2)[\varphi]$ to differ only outside $\mathscr{O}^{\mathrm{ret}}_{\mathrm{supp}\,F, \mathrm{supp}\,G}$ (resp. $\mathscr{O}^{\mathrm{adv}}_{\mathrm{supp}\,F, \mathrm{supp}\,G}$) for all $\varphi \in \mathscr{U}$. As for $\{F, G\}_{\mathscr{L}}$, we have from (100) and (101) that

$$\begin{aligned} \{F, G\}_{\mathscr{L}_1}(\varphi) - \{F, G\}_{\mathscr{L}_2}(\varphi) &= \Big\langle F^{(1)}[\varphi], (\Delta_{\mathscr{L}_1}[\varphi] - \Delta_{\mathscr{L}_2}[\varphi])G^{(1)}[\varphi] \Big\rangle \\ &= \Big\langle F^{(1)}[\varphi], (\Delta^{\mathrm{ret}}_{\mathscr{L}_1}[\varphi] - \Delta^{\mathrm{ret}}_{\mathscr{L}_2}[\varphi])G^{(1)}[\varphi] \Big\rangle \\ &\quad - \Big\langle F^{(1)}[\varphi], (\Delta^{\mathrm{adv}}_{\mathscr{L}_1}[\varphi] - \Delta^{\mathrm{adv}}_{\mathscr{L}_2}[\varphi])G^{(1)}[\varphi] \Big\rangle \\ &= 0 \end{aligned} \tag{102}$$

for all $\varphi \in \mathscr{U}$, as asserted. □

We have now the following strengthening of Proposition 3.2.12 and Theorem 3.2.15, which is crucial to this whole Subsection and justifies the christening "microcausal" given to the elements of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$. We shall take advantage of the fact that, thanks to Theorem 3.2.15, we may replace $E(\mathscr{L})[\varphi]$ by its *cutoff version*

$$E'(\mathscr{L})[\varphi_0]\varphi + f(E(\mathscr{L})[\varphi] - E'(\mathscr{L})[\varphi_0]\varphi) \tag{103}$$

with any $f \in \mathscr{C}^\infty_c(\mathscr{M})$ such that $f \equiv 1$ in a neighborhood of $(J^+(\operatorname{supp} F, g) \cup J^-(\operatorname{supp} F, g)) \cap (J^+(\operatorname{supp} G, g) \cup J^-(\operatorname{supp} G, g))$ while keeping $\{F, G\}_{\mathscr{L}}(\varphi)$ *unaltered* for all $\varphi, \varphi_0 \in \mathscr{U}$. The term in the right-hand side of (103) proportional to the cutoff function f corresponds to the nonlinear (interaction) part of $E(\mathscr{L})$ around the background field configuration φ_0.

3.2.16. Proposition. *Let $\mathscr{U}, \mathscr{L}$ be as in Proposition 3.2.12, and $F, G \in \mathscr{F}((\mathscr{M},g),\mathscr{U})$. Then $\{F, G\}_{\mathscr{L}}$ also belongs to $\mathscr{F}((\mathscr{M},g),\mathscr{U})$.*

Proof. We look at the derivatives of $\{F, G\}_{\mathscr{L}}$. To that end, we shall replace $E(\mathscr{L})$ by its cutoff version (103) in order to make the distribution kernel of $D^2E(\mathscr{L})[\varphi]$ *compactly supported*. This will allow us to obtain a technically more convenient formula for the derivatives of the causal propagator. In what follows we shall use the same notation for the cutoff Euler-Lagrange operator for simplicity. Since $\Delta_{\mathscr{L}}[\varphi] = \Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi] - \Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]$, formulae (83) and (84) together imply

$$D\Delta_{\mathscr{L}}[\varphi](\vec{\varphi}) = -\Delta_{\mathscr{L}}[\varphi]D^2E(\mathscr{L})[\varphi](\vec{\varphi})\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi] - \Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]D^2E(\mathscr{L})[\varphi](\vec{\varphi})\Delta_{\mathscr{L}}[\varphi]\ . \tag{104}$$

In particular, such a formula implies that $D\Delta_{\mathscr{L}}[\varphi](\vec{\varphi})$ has the same wave front set as $\Delta_{\mathscr{L}}[\varphi]$. As for higher orders, one obtains that

$$\begin{aligned} &D^k\Delta_{\mathscr{L}}[\varphi](\vec{\varphi}_1,\dots,\vec{\varphi}_k) \\ &\quad= \sum_{l=0}^{k}(-1)^l \sum_{\{I_1,\dots,I_l\}\in P_k}\sum_{\sigma\in S_l}\sum_{m=0}^{l}\left(\prod_{j=1}^{m}\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi_0]D^{|I_{\sigma(j)}|+1}E(\mathscr{L})[\varphi_0](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\right) \\ &\qquad\cdot\Delta_{\mathscr{L}}[\varphi]\left(\prod_{j=m+1}^{l}D^{|I_{\sigma(j)}|+1}E(\mathscr{L})[\varphi_0](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi_0]\right)\ . \end{aligned} \tag{105}$$

and hence the k-th order functional derivative of the Peierls bracket at φ is formally given by

$$\begin{aligned} D^k\{F,G\}_{\mathscr{L}}[\varphi](\vec{\varphi}_1,\dots,\vec{\varphi}_k) = &\sum_{\{J_1,J_2,J_3\}\subset P_k} F^{(|J_1|+1)}[\varphi]((\otimes_{j_1\in J_1}\vec{\varphi}_{j_1}) \\ &\otimes D^{|J_2|}\Delta_{\mathscr{L}}[\varphi]((\otimes_{j_2\in J_2}\vec{\varphi}_{j_2})\otimes G^{(|J_3|+1)}[\varphi](\otimes_{j_3\in J_3}\vec{\varphi}_{j_3}))) \end{aligned} \tag{106}$$

with $D^k\Delta_{\mathscr{L}}[\varphi](\vec{\varphi}_1,\dots,\vec{\varphi}_k)$ given as above. Moreover, since F and G are microcausal, the wave front sets of their derivatives contain no elements where either

- All covectors are in the closed forward light cone $\overline{V}_+$, or
- All are in the closed backward light cone $\overline{V}_-$.

Recall as well that since $D^kE(\mathscr{L})[\varphi]$ is a k-linear partial differential operator with distribution kernel $D^{k+1}\mathscr{L}(1)[\varphi]$, we conclude that (see the proof of Proposition 3.2.14 for more details)

$$\mathrm{WF}(D^{k+1}\mathscr{L}(1)[\varphi]) \subset N^*\Delta_{k+1}(\mathscr{M}) \smallsetminus 0\ ,$$

where

$$N^*\Delta_k(\mathscr{M}) = \{(x_1,\ldots,x_k;\xi_1,\ldots,\xi_k) \in T^*\mathscr{M}^k \mid x_1 = \cdots = x_k,\, \xi_1+\cdots+\xi_k = 0\}\ , \quad k \geq 2$$

is the *conormal bundle* to the (small) diagonal $\Delta_k(\mathscr{M})$ of $\mathscr{M}^k$.

By a reasoning similar to that employed in the proof of Proposition 3.2.12, we notice that due to (105) each term in the right-hand side of (106) before smearing with $\vec{\varphi}_1,\ldots,\vec{\varphi}_k$ can be seen as a string of compositions of:

(i) $l+1$ propagators either of the form $\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]$, $\Delta_{\mathscr{L}}[\varphi]$ or $\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]$; and
(ii) $l+2$ k_i-linear operators, $i=0,\ldots,l+1$ whose distribution kernels are either of the form $F^{(k_0+1)}[\varphi]$, $D^{k_i+2}\mathscr{L}(1)[\varphi]$ for $1\leq i\leq l$ or $G^{(k_{l+1}+1)}[\varphi]$,

for each $l=1,\ldots,k$ with $k_0+\cdots+k_{l+1}=k$. Moreover, the obtained distributions are once again compactly supported. The pairing of variables in such a composition for each term in the right-hand side of (105) is of the following form:

- The first variable of the kernel of the first propagator pairs with the first variable of $F^{(k_1+1)}[\varphi]$;
- The first variable of $D^{k_i+2}\mathscr{L}(1)[\varphi]$ pairs with the second variable of the kernel of the i-th propagator;
- The second variable of $D^{k_i+2}\mathscr{L}(1)[\varphi]$ pairs with the first variable of the kernel of the $(i+1)$-th propagator;
- The second variable of the kernel of the last propagator pairs with the first variable of $G^{(k_{l+1}+1)}[\varphi]$.

In particular, the kernel of the causal propagator $\Delta_{\mathscr{L}}[\varphi]$ has its first variable paired with the second variable of $D^{k_m+2}\mathscr{L}(1)[\varphi]$ and its second variable paired with the first variable of $D^{k_{m+1}+2}\mathscr{L}(1)[\varphi]$.

Suppose now that $(\xi_1,\ldots,\xi_k) \in \overline{V}^k_{+,g}(x_1,\ldots,x_k)$ is in $\mathrm{WF}(D^k\{F,G\}_{\mathscr{L}}[\varphi])$. If $(y_m,z_m;\eta_m,\zeta_m) \in \mathrm{WF}(\Delta_{\mathscr{L}}[\varphi])$, then either η_m or ζ_m is a past directed null covector w.r.t. $\hat{g}_{\mathscr{L}}[\varphi]$. Suppose it is η_m, so that $\eta_m \in \overline{V}_{-,g}(y_m)$ – then by Theorem 8.2.14, pp. 269–270 of [50] we must have that

$$\begin{aligned}(z_{m-1},y_m,x_{k_0+\cdots+k_{m-1}+1},\ldots,x_{k_0+\cdots+k_m};\zeta_{m-1},-\eta_m,\xi_{k_0+\cdots+k_{m-1}+1},\ldots,\xi_{k_0+\cdots+k_m})\\ \in \mathrm{WF}(D^{k_m+2}\mathscr{L}(1)[\varphi])\ ,\end{aligned}$$

implying that $z_{m-1}=y_m$ and $\zeta_{m-1} \in \overline{V}_{-,g}(z_{m-1})$. Now, if $(y_{m-1},z_{m-1};\eta_{m-1},\zeta_{m-1}) \in \mathrm{WF}(\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi])$ for some (y_{m-1},η_{m-1}), then either $(y_{m-1},\eta_{m-1}) = (z_{m-1},\zeta_{m-1})$ or ζ_{m-1} is null past directed and therefore η_{m-1} is null future directed. In either case, we have that $\eta_{m-1} \in \overline{V}_{+,g}(y_{m-1})$. Repeating the above procedure backwards as many times as needed as dictated by Theorem 8.2.14, pp. 269–270 of [50], we conclude that

$$(x_1,\ldots,x_{k_0},y_1;\xi_1,\ldots,\xi_{k_0},\eta_1) \in \mathrm{WF}(F^{(k_1+1)}[\varphi])$$

with $\eta_1 \in \overline{V}_{+,g}(y_1)$, which is absurd since F is assumed to be microcausal. Likewise, if instead ζ_m is null past directed, proceeding as above but forwards we conclude that

$$(z_l,x_{k_0+\cdots+k_l+1},\ldots,x_{k_0+\cdots+k_{l+1}};\zeta_l,\xi_{k_0+\cdots+k_l+1},\ldots,\xi_{k_0+\cdots+k_{l+1}}) \in \mathrm{WF}(G^{(k_{l+1}+1)}[\varphi])$$

with $\zeta_l \in \overline{V}_{+,g}(z_l)$, which is absurd since G is assumed to be microcausal. In the same fashion, we conclude that no $(\xi_1, \dots, \xi_k) \in \overline{V}^k_{-,g}(x_1, \dots, x_k)$ can belong to $\mathrm{WF}(D^k\{F,G\}_{\mathscr{L}}[\varphi])$. In particular, we see that no k-tuple of zero covectors can arise from the above procedure, hence again by Theorem 8.2.14, pp. 269–270 of [50] the (compactly supported) distribution $D^k\{F,G\}_{\mathscr{L}}[\varphi]$ is well defined. The proof is complete. $\square$

We stress that the presence of $\Delta_{\mathscr{L}}[\varphi]$ is crucial for the propagation argument underlying the proof of Proposition 3.2.16 to work, since it prevents the appearance of spacelike covectors which may disrupt the propagation procedure. Such an argument would not work if we had only retarded or only advanced propagators in each term of (106), because their wave front set may have elements over the diagonal whose covectors are spacelike. On the other hand, as the proof of Proposition 3.2.12 shows, in the case of microlocal F, G the clash of (spacelike) covectors though the propagation procedure is prevented by the fact that the wave front sets of $F^{(k)}[\varphi]$ and $G^{(l)}[\varphi]$ are conormal to $\Delta_k(\mathscr{M})$ and $\Delta_l(\mathscr{M})$ respectively for all $k, l > 0$. More generally, if $\mathscr{M}$ is parallelizable (e.g. if $(\mathscr{M}, g)$ is Minkowski space-time or if $d = 4$ [82]) then one may define for each $k \geq 2$ the sets

$$N^k(\mathscr{M}) = \{(x_1, \dots, x_k; \xi_1, \dots, \xi_k) \in T^*\mathscr{M}^k \smallsetminus 0 \mid \xi_1 + \cdots + \xi_k = 0\} \ , \ N^1(\mathscr{M}) = \varnothing \ .$$

If to deem F, G as microcausal we required in addition to Definition 3.2.13 that $\mathrm{WF}(F^{(k)}[\varphi])$, $\mathrm{WF}(G^{(k)}[\varphi]) \subset N^k(\mathscr{M})$ for all $k \geq 1$, one would be able to conclude by the same reasoning as in the proof of Proposition 3.2.12 that $\mathsf{R}_{\mathscr{L}}(F,G)$ and $\mathsf{A}_{\mathscr{L}}(F,G)$ are smooth, in fact even microcausal in this strengthened sense. This was the path followed e.g. by [34] in Minkowski space-time, see discussion between formulae (8) and (9), pp. 280 therein. However, it is clear that the definition of $N^k(\mathscr{M})$ is tied to a choice of global trivialization for $T^*\mathscr{M}$ (tacitly assumed therein), which is natural in the case of Minkowski space-time but generally no longer so, thus such requirement seems unnatural in curved space-times.

3.2.17. Corollary. *The Peierls bracket $F, G \mapsto \{F,G\}_{\mathscr{L}}$ defines a Lie bracket on $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$ for any globally hyperbolic metric g on $\mathscr{M}$ such that $g \gtrsim \hat{g}_{\mathscr{L}}[\varphi]$ for all $\varphi \in \mathscr{U}$.*

Proof. $\{\cdot,\cdot\}_{\mathscr{L}}$ is clearly bilinear. Antisymmetry of $\{\cdot,\cdot\}_{\mathscr{L}}$ follows from the argument right after Definition 3.2.11. All that is left to us is to prove that the Jacobi identity holds, that is,

$$\{F, \{G,H\}_{\mathscr{L}}\}_{\mathscr{L}} + \{G, \{H,F\}_{\mathscr{L}}\}_{\mathscr{L}} + \{H, \{F,G\}_{\mathscr{L}}\}_{\mathscr{L}} = 0 \tag{107}$$

for any $F, G, H \in \mathscr{F}((\mathscr{M}, g), \mathscr{U})$. To that end, we argue as in the proof of Proposition 3.2.16 and replace once more $E(\mathscr{L})$ by the cutoff version (103) while keeping the same notation, this time with the cutoff function f such that $f \equiv 1$ in a neighborhood of the (compact) region $\mathscr{O}_{\mathrm{supp}\, F, \mathrm{supp}\, G, \mathrm{supp}\, H}$, where for $\varnothing \neq K, L, M \subset \mathscr{M}$ we set

$$\mathscr{O}_{K,L,M} = \mathscr{O}_{K,L} \cup \mathscr{O}_{K,M} \cup \mathscr{O}_{L,M} \cup \mathscr{O}_{\mathscr{O}_{K,L},M} \cup \mathscr{O}_{\mathscr{O}_{L,M},K} \cup \mathscr{O}_{\mathscr{O}_{M,K},L} \ .$$

with $\mathscr{O}_{K,L}$ defined as in (93). It is clear from Theorem 3.2.15 that all Peierls brackets involved in the left-hand side of (107) remain unaltered by the cutoff. Now we have that

$$\begin{aligned}\{F,\{G,H\}_{\mathscr{L}}\}_{\mathscr{L}}(\varphi) &= H^{(2)}[\varphi](\Delta_{\mathscr{L}}[\varphi]G^{(1)}[\varphi],\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi]) \\ &\quad - G^{(2)}[\varphi](\Delta_{\mathscr{L}}[\varphi]H^{(1)}[\varphi],\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi]) \\ &\quad - G^{(1)}[\varphi](D\Delta_{\mathscr{L}}[\varphi](\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi])H^{(1)}[\varphi])\ .\end{aligned} \tag{108}$$

Consider the first two terms in the right-hand side of (108). Summing them along all three cyclic permutations of F, G, H yields zero thanks to the symmetry of second-order derivatives of functionals in their linear entries, so one is only left to show that

$$\begin{aligned}&G^{(1)}[\varphi](D\Delta_{\mathscr{L}}[\varphi](\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi])H^{(1)}[\varphi]) + F^{(1)}[\varphi](D\Delta_{\mathscr{L}}[\varphi](\Delta_{\mathscr{L}}[\varphi]H^{(1)}[\varphi])G^{(1)}[\varphi]) \\ &\qquad + H^{(1)}[\varphi](D\Delta_{\mathscr{L}}[\varphi](\Delta_{\mathscr{L}}[\varphi]G^{(1)}[\varphi])F^{(1)}[\varphi]) = 0\ .\end{aligned} \tag{109}$$

Inserting into (109) the formula (104) for the derivative of $\Delta_{\mathscr{L}}[\varphi]$ obtained in the proof of Proposition 3.2.16 we find that

$$\begin{aligned}&G^{(1)}[\varphi](D\Delta_{\mathscr{L}}[\varphi](\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi])H^{(1)}[\varphi]) \\ &\quad = -G^{(1)}[\varphi](\Delta_{\mathscr{L}}[\varphi]D^2E(\mathscr{L})[\varphi](\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi])\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]H^{(1)}[\varphi]) \\ &\qquad - G^{(1)}[\varphi](\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]D^2E(\mathscr{L})[\varphi](\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi])\Delta_{\mathscr{L}}[\varphi]H^{(1)}[\varphi]) \\ &\quad = D^3\mathscr{L}(1)[\varphi](\Delta_{\mathscr{L}}[\varphi]G^{(1)}[\varphi],\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]H^{(1)}[\varphi],\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi]) \\ &\qquad - D^3\mathscr{L}(1)[\varphi](\Delta_{\mathscr{L}}[\varphi]H^{(1)}[\varphi],\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]G^{(1)}[\varphi],\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi])\ ,\end{aligned} \tag{110}$$

where in the last identity we have exploited the symmetry of $D^3\mathscr{L}(1)[\varphi]$ in its first two entries. Summing the last formula of (110) along all three cyclic permutations of F, G, H yields zero once more thanks to the symmetry of $D^3\mathscr{L}(1)[\varphi]$ in its first and last entries. The proof is complete. □

Notice that the arguments employed in the proofs of Proposition 3.2.16 and Corollary 3.2.17 rely on the compactness of the support of the distribution kernel of $D^2E(\mathscr{L})[\varphi]$ through the formula (104) for the derivative of $\Delta_{\mathscr{L}}[\varphi]$, for therein one adds and subtracts a term of the form

$$\Delta^{\mathrm{adv}}_{\mathscr{L}}[\varphi]D^2E(\mathscr{L})[\varphi](\vec{\varphi})\Delta^{\mathrm{ret}}_{\mathscr{L}}[\varphi]$$

which is otherwise ill defined. However, as argued right after the proof of Theorem 3.2.15, this entails no loss of generality since we can perform a suitable cutoff of the nonlinear part of $E(\mathscr{L})$ through (103).

We shall prove in Section 4 that $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ is closed under products and that the Peierls bracket satisfies Leibniz's rule (Theorem 4.1.4). In other words, $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ becomes a *Poisson* algebra when endowed with the Peierls bracket associated to $\mathscr{L}$.

4. First structural results

With the body of results of Sections 2 and 3 at hand, we can start a detailed and motivated discussion of the mathematical structures underlying our approach.

4.1. **Topology of the space of microcausal functionals.** We can endow $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ with a topology which, despite being quite weak, accommodates rather well our algebraic operations. The weakest possible choice is the topology of pointwise convergence of functionals and their derivatives of all orders, which is the locally convex topology on $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ induced by the separating system of seminorms

$$F \mapsto |F^{(k)}[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)| \ , \quad \varphi\in\mathscr{U}\,,\ \vec{\varphi}_1,\ldots,\vec{\varphi}_k\in\mathscr{C}^\infty(\mathscr{M}),\ k\in\mathbb{N}\ .$$

Equivalently, this topology is the initial locally convex topology on $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ induced by the linear maps

$$F\mapsto\begin{cases}F(\varphi)\in\mathbb{C} & (k=0)\\ F^{(k)}[\varphi]\in\mathscr{E}'(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}) & (k\geq 1)\end{cases}\ , \quad \varphi\in\mathscr{U}\ , \tag{111}$$

where the space $\mathscr{E}'(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M})$ of d-form-valued distributions of compact support on $\mathscr{M}^k$ is the topological dual of $\mathscr{C}^\infty(\mathscr{M}^k)$. This choice, however, ignores the extra information on the wave front sets of $F^{(k)}[\varphi]$ which enters Definition 3.2.13 for microcausal functionals. A more natural choice is to replace the spaces of general, compactly supported distribution densities in (111) for each $k\geq 1$ by the following subspaces:

$$\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)=\{u\in\mathscr{E}'(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)\mid \mathrm{WF}(u)\subset\Upsilon_{k,g}\}\ . \tag{112}$$

These, however, are not standard spaces of compactly supported distributions with wave front sets within a prescribed (closed) cone, for $\Upsilon_{k,g}$ as defined in (94) is an *open* conic subset of $T^*\mathscr{M}^k\smallsetminus 0$. Therefore, one cannot immediately endow $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)$ with the Hörmander topology (see, for instance, Section 8.2 of [50]). It is possible, on the other hand, to define $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)$ as an inductive limit of an increasing sequence of spaces of compactly supported distributions with wave front sets contained in an increasing sequence of *closed* conic subsets of $T^*\mathscr{M}^k\smallsetminus 0$, each of these spaces being endowed with the Hörmander topology. The key result which allows us to do this is the following

4.1.1. Lemma. *For each $k=1,2,\ldots$ there is a countable family $\{\Gamma_{k,m}\}_{m\in\mathbb{N}}$ of closed conic subsets of $T^*\mathscr{M}^k$ such that $\Gamma_{k,m}\subset\mathring{\Gamma}_{k,m+1}$ and $\cup_{m=0}^\infty\Gamma_{k,m}=\Upsilon_{k,g}$ is given by* (98).

Proof. Let ω be a future directed timelike covector field in $(\mathscr{M},g)$ and $\epsilon>0$ such that $g_\epsilon\doteq g-\epsilon u\otimes u$ is a Lorentzian metric. We have that $g<g_{\epsilon'}<g_\epsilon$ and hence $V_{\pm,g_\epsilon}(x)\supset\overline{V}_{\pm,g_{\epsilon'}}(x)$ for all $0<\epsilon'<\epsilon$, $x\in M$. Let now $(\epsilon_m)_{m\in\mathbb{N}}$ be a sequence of positive real numbers such that $\epsilon_0=\epsilon$, $\epsilon_{m+1}<\epsilon_m$ and $\epsilon_m\overset{m\to\infty}{\longrightarrow}0$. We conclude that, for all $x\in\mathscr{M}$,

$$\begin{aligned}\complement(\overline{V}_{+,g}(x)\cup\overline{V}_{-,g}(x)) &= \left(\bigcup_{m=0}^\infty \complement(V_{+,g_{\epsilon_m}}(x)\cup V_{-,g_{\epsilon_m}}(x))\right)\smallsetminus\{0\}\\ &= \left(\bigcup_{m=0}^\infty \complement(V_{+,g_{\epsilon_m}}(x)\cup V_{-,g_{\epsilon_m}}(x))\smallsetminus\{0\}\right)\ .\end{aligned}$$

The above argument settles the case $k=1$. For $k>1$, we can write $\complement(\overline{V}^k_{+,g}(x_1,\dots,x_k)\cup\overline{V}^k_{-,g}(x_1,\dots,x_k))$ as a union of subsets of the form $\Omega=\prod_{j=1}^k W_j$, such that the possibilities for Ω fall in exactly one of the following three categories:

(a) $W_j=\complement(\overline{V}_{+,g}(x_j)\cup\overline{V}_{-,g}(x_j))$ for at least one j, and all $W_{j'}$'s which are not of this form are of the form $W_{j'}=\overline{V}_{+,g}(x_{j'})\cup\overline{V}_{-,g}(x_{j'})$. There are $\sum_{k'=1}^k\binom{k}{k'}=2^k-1$ such Ω's.

(b) For all $j=1,\dots,k$, we have either $W_j=\overline{V}_{+,g}(x_j)\smallsetminus\{0\}$ or $W_j=\overline{V}_{-,g}(x_j)\smallsetminus\{0\}$, and there is at least one pair $j,j'\subset\{1,\dots,k\}$, such that $W_j=\overline{V}_{+,g}(x_j)\smallsetminus\{0\}$ and $W_{j'}=\overline{V}_{-,g}(x_{j'})\smallsetminus\{0\}$. There are $\sum_{k'=1}^{k-1}\binom{k}{k'}=2^k-2$ such Ω's (we remark that this number is zero for $k=1$).

(c) $W_j=\{0\}$ for at least one j, all $W_{j'}$'s which are not of this form are either of the form $W_{j'}=\overline{V}_{+,g}(x_{j'})\smallsetminus\{0\}$ or $W_{j'}=\overline{V}_{-,g}(x_{j'})\smallsetminus\{0\}$, and there is at least one pair $j',j''\subset\{j=1,\dots,k\mid W_j\neq\{0\}\}$ such that $W_{j'}=\overline{V}_{+,g}(x_{j'})\smallsetminus\{0\}$ and $W_{j''}=\overline{V}_{-,g}(x_{j''})\smallsetminus\{0\}$. There are

$$\begin{aligned}\sum_{k'=1}^{k-2}(2^{k-k'}-2)\binom{k}{k'}&=2^k\left(\frac{3^k}{2^k}-1-\frac{1}{2^k}-\frac{2k}{2^k}\right)-2(2^k-2-k)\\&=3^k-3\cdot2^k+3\end{aligned}$$

such Ω's (we remark that this number is zero for $k=1,2$).

Let us enumerate the 3^k-2^k subsets Ω listed above, so that the first 2^k-1 ones are of type (a), and the remaining ones are of types (b) and (c):

$$\begin{aligned}\complement(\overline{V}^k_{+,g}(x_1,\dots,x_k)\cup\overline{V}^k_{-,g}(x_1,\dots,x_k))&=\bigcup_{l=1}^{3^k-2^k}\Omega_l\\&=\left(\bigcup_{l=1}^{2^k-1}\Omega_l\right)\cup\left(\bigcup_{l=2^k}^{3^k-2^k}\Omega_l\right)\ ,\\ \Omega_l&=\prod_{j=1}^k W_{j,l}\ .\end{aligned}$$

Let now $l<2^k$. We can write Ω_l as the countable union of an increasing sequence of closed conic subsets of $T^*_{(x_1,\dots,x_k)}\mathscr{M}^k\smallsetminus 0$

$$\Omega_l=\bigcup_{m=0}^{\infty}\Omega_{l,m}\ ,\ \Omega_{l,m}=\prod_{j=1}^k W_{j,l,m}\ ,$$

where

$$W_{j,l,m}=\begin{cases}\complement(V_{+,g_{\epsilon_m}}(x_j)\cup V_{-,g_{\epsilon_m}}(x_j))\smallsetminus\{0\} & \text{if } W_{j,l}=\complement(\overline{V}_{+,g}(x_j)\cup\overline{V}_{-,g}(x_j))\ ,\\ W_{j,l} & \text{if } W_{j,l}=\overline{V}_{+,g}(x_j)\cup\overline{V}_{-,g}(x_j)\ .\end{cases}$$

If $l \geq 2^k$, Ω_l is already a closed conic subset of $T^*_{(x_1,\ldots,x_k)}\mathscr{M}^k \setminus 0$. Finally, define

$$\Gamma_{k,m}(x_1,\ldots,x_k) = \left(\bigcup_{l=1}^{2^k-1} \Omega_{l,m}\right) \cup \left(\bigcup_{l=2^k}^{3^k-2^k} \Omega_l\right) .$$

By construction, $\Gamma_{k,m}(x_1,\ldots,x_k)$ is a closed conic subset of $T^*_{(x_1,\ldots,x_k)}\mathscr{M}^k \setminus 0$, $\Gamma_{k,m}(x_1,\ldots,x_k) \subset \mathring{\Gamma}_{k,m+1}(x_1,\ldots,x_k)$ and

$$\complement(\overline{V}^k_{+,g}(x_1,\ldots,x_k) \cup \overline{V}^k_{-,g}(x_1,\ldots,x_k)) = \bigcup_{m=0}^{\infty} \Gamma_{k,m}(x_1,\ldots,x_k)$$

for all $(x_1,\ldots,x_k) \in \mathscr{M}^k$. Taking $\Gamma_{k,m}$ as the disjoint union of the $\Gamma_{k,m}(x_1,\ldots,x_k)$'s for all $(x_1,\ldots,x_k) \in \mathscr{M}^k$ gives the thesis. $\square$

4.1.2. Corollary. *One can write* $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ *for all* $k = 1, 2, \ldots$ *as the countable inductive limit*

$$\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k) = \varinjlim_{m\in\mathbb{N}} \mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k) \tag{113}$$

of the spaces $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$. *Let* $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ *be endowed with the locally convex inductive limit topology induced by the Hörmander topology on each* $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ *for all* $k = 1, 2, \ldots$*; then* $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ *is nuclear for all such* k.

Proof. By Lemma 4.1.1, one has the inclusions

$$\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k) \subset \mathscr{E}'_{\Gamma_{k,m'}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$$

for all $m < m'$. Since, given any closed conic subset $\Gamma \subset T^*\mathscr{M}^k \setminus 0$, one can construct $u \in \mathscr{E}'_\Gamma = \mathscr{E}'_\Gamma(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ with $\mathrm{WF}(u) = \Gamma$ (Theorem 8.1.4, pp. 255–256 of [50]), the above set inclusion is proper for all $m < m'$. For the last statement, we recall that, for any given non-void, closed conic subset Γ of the cotangent bundle minus the range of its zero section, the Hörmander topology on $\mathscr{E}'_\Gamma$ is the initial topology induced by the linear maps $u \mapsto u(f) \in \mathbb{C}$ and $u \mapsto Pu \in \Gamma^\infty_c(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$, where f runs through all smooth functions and P runs through all properly supported pseudodifferential operators of order zero on the vector bundle $\wedge^{kd}T^*\mathscr{M}^k$ over $\mathscr{M}^k$ such that $\mathrm{WF}(P) \cap \Gamma = \varnothing$, where

$$\begin{aligned}\mathrm{WF}(P) = \{&(x_1,\ldots,x_k;\xi_1,\ldots,\xi_k) \in T^*\mathscr{M}^k \setminus 0 \mid \\ &(x_1,\ldots,x_k,x_1,\ldots,x_k;\xi_1,\ldots,\xi_k,-\xi_1,\ldots,-\xi_k) \in \mathrm{WF}(K_P)\}\end{aligned}$$

denotes the *microsupport* of P (see e.g. Proposition 18.1.26 and formulas (18.1.34), (18.1.35), pp. 88 as well as the remark following Theorem 18.1.28, pp. 89–90 of [51]). Here K_P is the Schwartz kernel of P. For the convenience of the reader, we recall that (a) $\mathrm{WF}(K_P) \subset N^*\Delta_2(\mathscr{M}^k)$ (see e.g. Theorem 18.1.16, pp. 80 of [51]), (b) P being properly supported means that the restrictions to $\operatorname{supp} K_P$ of the canonical projections onto the first k and the last k arguments are proper maps, which entails that Pu is compactly supported if u is, and (c) $\mathrm{WF}(P) \cap \Gamma = \varnothing$ implies that Pu is smooth (see e.g. Theorem 8.2.13, pp. 268–269 of [50]). The above inductive limit topology on $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ is strictly finer than the topology induced from $\mathscr{E}'(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$. Since the latter is Hausdorff, we conclude that the former is also Hausdorff. Moreover, since

$\mathbb{C}$ is finite-dimensional and $\Gamma^\infty_c(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ is nuclear, it follows from the permanence of nuclearity for initial topologies (Proposition 5.2.3, pp. 92 of [76]) that $\mathscr{E}'_\Gamma$ is nuclear as well. By Proposition 4.2.1, pp. 76 of [54] together with Theorems 5.1.1, pp. 85 and 5.2.2, pp. 91–92 of [76], any Hausdorff countable inductive limit of nuclear locally convex spaces is nuclear. Therefore, $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ must be nuclear for all k, as claimed. □

4.1.3. Remark (Stefan Waldmann, personal communication). We remark that the inclusion

$$\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k) \subset \mathscr{E}'_{\Gamma_{k,m+1}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$$

although being a proper injection, is *not* a topological embedding. The reason is the following: the space $\Gamma^\infty_c(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ of test densities is dense in the Hörmander topology of $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ for all $m \in \mathbb{N}$. Since by Theorem 8.1.4 of [50] one can find $u_m \in \mathscr{E}'_{\Gamma_{k,m+1}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ which does not belong to $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$, there is a sequence $(v_{n,m} \in \Gamma^\infty_c(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k))_{n\in\mathbb{N}}$ converging to u_m in the Hörmander topology of $\mathscr{E}'_{\Gamma_{k,m+1}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$. If $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ were a closed subspace in this topology, then u_m would have to be an element of this subspace, which is false by assumption. In fact, even more is true: since $\Gamma^\infty_c(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ is dense in the Hörmander topology of $\mathscr{E}'_{\Gamma_{k,m+1}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$, so is $\mathscr{E}'_{\Gamma_{k,m}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$. Hence, the inductive limit (113) cannot be a *strict* one.

From now on we tacitly assume that $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ is endowed with the topology defined in Corollary 4.1.2 for all k. Once this is done, we may proceed to proving the main result of this Subsection.

4.1.4. Theorem. *Let $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ be open in the compact-open topology, and let $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ be endowed with the initial topology induced by the linear maps*

$$F \mapsto F(\varphi) \in \mathbb{C}\ , \tag{114}$$

$$F \mapsto F^{(k)}[\varphi] \in \mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)\ ,\ k = 1,2,\dots\ , \tag{115}$$

*with φ running through all elements of $\mathscr{U}$. Then $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ is a nuclear locally convex vector space over the complex numbers which is also a Poisson *-algebra when endowed with the Peierls bracket associated to a microlocal generalized Lagrangian of first order on $\mathscr{U}$ with normally hyperbolic Euler-Lagrange operator. As a consequence, the Poisson *-subalgebra $\mathscr{F}_0(\mathscr{M},\mathscr{U})$ and the self-adjoint linear subspace $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M},\mathscr{U})$ are also nuclear locally convex subspaces when endowed with the relative topology. Moreover, the involution of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ is continuous.*

Proof. That $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ is a nuclear locally convex space follows from the permanence of nuclearity for initial topologies (Proposition 5.2.3, pp. 92 of [76]) together with Corollary 4.1.2. Involution is obviously well-defined, continuous and commutes with the Peierls bracket; Proposition 3.2.16 and Corollary 3.2.17 show that the Peierls bracket $\{\cdot,\cdot\}_\mathscr{L}$ associated to $\mathscr{L}$ is a Lie bracket on $\mathscr{F}((\mathscr{M},g),\mathscr{U})$. It remains to check that $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ is closed under products – Leibniz's rule for $\{\cdot,\cdot\}_\mathscr{L}$

$$\{F,GH\}_\mathscr{L} = \{F,G\}_\mathscr{L}H + G\{F,H\}_\mathscr{L} \tag{116}$$

will then follow from Leibniz's rule (A.4) for functional derivatives of pointwise products of functionals (see also the discussion right after Theorem 4.2.1).

Take $F, G \in \mathscr{F}((\mathscr{M}, g), \mathscr{U})$, and consider their pointwise product $(F \cdot G)(\varphi) = F(\varphi)G(\varphi)$. Now, by Leibniz's rule for derivatives of order k,

$$
\begin{aligned}
&(F \cdot G)^{(k)}[\varphi](\vec{\varphi}_1, \dots, \vec{\varphi}_k) \\
&\qquad = \sum_{\pi \in \mathscr{P}_k} \sum_{l=0}^{k} F^{(k-l)}[\varphi](\vec{\varphi}_{\pi(1)}, \dots, \vec{\varphi}_{\pi(k-l)}) G^{(l)}[\varphi](\vec{\varphi}_{\pi(k-l+1)}, \dots, \vec{\varphi}_{\pi(k)}) \ ,
\end{aligned}
$$

where $\mathscr{P}_k$ is the group of permutations of k elements. By Theorem 8.2.9, pp. 267 of [50], the wave front set of each distribution appearing in the above sum is given by

$$
\begin{aligned}
\mathrm{WF}(F^{(k-l)}[\varphi] \otimes G^{(l)}[\varphi]) \subset \ & \mathrm{WF}(F^{(k-l)}[\varphi]) \times \mathrm{WF}(G^{(l)}[\varphi]) \\
& \cup \Big(\mathrm{WF}(F^{(k-l)}[\varphi]) \times (\mathrm{supp}\,(G^{(l)}[\varphi]) \times \{0\})\Big) \\
& \cup \Big((\mathrm{supp}\, F^{(k-l)}[\varphi]) \times \{0\}) \times \mathrm{WF}(G^{(l)}[\varphi])\Big) \ .
\end{aligned}
$$

By direct inspection the right-hand side is included in the open set $\Upsilon_{k,g}$, as it should. The wave front set of $(F \cdot G)^{(k)}[\varphi]$ is clearly contained in the union of all the wave front sets of the components, which satisfies again the requested bound by the closedness of the wave front sets. The remaining claims follow immediately from the permanence of nuclearity under taking linear subspaces (Proposition 5.1.1, pp. 85 of [76]). □

4.2. **$\mathscr{C}^\infty$-ring structure and its consequences.** Actually, one can strengthen Theorem 4.1.4 considerably:

4.2.1. Theorem (Smooth functional calculus). *Given $F_1, \dots, F_n \in \mathscr{F}((\mathscr{M}, g), \mathscr{U})$, let $V \subset \mathbb{R}^{2n} \cong \mathbb{C}^n$ be an open set containing the range of $(F_1, \dots, F_n)$, and let $\psi : V \to \mathbb{C}$ be a smooth map. Then $\psi \circ (F_1, \dots, F_n) \in \mathscr{F}((\mathscr{M}, g), \mathscr{U})$ with $\mathrm{supp}\,(\psi \circ (F_1, \dots, F_n)) \subset \cup_{j=1}^n \mathrm{supp}\, F_j$.*

Proof. Smoothness of $\psi \circ (F_1, \dots, F_n)$ follows from Faà di Bruno's formula (A.7). The validity of the aforementioned support property follows from an argument similar to that used in the proof of Lemma 2.3.3 for products (i.e. $\psi(z_1, z_2) = z_1 z_2$), so we are only left with proving that the wave front set of the functional derivative of $\psi \circ (F_1, \dots, F_n)$ of order k is contained in $\Upsilon_{k,g}$ for all $k \geq 1$. This fact then follows from Faà di Bruno's formula (A.7) together with an argument similar to that used for products in Theorem 4.1.4. □

In particular, $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$ is a $\mathscr{C}^\infty$*-ring* [72]. To our knowledge, this is the first non-trivial example in which such a structure appears in applications outside pure mathematics. Moreover, the Peierls bracket acts as a $\mathscr{C}^\infty$-derivation on $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$, that is, if $\psi, F_1, \dots, F_n$ are as in Theorem 4.2.1 and $G \in \mathscr{F}((\mathscr{M}, g), \mathscr{U})$, then

(117)

$$
\{\psi(F_1, \dots, F_n), G\}_{\mathscr{L}} = \sum_{j=1}^{n} \left[\frac{\partial \psi}{\partial \mathrm{Re} z_j}(F_1, \dots, F_n)\{\mathrm{Re} F_j, G\}_{\mathscr{L}} + \frac{\partial \psi}{\partial \mathrm{Im} z_j}(F_1, \dots, F_n)\{\mathrm{Im} F_j, G\}_{\mathscr{L}} \right] .
$$

The above formula follows immediately from the chain rule (A.3) and yields Leibniz's rule for the Peierls bracket as a special case.

4.2.2. REMARK. A consequence of Theorem 4.2.1 is that the topology of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ given in Corollary 4.1.2 is *not* sequentially complete. To see this, let $F:\mathscr{U}\ni\varphi\mapsto F(\varphi)\doteq\int_{\mathscr{M}}\varphi\omega$, where ω is a smooth real-valued d-form of compact support in $\mathscr{M}$. Let (f_n) be a sequence of even smooth functions $f_n:\mathbb{R}\to[0,1]$ supported in $[-2,2]$ which converges pointwise to the characteristic function $\chi_{[-1,1]}$ of $[-1,1]$ and whose derivatives of all orders converge pointwise to zero (e.g. take $f_n(|x|)=1$ for $|x|\leq 1+(4n)^{-1}$ and $f_n(|x|)=0$ for $|x|\geq 1+(2n)^{-1}$). Defining $F_n\doteq f_n\circ F$ gives a sequence (F_n) of elements of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$, whose functional derivatives of order $k\geq 1$ are given by Faà di Bruno's formula (A.7) as

$$F_n^{(k)}[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)=f_n^{(k)}(F(\varphi))\left(\int_{\mathscr{M}}\vec{\varphi}_1\omega\right)\cdots\left(\int_{\mathscr{M}}\vec{\varphi}_k\omega\right)\ . \tag{118}$$

Hence, the functional derivatives of all orders of the elements of the sequence (F_n) converge to zero in the respective topologies for all $\varphi\in\mathscr{U}$. The sequence $(F_n(\varphi))$, however, converges pointwise to $\chi_{[-1,1]}\circ F(\varphi)$, which defines a functional on $\mathscr{U}$ which is in general *not even continuous*, let alone microcausal. By the Stone-Weierstrass theorem in the interval $[-2,2]$ [54], there is even a sequence of functionals $F_n\in\mathscr{F}((\mathscr{M},g),\mathscr{U}\cap F^{-1}((-2,2)))$ which lies in the *-subalgebra of $\mathscr{F}((\mathscr{M},g),\mathscr{U}\cap F^{-1}((-2,2)))$ generated by $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M},\mathscr{U}\cap F^{-1}((-2,2)))$ and converges to $\chi_{[-1,1]}\circ F$ in the topology of $\mathscr{F}((\mathscr{M},g),\mathscr{U}\cap F^{-1}((-2,2)))$.

4.2.3. REMARK. In view of the counterexample discussed in Remark 4.2.2, it would be desirable to find a stronger topology on $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ which is compatible with its Poisson *-algebraic and $\mathscr{C}^\infty$-ring structures, and (at least sequentially) complete. It is clear from this counterexample that even if we follow the proposal of [28] and replace the (weak) seminorms $|F^{(k)}[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)|$ by the *strong* seminorms

$$F\mapsto\sup\left\{\left|F^{(k)}[\varphi](\vec{\varphi})\right|\ \middle|\ \vec{\varphi}\in\mathscr{B}\right\}\ ,$$

where φ runs over $\mathscr{U}$ and $\mathscr{B}$ runs over all closed and bounded subsets of $\mathscr{C}^\infty(\mathscr{M}^k)$, we still get sequential incompleteness since the functional derivatives of each element in the sequence we have constructed have *empty* wave front sets and therefore weak convergence of the derivatives entails their strong convergence by the Banach-Steinhaus theorem. We point that the phenomenon described in Remark 4.2.2 is *independent* of the actual failures of sequential completeness for $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)$ in either the weak or strong topologies, which were shown in [28]. Therefore, this phenomenon *cannot* be circumvented by allowing the functional derivatives of microcausal functionals to take values in the completions of $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)$ in the strong topology for each k, as advocated in [14, 26, 27].

A seemingly better way out is to take full advantage of the Michal-Bastiani notion of differentiability and replace the seminorms $|F^{(k)}[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)|$ by the even stronger seminorms

$$F\mapsto\sup\left\{\left|F^{(k)}[\varphi](\vec{\varphi})\right|\ \middle|\ \vec{\varphi}\in\mathscr{B}\right\}\ ,$$

where $\mathscr{B}$ is as above and $\mathscr{K}$ runs over the compact subsets of $\mathscr{U}$. In other words, we require now uniform convergence of functional derivatives of all orders in compact subsets (this topology is called *Bastiani topology* in [14]). Since $\mathscr{C}^\infty(\mathscr{M})$ is semi-Montel, we have that $\mathscr{K} \times \mathscr{B}$ is compact. Therefore, since $\mathscr{U} \times \mathscr{C}^\infty(\mathscr{M}^k)$ is metrizable and hence compactly generated[8], we conclude that the completion of $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$ in this stronger topology does correspond to allowing the functional derivatives of each order $k \in \mathbb{N}$ to take values in the completion of $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k \to \mathscr{M}^k)$ in the strong topology (see e.g. Proposition 16.6.2, pp. 361 of [54]). Thanks to the results of [13], one then has separate continuity of the pointwise product and the Peierls bracket on $\mathscr{F}((\mathscr{M}, g), \mathscr{U})$ with respect to this topology and thus these bilinear operations extend (separately) continuously to the completion (see also [14, 27] for related results). By Faà di Bruno's formula (A.7), separate continuity also holds for the $\mathscr{C}^\infty$-ring operations. It is not clear, however, whether *nuclearity* survives in this stronger topology. For instance, as Meise has shown [69], the space of MB-smooth functionals on $\mathscr{U}$ endowed with the topology of uniform convergence of functional derivatives on compact subsets of $\mathscr{U}$ *cannot* be nuclear despite being complete.

Fortunately, there is a middle course able to get the best of both worlds, thanks to the coincidence of MB smoothness and convenient smoothness in Fréchet spaces (see Remark A.4 below). We start from the simple but important observation (see e.g. Lemma 3.11, pp. 30 of [63]) that the space $\mathscr{C}^\infty(\mathscr{U}, \mathbb{C})$ of (conveniently) smooth maps from $\mathscr{U} \subset \mathscr{C}^\infty(\mathscr{M})$ open to $\mathbb{C}$ is the projective limit

$$
\begin{aligned}
\mathscr{C}^\infty(\mathscr{U}, \mathbb{C}) &= \varprojlim_{\gamma \in \mathscr{C}^\infty(\mathbb{R}, \mathscr{U})} \mathscr{C}^\infty(\mathbb{R}, \mathbb{C}) \\
&= \Bigg\{ (F_\gamma)_\gamma \in \prod_{\gamma \in \mathscr{C}^\infty(\mathscr{U}, \mathbb{C})} \mathscr{C}^\infty(\mathbb{R}, \mathbb{C}) \;\Bigg|\; F_\gamma \circ \kappa = F_{\gamma \circ \kappa} \\
&\qquad \text{for all } \kappa \in \mathscr{C}^\infty(\mathbb{R}, \mathbb{R}) \Bigg\}
\end{aligned}
$$

along the preordered set $(\mathscr{C}^\infty(\mathbb{R}, \mathscr{U}), \preccurlyeq)$ with preorder $\preccurlyeq$ given by smooth reparametrization:

$$
\gamma \preccurlyeq \tilde{\gamma} \;\Leftrightarrow\; \gamma = \tilde{\gamma} \circ \kappa \text{ for some } \kappa \in \mathscr{C}^\infty(\mathbb{R}, \mathbb{R}) \ .
$$

To see the second identity, notice that any $(F_\gamma)_\gamma \in \prod_{\gamma \in \mathscr{C}^\infty(\mathscr{U}, \mathbb{C})} \mathscr{C}^\infty(\mathbb{R}, \mathbb{C})$ such that $F_\gamma \circ \kappa = F_{\gamma \circ \kappa}$ for all $\kappa \in \mathscr{C}^\infty(\mathbb{R}, \mathbb{R})$ defines a map $\mathscr{U} \ni \varphi \mapsto F(\varphi) = F_\varphi$, where we identify φ with the constant curve $\mathbb{R} \ni t \mapsto \varphi(t) \equiv \varphi \in \mathscr{U}$. One immediately sees that $F_\gamma(t_0) = F(\gamma(t_0))$ for all $\gamma \in \mathscr{C}^\infty(\mathbb{R}, \mathscr{U})$, $t_0 \in \mathbb{R}$ by means of the constant reparametrization $\kappa(t) \equiv t_0$. Conversely, any $F \in \mathscr{C}^\infty(\mathscr{U}, \mathbb{R})$ gives rise to such an $(F_\gamma)_\gamma$ by setting $F_\gamma = \gamma^* F = F \circ \gamma$ for all $\gamma \in \mathscr{C}^\infty(\mathbb{R}, \mathscr{U})$ – one then obviously has $F_\gamma \circ \kappa = F \circ \gamma \circ \kappa = F_{\gamma \circ \kappa}$ for all $\kappa \in \mathscr{C}^\infty(\mathbb{R}, \mathbb{R})$. As such, it is natural to impose on $\mathscr{C}^\infty(\mathscr{U}, \mathbb{C})$ the initial topology induced from the compact-open topology of $\mathscr{C}^\infty(\mathbb{R}, \mathbb{C})$ through the pullbacks γ^* by all $\gamma \in \mathscr{C}^\infty(\mathbb{R}, \mathscr{U})$ as in Definition 3.11, pp. 30 of [63], which is just the induced subspace topology from the direct product $\prod_{\gamma \in \mathscr{C}^\infty(\mathscr{U}, \mathbb{C})} \mathscr{C}^\infty(\mathbb{R}, \mathbb{C})$. Since $\mathscr{C}^\infty(\mathscr{U}, \mathbb{C})$ is a *closed* subspace of the latter and the compact-open topology of $\mathscr{C}^\infty(\mathbb{R}, \mathbb{C})$ is nuclear and

[8] Recall that a completely regular topological space X is said to be *compactly generated* or a *k-space* if the topology of X coincides with the final topology induced by the inclusions of compact subsets of X. This is equivalent to the space of continuous real-valued functions on X being complete with respect to the topology of uniform convergence on compact subsets of X (see e.g. Theorem 3.6.4, pp. 70 of [54]).

complete, it follows from the permanence of nuclearity for initial topologies (Proposition 5.2.3, pp. 92 of [76]) and the permanence of completeness for closed subspaces and products (respectively Propositions 3.2.5 and 3.2.6, pp. 59 of [54]) that this topology on $\mathscr{C}^\infty(\mathscr{U},\mathbb{C})$ is also nuclear and complete, as desired. Likewise, since convenient smoothness and MB smoothness coincide on $\mathscr{U}$, the topology induced on the (closed) subspace $\mathscr{F}_{00}(\mathscr{M},\mathscr{U})\cap\mathscr{C}^\infty(\mathscr{U},\mathbb{C})$ is nuclear (due to the permanence of nuclearity for linear subspaces, see Proposition 5.1.1, pp. 85 of [76]), complete and finer than the topology of pointwise convergence of all derivatives. To see the latter, notice that this topology is induced by the so-called *(strong) convenient seminorms*

$$F\mapsto\sup\left\{\left|F^{(k)}[\gamma(t)](\vec{\varphi})\right|\;\middle|\;t\in[a,b],\,a<b\in\mathbb{R},\,\gamma\in\mathscr{C}^\infty(\mathbb{R},\mathscr{U}),\,\vec{\varphi}\in\mathscr{B}\right\}\ ,$$

with $\mathscr{B}$ as before. In other words, we consider only the "at most one-dimensional" compact subsets $\mathscr{K}=\gamma([a,b])\subset\mathscr{U}$, $a<b\in\mathbb{R}$, $\gamma\in\mathscr{C}^\infty(\mathbb{R},\mathscr{U})$, which of course include all singleton subsets of $\mathscr{U}$ through all constant curves into $\mathscr{U}$. Substituting the convenient seminorms for $|F^{(k)}[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)|$ in $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ then yields a nuclear locally convex topology in the latter, which we suggestively call the *(strong) convenient topology* and whose completion amounts once more to allowing $F^{(k)}[\varphi]$ to take values in the completion of $\mathscr{E}'_{\Upsilon_{k,g}}(\wedge^{kd}T^*\mathscr{M}^k\to\mathscr{M}^k)$ in the strong topology for all $\varphi\in\mathscr{U}$, $k\in\mathbb{N}$. Unlike before, thanks to the permanence of nuclearity for completions (Proposition 5.3.1, pp. 93 of [76]) we can be sure that the completion of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ in the convenient topology is also nuclear. A similar proposal has been put forward in [14, 27] by including all smooth maps with finite (but otherwise arbitrary) dimensional domains and $\mathscr{U}$ as codomain in addition to just smooth curves into $\mathscr{U}$. The aforementioned continuity of the Poisson *-algebraic operations of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ still survives, of course.

Finally, we recall the important fact that $\mathscr{F}_{\mu\mathrm{loc}}(\mathscr{M},\mathscr{U})\subset\mathscr{F}((\mathscr{M},g),\mathscr{U})$ contains the squared Sobolev seminorms

$$\varphi\mapsto F_{k,f}(\varphi)=\|\varphi\|^2_{2,k,f}\ ,$$

defined in (5), for all $f\in\mathscr{C}^\infty_c(\mathscr{M})$. This together with Theorem 4.2.1 yields:

4.2.4. Proposition. *The following facts hold true:*

(i) *Given any open set $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ in the compact-open topology and $\varphi_0\in\mathscr{U}$, there is $F\in\mathscr{F}((\mathscr{M},g),\mathscr{C}^\infty(\mathscr{M}))$ such that $F(\varphi_0)=1$, $0\leq F\leq 1$, and $F\equiv 0$ in $\mathscr{C}^\infty(\mathscr{M})\smallsetminus\mathscr{U}$. In particular, one can completely recover the compact-open topology of $\mathscr{C}^\infty(\mathscr{M})$ from the complements of zero sets of elements of $\mathscr{F}((\mathscr{M},g),\mathscr{C}^\infty(\mathscr{M}))$.*

(ii) *Any $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ open in the compact-open topology admits locally finite partitions of unity whose elements belong to $\mathscr{F}((\mathscr{M},g),\mathscr{U})$.*

(iii) *Given any open set $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ in the compact-open topology, the algebra $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ separates the points of $\mathscr{U}$, that is, for any $\varphi_1,\varphi_2\in\mathscr{U}$ there is an $F\in\mathscr{F}((\mathscr{M},g),\mathscr{U})$ such that $F(\varphi_1)\neq F(\varphi_2)$.*

(iv) *Given any open set $\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})$ in the compact-open topology, any unital *-morphism $\omega:\mathscr{F}((\mathscr{M},g),\mathscr{U})\to\mathbb{C}$ (i.e. a* *-character *on $\mathscr{F}((\mathscr{M},g),\mathscr{U})$) is given by the evaluation functional at some $\varphi\in\mathscr{U}$ (by (iii), φ must be unique).*

(v) *Given any open sets $\mathscr{U},\mathscr{V}\subset\mathscr{C}^\infty(\mathscr{M})$ in the compact-open topology, any continuous unital *-morphism $\alpha:\mathscr{F}((\mathscr{M},g),\mathscr{U})\to\mathscr{F}((\mathscr{M},g),\mathscr{V})$ is the pullback of a unique smooth map $\alpha^*:\mathscr{V}\to\mathscr{U}$.*

Proof. (i) Let $\chi:\mathbb{R}\to[0,1]$ be an even smooth function such that $\chi(t)=0$ for $|t|\geq 1$ and $\chi(t)=1$ $|t|\leq\frac{1}{2}$. There are $k\in\mathbb{N}$, $f\in\mathscr{C}^\infty_c(\mathscr{M})$ and $R>0$ such that $\varphi_0\in\{\varphi\in\mathscr{C}^\infty(\mathscr{M})\mid F_{k,f}(\varphi-\varphi_0)<R^2\}\subset\mathscr{U}$. Set $F(\varphi)=\chi(R^{-2}F_{k,f}(\varphi-\varphi_0))$, and we are done by Theorem 4.2.1.

(ii) Recall that, since $\mathscr{C}^\infty(\mathscr{M})$ is a nuclear Fréchet space, it follows that $\mathscr{C}^\infty(\mathscr{M})$ is separable, hence second countable and Lindelöf. $\mathscr{U}$ is then a second countable metric space, hence also separable and Lindelöf. Since (i) holds, the result then follows from Theorem 16.10, pp. 171–172 of [63].

(iii) $\mathscr{U}$ is Hausdorff, hence the result follows immediately from (i).

(iv) By the proof of (ii), we know that $\mathscr{U}$ is Lindelöf. Since (i) implies that $\mathscr{U}$ is completely regular, it follows that it must be *realcompact*, that is, any $\mathbb{R}$-algebra homomorphism from the $\mathbb{R}$-valued continuous functions on $\mathscr{U}$ into $\mathbb{R}$ is given by evaluation at some $\varphi\in\mathscr{U}$ (see [36], Theorem 3.11.12, pp. 216). The result then follows for the $\mathbb{R}$-subalgebra of real-valued elements of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ by combining (ii) with Theorem 17.6, pp. 187–188, Remark 18.1, pp. 188–189 and Proposition 18.3, pp. 191 of [63]. The general case is immediate.

(v) Notice that the pullback of any *-character by α is also a *-character, hence by (iii)-(iv) α^* as above is really the pullback by α (thus also justifying our notation). Moreover, the action of α on functionals of the form $\mathscr{U}\ni\varphi\mapsto\int_{\mathscr{M}}f\varphi\mathrm{d}\mu_g$, $f\in\mathscr{C}^\infty_c(\mathscr{M})$, shows that α^* must be smooth on $\mathscr{V}$.

□

Some comments about the meaning of Proposition 4.2.4 are in order. Proposition 4.2.4 (ii) shows that we can "glue together" microcausal functionals defined on an open covering of $\mathscr{C}^\infty(\mathscr{M})$, that is, the assignment

$$\mathscr{U}\subset\mathscr{C}^\infty(\mathscr{M})\text{ open }\to\mathscr{F}((\mathscr{M},g),\mathscr{U})\ , \tag{119}$$

together with the restriction morphisms induced by inclusions between pairs of open subsets in $\mathscr{C}^\infty(\mathscr{M})$ in the compact-open topology, constitute a *sheaf* of *-algebras over the topological space $\mathscr{C}^\infty(\mathscr{M})$. However, multiplying $F\in\mathscr{F}((\mathscr{M},g),\mathscr{U})$ by a "bump" functional as given by Proposition 4.2.4 (i) improves the localization of F in field configuration space at the cost of *losing* information about the *space-time* support of F. This must be kept in mind when multiplying F by the elements of a partition of unity on $\mathscr{U}$ belonging to $\mathscr{F}((\mathscr{M},g),\mathscr{U})$. A more conceptual discussion of the interplay between these two notions of localization will take place in future work.

4.3. **On-shell ideals.**

4.3.1. DEFINITION. Let $\mathscr{U},\mathscr{L}$ be as in Proposition 3.2.12. We define the *on-shell ideal* of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$ associated to $\mathscr{L}$ as the subspace $\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})\subset\mathscr{F}((\mathscr{M},g),\mathscr{U})$ of all microcausal functionals F of the form

$$F(\varphi)=X[\varphi]E(\mathscr{L})[\varphi]\ ,\quad \varphi\in\mathscr{U}\ , \tag{120}$$

where $X:\mathscr{U}\times\Gamma^\infty(\wedge^{kd}T^*\mathscr{M}\to\mathscr{M})\ni(\varphi,\omega)\mapsto X[\varphi]\omega\in\mathbb{C}$ is jointly smooth and linear with respect to ω.

It is clear that $F(\varphi)=0$ for all $F\in\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})$ and all $\varphi\in\mathscr{U}$ such that $E(\mathscr{L})[\varphi]=0$. A key consequence of (120) is the following

4.3.2. PROPOSITION. *$\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})$ is a Poisson *-ideal of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$.*

Proof. It is clear that $\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})$ is a *-ideal of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$, so what is left is to show that $\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})$ is also a Lie ideal of $\mathscr{F}((\mathscr{M},g),\mathscr{U})$. Let $G\in\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})$, so that $G(\varphi)=X[\varphi]E(\mathscr{L})[\varphi]$ with X as in Definition 4.3.1. By the chain rule (A.3) applied to the pair of maps $X,(\mathbb{1},E(\mathscr{L}))$, we get that

$$G^{(1)}[\varphi](\vec{\varphi})=DX[\varphi](\vec{\varphi})E(\mathscr{L})[\varphi]+X[\varphi]E'(\mathscr{L})[\varphi]\vec{\varphi}\ ,\quad \vec{\varphi}\in\mathscr{C}^\infty(\mathscr{M})\ , \tag{121}$$

where DX is defined as in (A.10). Let now $F\in\mathscr{F}((\mathscr{M},g),\mathscr{U})$. Then

$$\begin{aligned}\{F,G\}_{\mathscr{L}}(\varphi)&=\left\langle F^{(1)}[\varphi],\Delta_{\mathscr{L}}[\varphi]G^{(1)}[\varphi]\right\rangle\\&=\left\langle F^{(1)}[\varphi],DX[\varphi](\vec{\varphi})E(\mathscr{L})[\varphi]\right\rangle-X[\varphi]E'(\mathscr{L})[\varphi]\Delta_{\mathscr{L}}[\varphi]F^{(1)}[\varphi]\\&=\left\langle F^{(1)}[\varphi],DX[\varphi](\vec{\varphi})E(\mathscr{L})[\varphi]\right\rangle\end{aligned}$$

and therefore $\{F,G\}_{\mathscr{L}}\in\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})$, as desired. □

One is then led to the

4.3.3. DEFINITION. Let $\mathscr{U},\mathscr{L}$ as in Proposition 3.2.12. The quotient Poisson*-algebra

$$\mathscr{F}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U})\doteq\mathscr{F}((\mathscr{M},g),\mathscr{U})/\mathscr{J}_{\mathscr{L}}((\mathscr{M},g),\mathscr{U}) \tag{122}$$

is called the *on-shell algebra* over $\mathscr{U}$ associated to $\mathscr{L}$.

As stated in the introduction, the on-shell algebra correspond to our algebra of observables once we have imposed the equations of motion $E(\mathscr{L})[\varphi]=0$ on field configurations in $\mathscr{U}$. A natural question at this point is whether any $F\in\mathscr{F}((\mathscr{M},g),\mathscr{U})$ vanishing on solutions $\varphi\in\mathscr{U}$ of $E(\mathscr{L})[\varphi]=0$ is of the form (120). This question shall be addressed in future work.

5. FINAL CONSIDERATIONS

We have presented the very first steps into a novel, algebraic approach to classical field theory in which the main role is played by algebras of functionals over sets of field configurations on any globally hyperbolic space-time.

As a whole, our formalism can be extended to field theories living on any fiber bundle over space-time. In fact, extensions of parts of our framework have already appeared in the literature, including fermion fields [78], Yang-Mills models and gravity [38, 89]. These works also show that our formalism is capable of dealing with Lagrangians possessing local symmetries which constrain the dynamics – more precisely, a rigorous version of the classical Batalin-Vilkoviskiĭ approach to gauge theories can be provided within our setup [38]. Such subtleties are absent in the case of real scalar fields, which do not possess any "internal" structure. A full account of our framework encompassing all the above examples will be pursued in the future.

On a more technical side, treating the above examples will occasionally require (particularly in the case of fermion fields) extending the results concerning normally hyperbolic linear partial differential operators presented in this series of papers to more general hyperbolic systems. Theorem 3.2.3 can be extended to symmetrizable, first-order hyperbolic systems with very few changes in the arguments. Arguably, Theorem 3.2.4 could be reworked along the lines of the paper of Dencker [31] to encompass symmetrizable, first-order hyperbolic systems of real principal type, of which the Dirac operator is an example [78]. One could try to go even further and encompass the case of second-order regularly hyperbolic systems of Christodoulou [24], but the microlocal analysis of such systems is severely underdeveloped, due to the possibility of occurrence of bicharacteristics with varying multiplicity (e.g. birefringence in crystal optics; see [66] for the state of the art on these matters).

In this paper we have restricted ourselves to studying *linearized* dynamics. This, of course, is far from being the full story – the analysis of full *nonlinear* dynamics within our approach, to be undertaken in a followup publication [20], will be based on a *semi-global solvability* result for second-order, quasi-linear hyperbolic partial differential operators $P : \mathscr{C}^\infty(\mathscr{M}) \to \mathscr{C}^\infty(\mathscr{M})$. More precisely, for a suitably large family of compact regions K of the space-time manifold $\mathscr{M}$, that the equation

$$P(\varphi_0 + \varphi) = P(\varphi_0) + f$$

has a smooth solution φ in K for any $\varphi_0, f \in \mathscr{C}^\infty(K)$, f sufficiently small. Moreover, if we prescribe the Cauchy data for φ on a suitable Cauchy hypersurface crossing K, this solution must be unique. Such a result can be proved by combining a simple refinement (due to Klainerman [58, 59], see also Hintz and Vasy [49]) of classical energy estimates for second-order linear hyperbolic partial differential operators with a variant of the Nash-Moser-Hörmander inverse function theorem [45], pretty much in the spirit of the results by Bryant, Griffiths and Yang [21] and Tso [83]. Taking $f = P_0(\varphi_0) - P(\varphi_0)$, where P is a "small" perturbation of P_0, yields that setting $m_{P,P_0}(\varphi_0) \doteq \varphi_0 + \varphi$ with φ as above leads to the formula

$$P \circ m_{P,P_0} = P_0 \ .$$

A map m_{P,P_0} intertwining P and P_0 in the above sense is called a *Møller map*, in analogy with the Møller wave operators in quantum mechanical scattering theory. Møller maps in classical field theory were discussed formally in [15, 17, 34, 35] and will constitute the backbone of our take on nonlinear dynamics – in particular, since they act as Poisson maps with respect to the Peierls brackets associated to two Euler-Lagrange operators differing by a perturbation, they can be used to locally linearize a Peierls bracket around a given field configuration, pretty much like the Darboux-Weinstein theorem for regular, finite-dimensional Poisson manifolds [84]. We also hope that finer details of on-shell ideals might be elucidated with such methods.

The final release of the present paper was delayed because of incomplete proofs of Proposition 3.2.16 and Corollary 3.2.17 in previous versions. We hope that we have now clarified the validity of those statements. In the meantime, several papers appeared dealing with other side aspects of the present paper, namely [14, 26, 27, 28]. Some of these aspects were addressed in Remark 4.2.3.

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Appendix A. A short review of differential calculus on locally convex topological vector spaces

In this Appendix we list the basic definitions and results of differential calculus we need. Our basic references are [45] and [63], to whom we refer for more details and proofs. The first reference works only with Fréchet spaces, but the proofs of the results quoted below work in the general case with little or no change.

The notion of differentiability of curves in locally convex topological vector spaces is straightforward.

A.1. Definition. Let $\gamma : (a, b) \to \mathscr{F}$, $a < b \in \mathbb{R} \cup \{\pm\infty\}$ be a continuous curve into a locally convex topological vector space $\mathscr{F}$. We say that γ is a $\mathscr{C}^1$ *curve* if for all $t \in (a, b)$ the limit

$$\gamma'(t) \doteq \lim_{s\to 0} \frac{1}{s}(\gamma(t+s) - \gamma(t))$$

exists and defines a *continuous* curve $\gamma' : (a,b) \to \mathscr{F}$ (continuity of γ actually follows from these conditions alone, hence it does not hurt to assume it from the start). We also say that γ is a $\mathscr{C}^m$ curve, $m \geq 1$, if $\gamma^{(k)} \doteq (\gamma^{(k-1)})'$ exists and is continuous for all $1 \leq k \leq m$, where $\gamma^{(0)} \doteq \gamma$. If γ is a $\mathscr{C}^m$ curve for all m, we say that γ is a *smooth* curve.

We stress that there would be no loss of generality if we required the domain of smooth curves to be the whole real line: by the chain rule (A.3), $\gamma : (a,b) \to \mathscr{F}$ is smooth if and only if $\gamma \circ f : \mathbb{R} \to \mathscr{F}$ is smooth for any diffeomorphism $f : \mathbb{R} \to (a,b)$ (e.g. $f(\lambda) = \frac{b+a}{2} + \frac{b-a}{2}\tanh(\lambda)$). Once this is said, let us see how Definition A.1 is realized in the concrete cases that interest us.

- $\mathscr{F} = \mathscr{C}^\infty(\mathscr{M})$ (endowed with the compact-open topology): $\gamma : \mathbb{R} \to \mathscr{F}$ is smooth if and only if $\gamma(\lambda)(p) = \Phi(\lambda, p)$ for all $(\lambda, p) \in \mathbb{R} \times \mathscr{M}$, where $\Phi \in \mathscr{C}^\infty(\mathbb{R} \times \mathscr{M})$;
- $\mathscr{F} = \mathscr{C}^\infty_c(\mathscr{M})$ (endowed with the usual inductive limit topology): $\gamma : \mathbb{R} \to \mathscr{F}$ is smooth if and only if $\gamma(\lambda)(p) = \Phi(\lambda, p)$ for all $(\lambda, p) \in \mathbb{R} \times \mathscr{M}$, where $\Phi \in \mathscr{C}^\infty(\mathbb{R} \times \mathscr{M})$ is such that for any $a < b \in \mathbb{R}$ there is a compact subset $K \subset \mathscr{M}$ such that $\Phi(\lambda, p) = \Phi(a, p)$ for all $p \notin K$, $\lambda \in [a,b]$.

The notion of smooth curves allows one to introduce another topology on $\mathscr{F}$, given by the final topology induced by $\mathbb{R}$ through all smooth curves $\gamma : \mathbb{R} \to \mathscr{F}$. We call this topology the c^∞-topology on $\mathscr{F}$. This topology is necessarily finer than the original one, but it is not in general a vector space topology – the finest locally convex vector space topology on $\mathscr{F}$ that is coarser then the c^∞-topology is the bornologification of $\mathscr{F}$'s original topology. The c^∞- and the original locally convex vector space topologies coincide if $\mathscr{F}$ is e.g. metrizable (such as $\mathscr{C}^\infty(\mathscr{M})$), but are distinct for $\mathscr{F} = \mathscr{C}^\infty_c(\mathscr{M})$ if $\mathscr{M}$ is non-compact since then the c^∞-topology is not a vector space topology (see e.g. Proposition 4.26 (ii), pp. 45 of [63]).[9]

Given two locally convex vector spaces $\mathscr{F}_1$, $\mathscr{F}_2$, $\mathscr{U} \subset \mathscr{F}_1$ c^∞-open, we say that a map $\Phi : \mathscr{U} \to \mathscr{F}_2$ is *conveniently smooth* if $\Phi \circ \gamma$ is a smooth curve on $\mathscr{F}_2$ for every smooth curve $\gamma : \mathbb{R} \to \mathscr{U}$. We stress that conveniently smooth maps need not even be continuous (see [41] for a counterexample). A simple non-trivial example of a conveniently smooth map $\Phi : \mathscr{F} \to \mathscr{F}$ is, of course, the translation $\varphi \mapsto \Phi(\varphi) = \varphi + \varphi_0$ by a fixed element $\varphi_0 \in \mathscr{F}$. In particular, the coordinate change maps $\kappa_{\varphi_2} \circ \kappa^{-1}_{\varphi_1} : \mathscr{C}^\infty_c(\mathscr{M}) \to \mathscr{C}^\infty_c(\mathscr{M})$ in the affine flat manifold $\mathscr{C}^\infty(\mathscr{M})$ (endowed with the Whitney topology) are conveniently smooth for all $\varphi_1, \varphi_2 \in \mathscr{C}^\infty(\mathscr{M})$ such that $\varphi_1 - \varphi_2 \in \mathscr{C}^\infty_c(\mathscr{M})$. This shows that the atlas $\mathfrak{U}$ defined in (7) induces a smooth structure on $\mathscr{C}^\infty(\mathscr{M})$; the corresponding smooth manifold topology is, of course, the manifold topology generated by the c^∞-open subsets of the modelling vector space $\mathscr{C}^\infty_c(\mathscr{M})$, which is even finer than the Whitney topology. The connected components of this topology are, however, also of the form $\mathscr{C}^\infty_c(\mathscr{M}) + \varphi_0$, $\varphi_0 \in \mathscr{C}^\infty(\mathscr{M})$; therefore, the smooth curves in $\mathscr{C}^\infty(\mathscr{M})$ with respect to the smooth structure induced by the atlas $\mathfrak{U}$ must be of the form $\mathbb{R} \ni \lambda \mapsto \gamma(\lambda) = \varphi_0 + \gamma_0(\lambda)$, where $\gamma_0 : \mathbb{R} \to \mathscr{C}^\infty_c(\mathscr{M})$ is smooth. Hence, it is just fair to say that such γ is *a smooth curve with*

[9] Nonetheless, in this case the c^∞-topology coincides with the so-called *Kelleyfication* of $\mathscr{F}$, which is the final topology induced by all compact subsets of $\mathscr{F}$ through their respective inclusions (see e.g. Theorem 4.11 (3), pp. 39–40 of [63]). It is clear that the Kelleyfication of $\mathscr{F}$ coinciding with the original topology of $\mathscr{F}$ amounts to $\mathscr{F}$ being compactly generated (see footnote 8 above). This happens if e.g. $\mathscr{F}$ is metrizable.

respect to the Whitney topology, and the smooth structure induced by the atlas $\mathfrak{U}$, *the smooth structure on $\mathscr{C}^\infty(\mathscr{M})$ induced by the Whitney topology.*

A.2. REMARK. It can be shown [63] that, for $\mathscr{C}^\infty(\mathscr{M})$ endowed with the smooth structure induced by the Whitney topology, the bundles

$$T^{r,s}\mathscr{C}^\infty(\mathscr{M}) = (\otimes^s T^*\mathscr{C}^\infty(\mathscr{M})) \otimes (\otimes^r T\mathscr{C}^\infty(\mathscr{M}))$$

of tensors of contravariant rank r and covariant rank s are given at each $\varphi \in \mathscr{C}^\infty(\mathscr{M})$ by the space of bounded linear mappings from $\otimes^s_\beta \mathscr{C}^\infty_c(\mathscr{M})$ to $\otimes^r_\beta \mathscr{C}^\infty_c(\mathscr{M})$. Here $\otimes_\beta$ denotes the *bornological* tensor product, whose topology is the finest locally convex topology on the algebraic tensor product such that the canonical quotient map is *bounded*; this topology is finer than the projective tensor product topology. Nonetheless, $T\mathscr{C}^\infty(\mathscr{M})$ and $T^*\mathscr{C}^\infty(\mathscr{M})$ do assume the form given in Subsection 2.2 (see the proof of Theorem 42.17, pp. 447–448 of [63]). It also turns out that the particular structure of $\mathscr{C}^\infty_c(\mathscr{M})$, together with Theorems 6.14, pp. 72–73 and 28.7, pp. 280–281 of [63], imply that every kinematical tangent vector on $\mathscr{C}^\infty(\mathscr{M})$ is also an *operational* one, i.e. it defines a point derivation on (conveniently) smooth maps $F : \mathscr{C}^\infty(\mathscr{M}) \to \mathbb{R}$.

In principle, we could develop essentially all tools of differential calculus by using convenient smoothness. However, for the purposes of this paper, it is often preferrable to use a stronger concept of smoothness. Such a notion is provided, for instance, by Michal [70] and Bastiani [5]. This is also the notion employed in the accounts of infinite dimensional differential calculus done by Milnor [71] and Hamilton [45], and all the basic results of Calculus we present in the remainder of this Appendix are formulated in this context (see, however, Remark A.4 below). The basic definition is as follows (See also Definition 2.3.7 for the special case of real-valued maps):

A.3. DEFINITION. Let $\mathscr{F}_1, \mathscr{F}_2$ be locally convex topological vector spaces, $\mathscr{U} \subset \mathscr{F}_1$ open, and $F : \mathscr{U} \to \mathscr{F}_2$ a continuous map. We say that F is *(MB-)differentiable of order m* ("MB" stands for the names of Michal and Bastiani) if for all $k = 1, \dots, m$ the k-th order directional (Gâteaux) derivatives

$$F^{(k)}[\varphi](\vec{\varphi}_1, \dots, \vec{\varphi}_k) \doteq \frac{\partial^k}{\partial\lambda_1 \cdots \partial\lambda_k}\Big|_{\lambda_1 = \cdots = \lambda_k = 0} F\left(\varphi + \sum_{j=1}^k \lambda_j \vec{\varphi}_j\right) \tag{A.1}$$

exist as jointly continuous maps from $\mathscr{U} \times \mathscr{F}_1^k \ni (\varphi, \vec{\varphi}_1, \dots, \vec{\varphi}_k)$ to $\mathscr{F}_2$. If F is differentiable of order m for all $m \in \mathbb{N}$, we say that F is *(MB-)smooth.*[10]

The right-hand side of formula (A.1) should be understood as the differentiation of a k-parameter curve taking values in $\mathscr{F}_2$, for fixed $\varphi, \vec{\varphi}_1, \dots, \vec{\varphi}_k$. The argument of F inside the limit is guaranteed to lie inside $\mathscr{U}$ for sufficiently small $\lambda_1, \dots, \lambda_k$.

It follows from Definition A.3 that if $F : \mathscr{U} \subset \mathscr{F}_1 \to \mathscr{F}_2$ is MB-differentiable of order $m > 0$ then the maps $\mathscr{U} \ni \varphi \mapsto F^{(k)}[\varphi] \in \mathscr{L}^k(\mathscr{F}_1, \mathscr{F}_2)$ are *continuous* for all $1 \leq k \leq m$, where

[10] MB differentiability and MB smoothness are respectively listed in Keller's treatise [55] as "$\mathscr{C}^k_c$- and $\mathscr{C}^\infty_c$-differentiability". Here we avoid his nomenclature, for it clashes with the usual notation for differentiable and smooth functions with compact support.

$\mathscr{L}^k(\mathscr{F}_1, \mathscr{F}_2)$ is the locally convex topological vector space of all k-linear maps from $\mathscr{F}_1^k$ to $\mathscr{F}_2$ endowed with the compact-open topology. If $\mathscr{F}_1$ is semi-Montel (i.e. closed and bounded subsets of $\mathscr{F}_1$ are compact), such topology amounts to uniform convergence in bounded subsets of $\mathscr{F}_1^k$. If $\mathscr{F}_1^k$ is compactly generated (e.g. when $\mathscr{F}_1$ is metrizable, see e.g. Proposition 3.3.20, pp. 152 of [36] and footnote 9 above) and $\mathscr{F}_2$ is complete, then by Proposition 16.6.2, pp. 361 of [54] $\mathscr{L}^k(\mathscr{F}_1, \mathscr{F}_2)$ is also complete.

Given $\mathscr{U}$ an *arbitrary* (i.e. not necessarily open) subset of $\mathscr{F}_1$, we say that a continuous map $F : \mathscr{U} \to \mathscr{F}_2$ is differentiable of order m (resp. smooth) if there is $\mathscr{V} \supset \mathscr{U}$ open in the compact-open topology and a functional $\tilde{F} : \mathscr{V} \to \mathscr{F}_2$ extending F (i.e. $\tilde{F}|_{\mathscr{U}} = F$) such that $\tilde{F}$ is differentiable of order m (resp. smooth). For completely arbitrary $\mathscr{U}$, the derivatives of F on $\mathscr{U}$ depend on the choice of extension $\tilde{F}$ (take for instance $\mathscr{U} = \{\varphi\}$ for some $\varphi \in \mathscr{F}_1$). However, if $\mathscr{U}$ happens to have a nonvoid interior, then it is easily shown that the derivatives of F on $\mathscr{U}$ do not depend on the choice of extension. Under certain conditions on F, one can weaken this condition (see, for instance, Remark 2.3.9).

A.4. Remark. For Mackey-complete locally convex topological vector spaces (also called *c^∞-complete* or *convenient* topological vector spaces), convenient smoothness enjoys essentially all the rules of Calculus presented in the remainder of this Appendix assuming MB differentiability (see e.g. footnote 11 below). Moreover, for Fréchet spaces (which are convenient and whose topology coincides with the corresponding c^∞-topology) convenient and MB smoothness coincide (see e.g. Theorem 1, pp. 77 of [39] together with Theorem 2.14, pp. 20–21 of [63]).

Let $\gamma : [a,b] \to \mathscr{F}$, $a < b \in \mathbb{R}$, be a continuous curve segment in the *complete* locally convex topological vector space $\mathscr{F}$. We can define the *(Riemann) integral* of γ along $[a,b]$

$$\int_a^b \gamma(\lambda)\mathrm{d}\lambda \in \mathscr{F}$$

as the unique linear map from the space $\mathscr{C}([a,b],\mathscr{F})$ of continuous curves from $[a,b]$ to $\mathscr{F}$ into the space $\mathscr{F}$ such that[11]:

(1) For any continuous linear functional $u : \mathscr{F} \to \mathbb{R}$, we have that $u\left(\int_a^b \gamma(\lambda)\mathrm{d}\lambda\right) = \int_a^b u(\gamma(\lambda))\mathrm{d}\lambda$;

(2) For any continuous seminorm $\|\cdot\|$ on $\mathscr{F}$, we have that $\left\|\int_a^b \gamma(\lambda)\mathrm{d}\lambda\right\| \leq \int_a^b \|\gamma(\lambda)\|\mathrm{d}\lambda$;

(3) If $a < c < b \in \mathbb{R}$, then $\int_a^b \gamma(\lambda)\mathrm{d}\lambda = \int_a^c \gamma(\lambda)\mathrm{d}\lambda + \int_c^b \gamma(\lambda)\mathrm{d}\lambda$.

The *Fundamental Theorem of Calculus* holds for the Riemann integral of curves taking values in $\mathscr{F}$:

A.5. Theorem ([45], Theorems 2.2.3 and 2.2.2). *Let $\gamma_0 : [a,b] \to \mathscr{F}$ be a continuous curve, $a \leq t \leq b$, and define $\gamma_1(t) \doteq \int_a^t \gamma_0(\lambda)\mathrm{d}\lambda$. Then $\gamma_1 : [a,b] \to \mathscr{F}$ is a $\mathscr{C}^1$ curve, and $\gamma_1'(t) = \gamma_0(t)$. Conversely, if $\gamma_1 : [a,b] \to \mathscr{F}$ is a $\mathscr{C}^1$ curve, then $\gamma_1(b) - \gamma_1(a) = \int_a^b \gamma_1'(\lambda)\mathrm{d}\lambda$.* □

[11] However, as argued e.g. in Proposition 2.7, pp. 17 of [63], if γ is Lipschitz (i.e. the subset $\{(t-s)^{-1}(\gamma(t) - \gamma(s)) \mid t \neq s\ ,\ a \leq t, s \leq b\}$ is bounded) then it suffices to assume that $\mathscr{F}$ is convenient to get the Riemann integral of γ along $[a,b]$ with all the properties discussed in this Appendix.

A.6. COROLLARY ([45], Theorem 3.2.2). *Let $F : \mathscr{U} \subset \mathscr{F}_1 \to \mathscr{F}_2$ be a continuous map with $\mathscr{F}_2$ complete, $\varphi_0 \in \mathscr{U}$, and $\vec{\varphi} \in \mathscr{U} - \varphi_0 \doteq \{\varphi - \varphi_0 \in \mathscr{F}_1 \mid \varphi \in \mathscr{U}\}$. Assume that $\mathscr{U}$ is convex for simplicity. If F is differentiable of order one in the sense of Definition A.3, then*

$$F(\varphi_0 + \vec{\varphi}) - F(\varphi_0) = \int_0^1 F^{(1)}[\varphi_0 + \lambda\vec{\varphi}](\vec{\varphi})\mathrm{d}\lambda \ . \tag{A.2}$$

□

With the aid of the fundamental theorem of Calculus A.5, the following key results can be proven. First, the usual linearity property for first-order derivatives holds:

A.7. LEMMA ([45], Lemma 3.2.3 and Theorem 3.2.5). *Let $F : \mathscr{U} \subset \mathscr{F}_1 \to \mathscr{F}_2$ be a continuous map with $\mathscr{F}_2$ complete, $\varphi \in \mathscr{U}$. If F is differentiable of order one in the sense of Definition A.3, then for all scalars λ, μ and all $\vec{\varphi}, \vec{\varphi}' \in \mathscr{F}_1$ we have that*

$$F^{(1)}[\varphi](\lambda\vec{\varphi} + \mu\vec{\varphi}') = \lambda F^{(1)}[\varphi](\vec{\varphi}) + \mu F^{(1)}[\varphi](\vec{\varphi}') \ .$$

□

Next, the *chain rule* holds:

A.8. THEOREM ([45], Theorem 3.3.4). *Let $F : \mathscr{U} \subset \mathscr{F}_1 \to \mathscr{F}_2$, $G : \mathscr{V} \subset \mathscr{F}_2 \to \mathscr{F}_3$ be respectively continuous maps from open subsets $\mathscr{U}, \mathscr{V}$ of locally convex topological vector spaces $\mathscr{F}_1, \mathscr{F}_2$ into $\mathscr{F}_2$ and the locally convex topological vector space $\mathscr{F}_3$, such that $F(\mathscr{U}) \subset \mathscr{V}$. Suppose that $\mathscr{F}_2$ and $\mathscr{F}_3$ are complete. If F (resp. G) is once differentiable on $\mathscr{U}$ (resp. $\mathscr{V}$) in the sense of Definition A.3, then for all $\varphi \in \mathscr{U}$, $\vec{\varphi} \in \mathscr{F}_1$ we have that*

$$(G \circ F)^{(1)}(\varphi)(\vec{\varphi}) = G^{(1)}[F(\varphi)](F^{(1)}[\varphi](\vec{\varphi})) \ . \tag{A.3}$$

□

The chain rule (A.3) yields, after taking direct sums, the *Leibniz's rule* for derivatives of composition of n-tuples of maps $F_1, \ldots, F_n$ with a continuous n-linear map ψ

$$(\psi(F_1, \ldots, F_n))^{(1)}[\varphi](\vec{\varphi}) = \sum_{j=1}^{n} \psi(F_1[\varphi], \ldots, F_j^{(1)}[\varphi](\vec{\varphi}), \ldots, F_n[\varphi]) \ . \tag{A.4}$$

This, together with the fundamental theorem of Calculus (A.2), yields the *integration by parts formula* and, even more importantly, *Taylor's formula with (integral) remainder*

$$F(\varphi_0 + \vec{\varphi}) = \sum_{j=0}^{k} \frac{1}{j!} F^{(j)}[\varphi_0](\vec{\varphi}, \ldots, \vec{\varphi}) + \int_0^1 \frac{(1-\lambda)^k}{k!} F^{(k+1)}[\varphi_0 + \lambda\vec{\varphi}](\vec{\varphi}, \ldots, \vec{\varphi})\mathrm{d}\lambda \ . \tag{A.5}$$

To see this, note that Leibniz's rule implies the following key formula:

$$\begin{aligned} \frac{(1-\lambda)^{k-1}}{(k-1)!} F^{(k)}[\varphi_0 + \lambda\vec{\varphi}](\vec{\varphi}, \ldots, \vec{\varphi}) &= \frac{(1-\lambda)^k}{k!} F^{(k+1)}[\varphi_0 + \lambda\vec{\varphi}](\vec{\varphi}, \ldots, \vec{\varphi}) \\ &\quad - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left[\frac{(1-\lambda)^k}{k!} F^{(k)}[\varphi_0 + \lambda\vec{\varphi}](\vec{\varphi}, \ldots, \vec{\varphi})\right] \ . \end{aligned} \tag{A.6}$$

Integrating both sides of formula (A.6) from $\lambda = 0$ to $\lambda = 1$ by means of the fundamental theorem of Calculus (A.2) yields the fundamental induction step from $k-1$ to k. Since the case $k = 0$ of (A.5) is settled by the fundamental theorem of Calculus itself, we are done.

For the convenience of the reader, we prove the generalization of the chain rule (A.3) for higher derivatives, since this proof is not easy to find in the literature at the present level of generality. We follow the argument employed in [56].

A.9. Corollary (Faà di Bruno's formula). *Let $F : \mathscr{U} \subset \mathscr{F}_1 \to \mathscr{F}_2$, $G : \mathscr{V} \subset \mathscr{F}_2 \to \mathscr{F}_3$ satisfy the hypotheses of Theorem A.8. If F (resp. G) is m-times differentiable on $\mathscr{U}$ (resp. $\mathscr{V}$), then $G \circ F$ is also m-times differentiable on $\mathscr{U}$, and for all $1 \leq k \leq m$,*

$$(G \circ F)^{(k)}[\varphi](\vec{\varphi}_1, \dots, \vec{\varphi}_k) = \sum_{\pi \in P_k} G^{(|\pi|)}[F(\varphi)] \left(\bigotimes_{I \in \pi} F^{(|I|)}[\varphi](\otimes_{j \in I} \vec{\varphi}_j) \right) , \tag{A.7}$$

where P_k is the set of all partitions $\pi = \{I_1, \dots, I_l\}$ of $\{1, \dots, k\}$, that is, $I_j \neq \varnothing$, $I_j \cap I_{j'} = \varnothing$ for $j \neq j'$ and $\cup_{j=1}^{l} I_j = \{1, \dots, k\}$.

Proof. We proceed by induction on k. The case $k = 1$ is just the usual chain rule (A.3). Assume that the formula is valid up to order $k-1$ along $\vec{\varphi}_1, \dots, \vec{\varphi}_{k-1}$. Then for each partition π of $\{1, \dots, k-1\}$ in the above sum we have, by Leibniz's rule (A.4),

$$\begin{aligned}
&\left[G^{(|\pi|)} \circ F \left(\bigotimes_{I \in \pi} F^{(|I|)}(\otimes_{j \in I} \vec{\varphi}_j) \right) \right]^{(1)} [\varphi](\vec{\varphi}_k) \\
&\qquad = G^{(|\pi|+1)}[F(\varphi)] \left(F^{(1)}[\varphi](\vec{\varphi}_k) \otimes \bigotimes_{I \in \pi} F^{(|I|)}[\varphi](\otimes_{j \in I} \vec{\varphi}_j) \right) \\
&\qquad + \sum_{I' \in \pi} G^{(|\pi|)}[F(\varphi)] \left(F^{(|I'|+1)}[\varphi] \left(\vec{\varphi}_k \otimes \bigotimes_{j \in I'} \vec{\varphi}_j \right) \otimes \bigotimes_{I \in \pi \smallsetminus \{I'\}} F^{(|I|)}[\varphi](\otimes_{l \in I} \vec{\varphi}_l) \right) .
\end{aligned}$$

However, any partition π' of $\{1, \dots, k\}$ is either of the form $\pi' = \{\{k\}\} \cup \pi$ or $\pi' = (\pi \smallsetminus \{I'\}) \cup \{I' \cup \{k\}\}$ for some $I' \in \pi$, $\pi \in P_{k-1}$. Hence, summing the above identities over all such π gives the desired result. ☐

A consequence of Faà di Bruno's formula (A.7) is the generalization of Leibniz's rule (A.4) for higher order derivatives of composition of l-tuples of maps $F_1, \dots, F_l$ with a continuous l-linear map ψ

$$(\psi(F_1, \dots, F_l))^{(k)}[\varphi]\,(\vec{\varphi}_1, \dots, \vec{\varphi}_k) = \sum_{\{I_1, \dots, I_l\} \in \tilde{P}_{k,l}} \psi \left(F_1^{(|I_1|)}[\varphi](\otimes_{j \in I_1} \vec{\varphi}_j), \dots, F_l^{(|I_l|)}[\varphi](\otimes_{j \in I_l} \vec{\varphi}_j) \right) , \tag{A.8}$$

where $\tilde{P}_{k,l}$ is the set of all partitions $\pi = \{I_1, \dots, I_l\}$ of $\{1, \dots, k\}$ in l *possibly (but not all) empty* subsets, i.e. $I_j \cap I_{j'} = \varnothing$ for $j \neq j'$ and $\cup_{j=1}^{l} I_j = \{1, \dots, k\}$. As another application, we obtain the so-called *k-th order resolvent formula* (A.12) below which shall often be useful. Consider two MB-differentiable maps $F : \mathscr{U} \times \mathscr{F}_1 \to \mathscr{F}_2$, $G : \mathscr{U} \times \mathscr{F}_2 \to \mathscr{F}_1$ of order one, where $\mathscr{F}_1, \mathscr{F}_2$ are locally convex topological vector spaces and $\mathscr{U} \subset \mathscr{F}$ is a nonvoid open subset of the locally convex topological vector space $\mathscr{F}$. For notational convenience, we also occasionally write $F(\varphi,\vec{\varphi}) \doteq F[\varphi]\vec{\varphi}$, $G(\varphi,\vec{\psi}) \doteq G[\varphi]\vec{\psi}$. Suppose that both F and G are *linear* in their second arguments and satisfy

$$\begin{aligned} F[\varphi]G[\varphi]\vec{\psi} &= \vec{\psi}\ , \quad \forall\varphi\in\mathscr{U}\ ,\ \vec{\psi}\in\mathscr{F}_2\ , \\ G[\varphi]F[\varphi]\vec{\varphi} &= \vec{\varphi}\ , \quad \forall\varphi\in\mathscr{U}\ ,\ \vec{\varphi}\in\mathscr{F}_1\ . \end{aligned} \tag{A.9}$$

If we define

$$D_1^kF[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\vec{\varphi} = F^{(k)}[\varphi,\vec{\varphi}]((\vec{\varphi}_1,0),\ldots,(\vec{\varphi}_k,0))\ ,\quad D_1^1\doteq D_1\ ,\ D_1^0=\mathbb{1}\ , \tag{A.10}$$

then by the chain rule (A.3) applied to the pair of maps $F,(\mathbb{1},G)$ and (A.9) we have the *(first-order) resolvent formula*

$$D_1G[\varphi](\vec{\varphi}_1)\vec{\psi} = -G[\varphi]D_1F[\varphi](\vec{\varphi}_1)G[\varphi]\vec{\psi}\ . \tag{A.11}$$

It follows from the above formula that if in addition F is MB-smooth, then so is G. More precisely, in this case we obtain the following (not so pleasant) higher-order generalization of (A.11), obtained by induction on $k\geq 1$ from (A.11) and an argument analogous to the one used in the proof of Corollary A.9:

(A.12)

$$D_1^kG[\varphi]\,(\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\,\vec{\psi} = \sum_{l=1}^{k}(-1)^l\sum_{\{I_1,\ldots,I_l\}\in P_k}\sum_{\sigma\in S_l}\left(\prod_{j=1}^{l}G[\varphi]D^{|I_{\sigma(j)}|}F[\varphi](\otimes_{i\in I_{\sigma(j)}}\vec{\varphi}_i)\right)G[\varphi]\vec{\psi}\ .$$

Here, P_k is again the set of all partitions of $\{1,\ldots,k\}$ as in the statement of Corollary A.9, whereas S_l is the set of all permutations of $\{1,\ldots,l\}$.

Finally, one can show that the order of differentiation for higher order derivatives is irrelevant:

A.10. Theorem ([45], Theorem 3.6.2). *Let $F:\mathscr{U}\subset\mathscr{F}_1\to\mathscr{F}_2$ be a continuous map with $\mathscr{F}_2$ complete. If F is differentiable of order $m>1$ in the sense of Definition A.3, then $F^{(k)}[\varphi]$: $\mathscr{F}_1^k\ni(\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\mapsto F^{(k)}[\varphi](\vec{\varphi}_1,\ldots,\vec{\varphi}_k)\in\mathscr{F}_2$ is a symmetric, k-linear map for all fixed $\varphi\in\mathscr{U}$, $2\leq k\leq m$.* □

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