Conservation of the stress tensor in perturbative interacting quantum field theory in curved spacetimes

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Abstract

We propose additional conditions (beyond those considered in our previous papers) that should be imposed on Wick products and time-ordered products of a free quantum scalar field in curved spacetime. These conditions arise from a simple "Principle of Perturbative Agreement": For interaction Lagrangians L_1 that are such that the interacting field theory can be constructed exactly—as occurs when L_1 is a "pure divergence" or when L_1 is at most quadratic in the field and contains no more than two derivatives—then time-ordered products must be defined so that the perturbative solution for interacting fields obtained from the Bogoliubov formula agrees with the exact solution. The conditions derived from this principle include a version of the Leibniz rule (or "action Ward identity") and a condition on time-ordered products that contain a factor of the free field φ or the free stress-energy tensor T_{ab}. The main results of our paper are (1) a proof that in spacetime dimensions greater than 2, our new conditions can be consistently imposed in addition to our previously considered conditions and (2) a proof that, if they are imposed, then for *any* polynomial interaction Lagrangian L_1 (with no restriction on the number of derivatives appearing in L_1), the stress-energy tensor Θ_{ab} of the interacting theory will be conserved. Our work thereby establishes (in the context of perturbation theory) the conservation of stress-energy for an arbitrary interacting scalar field in curved spacetimes of dimension greater than 2. Our approach requires us to view time-ordered products as maps taking classical field expressions into the quantum field algebra rather than as maps taking Wick polynomials of the quantum field into the quantum field algebra.

1 Introduction

In [13] and [14], we took an axiomatic approach toward defining Wick powers and time-ordered products of a quantum scalar field, φ, in curved spacetime. We provided a list of axioms that these quantities are required to satisfy (see conditions T1-T9 of [14] or section 2 below) and then succeeded in proving both their uniqueness (up to specified renormalization ambiguities) [13] and their existence [13, 14].

Our previous analysis restricted attention to the case where the Wick powers and the factors appearing in the time-ordered products do not contain derivatives of the scalar field φ. In fact, however, as we already noted in [13, 14], our uniqueness and existence results extend straightforwardly to the case where the Wick powers and the factors appearing in the time-ordered products are arbitrary polynomial expressions in φ and its derivatives[1]. We excluded the explicit consideration of expressions containing derivatives partly for simplicity but also because it was clear to us that additional axioms should be imposed on these quantities—and, consequently, stronger uniqueness and existence theorems should be proven—but it was not clear to us precisely what form these additional axioms should take. The main purpose of this paper is to provide these additional axioms, to investigate some of their consequences—most notably, conservation of the stress-energy of the interacting field—and to prove the desired stronger existence and uniqueness results for our new strengthened set of axioms.

Some simple examples should serve to illustrate the issues involved in determining what additional conditions should be imposed. One obvious possible requirement is the "Leibniz rule". Consider, for example, the Wick monomials φ^2 and $\varphi\nabla_a\varphi$ in $D = 4$ spacetime dimensions. The uniqueness theorem of [13] applies to both of these expressions. It establishes that the first is unique up to the addition of $c_1 R\mathbb{1}$, where c_1 is an arbitrary constant and R denotes the scalar curvature. Similarly, the second is unique up to the addition of $c_2\nabla_a R\mathbb{1}$, where c_2 is an independent arbitrary constant. However, it would be natural to require that

$$\nabla_a\varphi^2 = 2\varphi\nabla_a\varphi \tag{1}$$

where the left side denotes the distributional derivative of φ^2. If we wished to impose eq. (1), then we would need to strengthen our previous existence theorem to show that eq. (1) can be imposed in addition to our previous axioms. (This is easily done.) Our above uniqueness result would then be strengthened in that we would have $c_1 = 2c_2$, i.e, c_1 and c_2 would no longer be independent. Note that the Leibniz rule eq. (1) has an obvious generalization to arbitrary Wick polynomials, but it is not so obvious, a priori, what form the Leibniz rule should take on factors occurring in time-ordered products.

A second "obvious" requirement that one might attempt to impose on Wick polynomials and time-ordered products is that they respect the equations of motion of the free

[1] Axiom T9 was explicitly stated in [14] only for the case of expressions that do not contain derivatives. Its generalization to expressions with derivatives is given in section 2 below.

field φ. Consider the case of a massless Klein-Gordon field, so that $\nabla^a \nabla_a \varphi = 0$. Then it would seem natural to require the vanishing of any Wick monomial containing a factor of $\nabla^a \nabla_a \varphi$—such as the Wick monomials $\varphi \nabla^a \nabla_a \varphi$ and $(\nabla_b \varphi)(\nabla^a \nabla_a \varphi)$. Similarly, it would be natural to require the vanishing of any time-ordered product with the property that any of its arguments contains a factor of this form. However, it turns out that—as we will explicitly prove in section 3 below—it is *not* possible to impose this "wave equation" requirement together with the Leibniz rule requirement of the previous paragraph.

Should one impose the Leibniz rule or the free equations of motion (or neither of them) on Wick polynomials or time-ordered products? If the Leibniz rule is imposed, what form should it take for time-ordered products? Should any conditions be imposed in addition to the Leibniz rule or, alternatively, to the free equations of motion? In this paper, we will take the view that these and other similar questions should *not* be answered by attempting to make aesthetic arguments concerning properties of Wick polynomials and time-ordered products for the free field theory defined by the free Lagrangian L_0. Rather, we will consider the properties of the interacting quantum field theory defined by adding to L_0 an interaction Lagrangian density L_1, which may contain an arbitrary (but finite) number of powers of φ and its derivatives. As discussed in detail e.g., in section 3 of [15] (see also subsection 4.1 below), an arbitrary interacting quantum field Φ_{L_1} (with Φ denoting an arbitrary polynomial in φ and its derivatives) is defined perturbatively by the Bogoliubov formula, which expresses Φ_{L_1} in terms of the free-field time-ordered products with factors composed of Φ and L_1. The main basic idea of this paper is to invoke the following simple principle, which we will refer to as the "Principle of Perturbative Agreement": *If the interaction Lagrangian L_1 is such that the quantum field theory defined by the full Lagrangian $L_0 + L_1$ can be solved exactly, then the perturbative construction of the quantum field theory must agree with the exact construction.*

There are two separate cases in which this principle yields nontrivial conditions. The first is where the interaction Lagrangian corresponds to a pure "boundary term", i.e., in differential forms notation, the interaction Lagrangian is of the form $\mathrm{d}\, B$, where B is a smooth $(D-1)$-form of compact support depending polynomially on φ and its derivatives. Such an "interaction" produces an identically vanishing contribution to the action, and the interacting quantum field theory is therefore identical to the free theory. As we shall show in subsection 3.1, the imposition of the requirement that all perturbative corrections vanish for any interaction Lagrangian of the form $\mathrm{d}\, B$ precisely yields the Leibniz rule for Wick polynomials and yields a generalization of the Leibniz rule for time-ordered products. This generalization states that, in effect, derivatives can be freely commuted through the "time ordering". We will refer to this condition as the generalized Leibniz rule and will label it as "T10". Our condition T10 corresponds to the "action Ward identity" proposed in [18, 9] and proven recently in the context of flat spacetime theories in [10]. In order for condition T10 to be mathematically consistent, it is necessary that we adopt the viewpoint of [2] and [8]—which we already adopted in [15] for other reasons—that time-ordered products are maps from *classical* field expressions (on which the classical equations of motion are *not* imposed) into the quantum algebra of observables. This viewpoint and the reasons that necessitate its adoption are explained in detail in section 2. A proof that condition T10 can be consistently imposed in addition to conditions T1-T9 is given in subsection 3.1.

The second case where the above principle yields nontrivial conditions is where the interaction Lagrangian is at most quadratic in the field and contains a total of at most two derivatives. This includes interaction Lagrangians consisting of terms of the form $J\varphi$, $V\varphi^2$, and $h^{ab}\nabla_a\varphi\nabla_b\varphi$, corresponding to the presence of an external classical source, a spacetime variation of the mass, and a variation of the spacetime metric. In all of these cases, the exact quantum field algebra of the theory with Lagrangian $L_0 + L_1$ can be constructed directly, in a manner similar to the theory with Lagrangian L_0. Our demand that perturbation theory reproduce this construction yields new, nontrivial conditions on time-ordered products (which are most conveniently formulated in terms of retarded products). The general form of this requirement, which we label as "T11", is formulated in subsection 4.1. A useful infinitesimal version of this condition for the case of an external current interaction—which we label as condition T11a—is derived in subsection 4.2, and a corresponding infinitesimal version for the case of a metric variation—which we label as condition T11b—is derived in subsection 4.3.

The consequences of our additional conditions are investigated in section 5. The main results proven there—which also constitute some of the main results of this paper—are that our conditions imply the following: (i) The free stress-energy tensor, T_{ab}, in the free quantum theory must be conserved. (ii) For an *arbitrary* polynomial interaction Lagrangian, L_1, (a) the interacting quantum field φ_{L_1} always satisfies the interacting equations of motion and (b) the interacting stress-energy tensor, $\Theta^{ab}_{L_1}$, of the interacting theory always is conserved. This is rather remarkable in that, a priori, one might have expected properties (i) and (ii) to be entirely independent of conditions T1-T11. Indeed, one might have expected that if one required that (i) and (ii) be satisfied in perturbation theory, one would obtain a further set of requirements on Wick polynomials and time-ordered products. The fact that no additional conditions are actually needed provides confirmation that T10 and T11 are the appropriate conditions that are needed to supplement our original conditions T1-T9. In effect, the analysis of section 5 shows the following: Suppose that the definition of time-ordered products satisfies T1-T10. Then, if the definition of time-ordered products is further adjusted, if necessary, so that in perturbation theory the quantum field satisfies the correct field equation in the presence of an arbitrary classical current source J (as required by T11a), then the interacting field also will satisfy the correct field equation for an arbitrary self-interaction. Furthermore, if, in perturbation theory, the stress-energy tensor remains conserved in the presence of an arbitrary metric variation (as is a consequence of T11b), it also will remain conserved in the presence of an arbitrary self-interaction.

Finally, in section 6, we prove that condition T11a and—in spacetimes of dimension $D > 2$—condition T11b can be consistently imposed, in addition to conditions T1-

T10. The proof that condition T11a can be consistently imposed is relatively straightforward, and is presented in subsection 6.1. The proof that condition T11b also can be imposed when $D > 2$ is much more complex technically, and is presented in the seven sub-subsections of 6.2. Despite its complexity, the proof is logically straightforward except for a significant subtlety that is treated in sub-subsection 6.2.6. Here we find that a potential obstruction to satisfying T11b arises from the requirement that time-ordered-products containing more than one factor of the stress-energy tensor be symmetric in these factors. We show that this potential obstruction does not actually occur for the theory of a scalar field, as treated here. However, this need not be the case for other fields, and, indeed, it presumably is the underlying cause of the inability to impose stress-energy conservation in certain parity violating theories in curved spacetimes of dimension $D = 4k + 2$, as found in [1]. For scalar fields, we are thereby able to show that condition T11b can be consistently imposed in curved spacetimes of dimension $D > 2$. However, for $D = 2$ a further difficulty arises from the simple fact that the freedom to modify the definition of $\varphi\nabla_a\nabla_b\varphi$ by the addition of an arbitrary local curvature term does not give rise to a similar freedom to modify the definition of T_{ab}, and we find that, as a consequence, condition T11b cannot be satisfied for a scalar field in $D = 2$ dimensions.

It is our view that conditions T1-T11 provide the complete characterization of Wick polynomials and time-ordered products of a quantum scalar field in curved spacetime.

Notation and Conventions. Our notation and conventions generally follow those of our previous papers [13]-[15]. The spacetime dimension is denoted as D, and $(M, \mathbf{g})$ always denotes an oriented, globally hyperbolic spacetime. We denote by $\boldsymbol{\epsilon} = \sqrt{-\mathbf{g}}\, \mathrm{d}\, x^0 \wedge \cdots \wedge \mathrm{d}\, x^{D-1}$ the volume element (viewed as a D-form, or density of weight 1) associated with $\mathbf{g}$. Abstract index notation is used wherever it does not result in exceedingly many indices. However, abstract index notation is generally not used for $\mathbf{g} = g_{ab}$ and $\boldsymbol{\epsilon} = \epsilon_{ab...c}$.

2 The nature and properties of time-ordered products

2.1 The construction of the free quantum field algebra and the nature of time-ordered products

Consider a scalar field φ on an arbitrary globally hyperbolic spacetime, $(M, \mathbf{g})$, with classical action

$$S_0 = \int L_0 = -\frac{1}{2} \int (g^{ab}\nabla_a\varphi\nabla_b\varphi + m^2\varphi^2 + \xi R\varphi^2)\boldsymbol{\epsilon}. \tag{2}$$

The equations of motion derived from this action have unique fundamental advanced and retarded solutions $\Delta^{\mathrm{adv/ret}}(x,y)$ satisfying

$$(\nabla^a \nabla_a - m^2 - \xi R)\Delta^{\mathrm{adv/ret}} = \delta, \tag{3}$$

together with the support property

$$\operatorname{supp} \Delta^{\mathrm{adv/ret}} \subset \{(x,y) \in M \times M \mid x \in J^{-/+}(y)\}, \tag{4}$$

where $J^{-/+}(S)$ is the causal past/future of a set S in spacetime. Here we view the distribution kernel of $\Delta^{\mathrm{adv/ret}}$ as undensitized, i.e., acting on test *densities* rather than *scalar* test functions[2], i.e., we view $\Delta^{\mathrm{adv/ret}}$ as a linear map from compactly supported, smooth *densities* to smooth *scalar* functions.

The quantum theory of the field φ is defined by constructing a suitable *-algebra of observables as follows: We start with the free *-algebra with identity $\mathbb{1}$ generated by the formal expressions $\varphi(f)$ and $\varphi(h)^*$ where f, h are smooth compactly supported densities on M. Now factor this free *-algebra by the following relations:

(i) $\varphi(\alpha_1 f_1 + \alpha_2 f_2) = \alpha_1 \varphi(f_1) + \alpha_2 \varphi(f_2)$, with $\alpha_1, \alpha_2 \in \mathbb{C}$;

(ii) $\varphi(f)^* = \varphi(\bar{f})$;

(iii) $\varphi((\nabla^a \nabla_a - m^2 - \xi R)f) = 0$; and

(iv) $\varphi(f_1)\varphi(f_2) - \varphi(f_2)\varphi(f_1) = \mathrm{i}\Delta(f_1, f_2)\mathbb{1}$, where Δ denotes the causal propagator for the Klein-Gordon operator,

$$\Delta = \Delta^{\mathrm{adv}} - \Delta^{\mathrm{ret}}. \tag{5}$$

We refer to the algebra, $\mathcal{A}(M, \mathbf{g})$, defined by relations (i)–(iv) as the CCR-algebra (for "canonical commutation relations"). Quantum states on the CCR-algebra $\mathcal{A}$ are simply linear maps ω from $\mathcal{A}$ into $\mathbb{C}$ that are normalized in the sense that $\omega(\mathbb{1}) = 1$ and that are positive in the sense that $\omega(a^* a)$ is non-negative for any $a \in \mathcal{A}$. This algebraic notion of a quantum state corresponds to the usual notion of a state as a normalized vector in a Hilbert space as follows: Given a representation, π, of $\mathcal{A}$ on a Hilbert space, $\mathcal{H}$, (so that each $a \in \mathcal{A}$ is represented as a linear operator $\pi(a)$ on $\mathcal{H}$), then any normalized vector state $|\psi\rangle \in \mathcal{H}$ defines a state ω in the above sense via taking expectation values, $\omega(a) = \langle \psi | \pi(a) | \psi \rangle$. Conversely, given a state, ω, the GNS construction establishes that one always can find a Hilbert space, $\mathcal{H}$, a representation, π of $\mathcal{A}$ on $\mathcal{H}$, and a vector $|\psi\rangle \in \mathcal{H}$ such that $\omega(a) = \langle \psi | \pi(a) | \psi \rangle$.

By construction, the only observables contained in $\mathcal{A}$ are the correlation functions of the quantum field φ. Even if we were only interested in considering the free quantum

[2]Consequently, the delta-distribution in eq. (3) is also undensitized.

field defined by the action eq. (2), there are observables of interest that are not contained in $\mathcal{A}$, such as the stress-energy tensor of the quantum field

$$T^{ab} = 2\boldsymbol{\epsilon}^{-1}\frac{\delta L_0}{\delta g_{ab}} = \nabla^a\varphi\nabla^b\varphi - \frac{1}{2}g^{ab}\nabla^c\varphi\nabla_c\varphi - \frac{1}{2}g^{ab}m^2\varphi^2 + \xi[G^{ab}\varphi^2 - 2\nabla^a(\varphi\nabla^b\varphi) + 2g^{ab}\nabla^c(\varphi\nabla_c\varphi)]. \quad (6)$$

We will refer to any polynomial expression, Φ, in φ and its derivatives as a "Wick polynomial". All Wick polynomials, such as T_{ab}, that involve quadratic or higher order powers of φ are intrinsically ill defined on account of the distributional character of φ. It is natural, however, to try to interpret Wick polynomials as arising from "unsmeared" elements of $\mathcal{A}$ that are then made well defined via some sort of "regularization" procedure. In Minkowski spacetime, a suitable regularization is accomplished by "normal ordering", which can be interpreted in terms of a subtraction of expectation values in the Minkowski vacuum state. However, in curved spacetime, regularization via "vacuum subtraction" is, in general, neither available (since there will, in general, not exist a unique, preferred "vacuum state") nor appropriate (since the resulting Wick polynomials will fail to be local, covariant fields [13]).

The necessity of going beyond observables in $\mathcal{A}$ becomes even more clear if one attempts to construct the theory of a self-interacting field (with a polynomial self-interaction) in terms of a perturbation expansion off of a free field theory. First, the interaction Lagrangian, L_1, itself will be a Wick polynomial and thereby corresponds to an observable that does not lie in $\mathcal{A}$. Second, the nth order perturbative corrections to φ—or, more generally, the nth order perturbative corrections to any Wick monomial Φ—are formally given by the Bogoliubov formula (see eq. (91) below), which expresses the Wick monomial Φ_{L_1}, for the interacting field as a sum of Φ and correction terms involving the "time-ordered products" of expressions containing one factor of Φ and n factors of L_1. For the case of two Wick monomials, Φ_1 and Φ_2, the time-ordered product is formally given by

$$\mathscr{T}(\Phi_1(x_1)\Phi_2(x_2)) = \vartheta(x_1^0 - x_2^0)\Phi_1(x_1)\Phi_2(x_2) + \vartheta(x_2^0 - x_1^0)\Phi_2(x_2)\Phi_1(x_1) \quad (7)$$

where ϑ denotes the step function. (The formal generalization of eq. (7) to time-ordered products with n-arguments is straightforward.) However, even if Wick monomials have been suitably defined, the time-ordered product (7) is not well defined since the Wick monomials also have a distributional character, and taking their product with a step function is, in general, ill defined. Nevertheless, in Minkowski spacetime, time-ordered products can be defined by well known renormalization procedures.

Thus, the perturbative construction of the quantum field theory of an interacting field requires the definition of Wick polynomials and time-ordered products, both of which necessitate enlarging the algebra of observables beyond the original CCR-algebra, $\mathcal{A}$. These steps were successfully carried out in [13, 14], based upon prior results obtained in [4, 5]. The first key step is to construct an algebra of observables, $\mathcal{W}(M, \mathbf{g})$, which is large enough to contain all Wick polynomials and time-ordered products. To do so, consider the following expressions in $\mathcal{A}(M, \mathbf{g})$:

$$\begin{aligned} W_n(u) &= \int u(x_1, \dots, x_n) :\prod_i^n \varphi(x_i) :_\omega \\ &\equiv \int u(x_1, \dots, x_n) \frac{\delta^n}{\mathrm{i}^n \delta f(x_1) \cdots \delta f(x_n)} e^{\mathrm{i}\varphi(f) + \frac{1}{2}\omega_2(f,f)} \Big|_{f=0}, \quad u \in C_0^\infty \end{aligned} \tag{8}$$

where ω_2 is the two-point function of an arbitrarily chosen Hadamard state. Thus, ω_2 is a distribution on $M \times M$ with antisymmetric part equal to $(\mathrm{i}/2)\Delta$, satisfying the spectrum condition given in eq. (31) and satisfying the Klein-Gordon equation in each entry, i.e., $(P \otimes 1)\omega_2 = 0 = (1 \otimes P)\omega_2$ where P is the Klein-Gordon operator associated with L_0,

$$P = \nabla^a \nabla_a - m^2 - \xi R. \tag{9}$$

It follows from the above relations (i)–(iv) in the CCR-algebra that $W_n(u)^* = W_n(\bar{u})$, and that

$$W_n(u) \cdot W_m(u') = \sum_{2k \le m+n} W_{n+m-2k}(u \otimes_k u'), \tag{10}$$

where the "k-times contracted tensor product" $\otimes_k$ is defined by

$$\begin{aligned} (u \otimes_k u')(x_1, \dots, x_{n+m-2k}) \stackrel{\text{def}}{=} \mathbf{S} \frac{n!m!}{(n-k)!(m-k)!k!} \int_{M^{2k}} u(y_1, \dots, y_k, x_1, \dots, x_{n-k}) \times \\ u'(y_{k+1}, \dots, y_{k+i}, x_{n-k+1}, \dots, x_{n+m-2k}) \prod_{i=1}^k \omega_2(y_i, y_{k+i}) \, \boldsymbol{\epsilon}(y_i) \boldsymbol{\epsilon}(y_{k+i}) \end{aligned} \tag{11}$$

where $\mathbf{S}$ denotes symmetrization in $x_1, \dots, x_{n+m-2k}$. If either $m < k$ or $n < k$, then the contracted tensor product is defined to be zero. The above product formula can be recognized as Wick's theorem for normal ordered products. The enlarged algebra $\mathcal{W}(M, \mathbf{g})$ is now obtained by allowing not only compactly supported smooth functions $u \in C_0^\infty$ as arguments of $W_n(u)$ but more generally any *distribution* u in the space

$$\mathcal{E}_n(M, \mathbf{g}) = \{u \in \mathcal{D}'(M^n) \mid \mathrm{WF}(u) \cap (V^+)^n = \mathrm{WF}(u) \cap (V^-)^n = \emptyset\}. \tag{12}$$

Here, $V^{+/-} \subset T^*M$ is the union of all future resp. past lightcones in the cotangent space over M, and $\mathrm{WF}(u)$ is the wave front [16] set of a distribution u. The key point is that Hadamard property of ω_2 and the wave front set condition on the u and u' imposed in the definition of the spaces $\mathcal{E}'_n(M, \mathbf{g})$ is necessary and sufficient in order to show that the distribution products appearing in the contracted tensor product are well-defined and give a distribution in the desired class $\mathcal{E}'_{m+n-2k}(M, \mathbf{g})$. Note that the definition of the algebra $\mathcal{W}(M, \mathbf{g})$ a priori depends on the choice of ω_2. However, it can be shown [13] that different choices give rise to *-isomorphic algebras. Thus, as an abstract algebra, $\mathcal{W}(M, \mathbf{g})$ is independent of the choice of ω_2.

Although the algebra $\mathcal{W}(M, \mathbf{g})$ is "large enough" to contain all Wick polynomials and time-ordered products, the above construction does not determine which elements of $\mathcal{W}(M, \mathbf{g})$ correspond to given Wick polynomials or time-ordered products. (In particular, the normal-ordered quantities W_n, eq. (8), with u taken to be a smooth function of one variable times a delta-function, clearly do not provide an acceptable definition of Wick powers, since they fail to define local, covariant fields [13].) In [13, 14], an axiomatic approach was then taken to determine which elements of $\mathcal{W}$ correspond to given Wick polynomials and time-ordered products. In other words, rather than attempting to define Wick polynomials and time-ordered products by the adoption of some particular regularization scheme, we provided a list of properties that these quantities should satisfy. We proved the existence of Wick polynomials and time-ordered products satisfying these properties and also proved their uniqueness up to expected renormalization ambiguities. As already discussed in the previous section, one of the main purposes of the present paper is to supplement this list of axioms with additional conditions applicable to Wick polynomials and time-ordered products containing derivatives, and to prove correspondingly stronger existence and uniqueness theorems.

We will shortly review the axioms that we previously gave in [13, 14]. However, before doing so, we shall explain a subtle but important shift in our viewpoint on the nature of Wick polynomials and time-ordered products.

A Wick polynomial is a distribution, valued in the quantum field algebra $\mathcal{W}$ that corresponds to a polynomial expression in the classical field φ and its derivatives. It is therefore natural to consider the classical algebra, $\mathcal{C}_{\text{class}}$, of real polynomial expressions in the (unsmeared) classical field $\varphi(x)$ and its derivatives, where we impose all of the normal rules of algebra (such as the associative, commutative, and distributive laws) and tensor calculus (such as the Leibniz rule) to the expressions in $\mathcal{C}_{\text{class}}$, and, in addition, we impose the wave equation on φ, i.e., we set $(\nabla^a \nabla_a - m^2 - \xi R)\varphi(x) = 0$. It would then be natural to view Wick polynomials as maps from $\mathcal{C}_{\text{class}}$ into distributions with values in $\mathcal{W}$. However, this viewpoint on Wick polynomials is, in general, inconsistent because of the existence of anomalies. Indeed, we already mentioned in the introduction that—as we will explicitly show in section 3.2 below—under our other assumptions, it will not be consistent to set to zero all Wick monomials containing a factor of $(\nabla^a \nabla_a - m^2 - \xi R)\varphi(x)$, even though elements of $\mathcal{C}_{\text{class}}$ that contain such a factor vanish.

This difficulty has a simple remedy: We can instead define a classical field algebra of polynomial expressions in the unsmeared field $\varphi(x)$ and its derivatives where we no longer impose the wave equation. More precisely, let $\mathcal{V}_{\text{class}}$ denote the real vector space of all classical polynomial tensor expressions[3] involving φ, its symmetrized covariant derivatives[4] $(\nabla)^k\varphi$, the metric, and arbitrary curvature tensors C,

$$\mathcal{V}_{\text{class}} = \text{span}_{\mathbb{R}}\{\Phi = C \cdot (\nabla)^{r_1}\varphi \cdots (\nabla)^{r_k}\varphi; \quad k, r_i \in \mathbb{N}\}. \tag{13}$$

where, as in the case of $\mathcal{C}_{\text{class}}$, we impose all of the normal rules of algebra and tensor calculus to the expressions in $\mathcal{V}_{\text{class}}$ but now we do *not* impose the field equation associated with L_0. We denote a generic monomial element in $\mathcal{V}_{\text{class}}$ by the capital greek letter Φ.

We also introduce the space $\mathcal{F}_{\text{class}}$ of all *classical* D-form functionals of the metric $\mathbf{g}$, the field φ and its derivatives, depending in addition on compactly supported (complex) tensor fields f,

$$\begin{aligned}\mathcal{F}_{\text{class}} = \text{span}\{A(x) = \boldsymbol{\epsilon}(x)\nabla^{c_1}\cdots\nabla^{c_m} f^{a_1\dots a_r}(x)\Phi_{a_1\dots a_r c_1\dots c_m}(x) \mid \\ f \text{ smooth, comp. supported tensor field on } M; \Phi \text{ a monomial in} \mathcal{V}_{\text{class}}\}.\end{aligned} \tag{14}$$

Again, we do not assume in the definition of $\mathcal{F}_{\text{class}}$ that the classical equations of motion for φ hold. In particular, we do *not* assume that expressions such as $f(\nabla^a\nabla_a - \xi R - m^2)\varphi$ are set to zero. We will often suppress the tensor indices and write a classical D-form functional $A \in \mathcal{F}_{\text{class}}$ simply as

$$A = f\Phi \in \mathcal{F}_{\text{class}}, \tag{15}$$

or $A = [(\nabla)^k f]\Phi$, if we want to emphasize that the functional depends on derivatives of f. We then view the Wick polynomials as linear maps from $\mathcal{F}_{\text{class}}$ into $\mathcal{W}$.

Following [2] and [8], we previously explicitly adopted the above viewpoint on Wick polynomials in [15]. This viewpoint does not constitute a significant departure from standard viewpoints, but merely provides a clearer framework for discussing anomalies. However, as we shall now explain, our viewpoint on time-ordered products—which corresponds to the viewpoint taken in [9]—does constitute a significant departure from viewpoints that are commonly taken.

As indicated above (see eq. (7)), it would appear natural to view the time-ordered product, $\mathscr{T}$, in n-factors as a multilinear map taking Wick polynomials into $\mathcal{W}$. Indeed, our previous papers [13]-[15] contain the phrase "Wick powers and their time-ordered products" in many places. However, the untenability of this view can be seen from the following simple example. Consider the quantum field theory defined by the classical Lagrangian density $L = L_0 + L_1$, with

$$L_1 = fP\varphi\boldsymbol{\epsilon} \tag{16}$$

[3]The coefficients of these polynomial expressions may have arbitrary polynomial dependence on the dimensionful parameter m^2 and may have arbitrary analytic dependence on the dimensionless parameter ξ. However, we will not normally explicitly write these possible dependences on the parameters appearing in the theory.

[4]The notation $(\nabla)^k t_{bc\dots d}$ is a shorthand for the symmetrized k-th derivative of a tensor, $\nabla_{(a_1}\cdots\nabla_{a_k)}t_{bc\dots d}$. We may write any expression containing k derivatives of a tensor field $t_{bc\dots d}$ in terms of symmetrized derivatives of $t_{bc\dots d}$ of kth and lower order and curvature.

for some smooth function, f, of compact support, where P stands for the Klein-Gordon operator associated with L_0, eq. (9). The classical equations of motion arising from the Lagrangian L are simply

$$P\varphi = Pf \tag{17}$$

i.e., φ satisfies the inhomogeneous wave equation with smooth source $J = Pf$. Clearly, the interacting quantum field, φ_{L_1}, also should satisfy the inhomogeneous wave equation with source $J = Pf\mathbb{1}$. By inspection, it follows that φ_{L_1} should be given in terms of the free quantum field φ by

$$\varphi_{L_1} = \varphi + f\mathbb{1} \tag{18}$$

Note that this interacting quantum field theory has a trivial S-matrix (since $\varphi_{L_1} = \varphi$ outside of the support of f), but the local field φ_{L_1} is, of course, affected by f in the region where $f \neq 0$.

Now compare eq. (18) with what is obtained from perturbation theory. As already noted above, in perturbation theory, φ_{L_1} is equal to the free quantum field $\varphi(x)$, plus a sum of corrections terms, where the n-th order correction term involves the quantity

$$\int \mathscr{T}\left(\varphi(x)\prod_{i=1}^{n} P\varphi(y_i)\right) f(y_1)\dots f(y_n)\boldsymbol{\epsilon}(y_1)\dots\boldsymbol{\epsilon}(y_n). \tag{19}$$

Since $P\varphi = 0$, it would appear that perturbation theory yields $\varphi_{L_1} = \varphi$ rather than eq. (18). Consequently, we are put in the position of having to choose (at least) one of the following three possibilities: (1) The exact solution (18) for the interacting field is wrong. (2) The Bogoliubov formula for the interacting quantum field is wrong, at least in the case of interactions involving derivatives of the field. (3) The time-ordered product eq. (19) can be nonvanishing even though the Wick monomial $P\varphi$ vanishes. In our view, choices (1) and (2) are far more unacceptable than (3), and we therefore choose option (3). The results of this paper (specifically, the existence theorem of section 6), will establish that it is mathematically consistent to make this choice.

Thus, we do *not* view the time-ordered products (with n factors) as an n-times multilinear map on Wick polynomials but rather as an n-times multilinear map

$$\mathscr{T}_{\mathbf{g}} : \underbrace{\mathcal{F}_{\text{class}} \times \cdots \times \mathcal{F}_{\text{class}}}_{n \text{ factors}} \to \mathcal{W}(M, \mathbf{g}), \tag{20}$$

$$(f_1\Phi_1, \dots, f_n\Phi_n) \to \mathscr{T}_{\mathbf{g}}\left(\prod_{i=1}^{n} f_i\Phi_i\right). \tag{21}$$

We note that, for a fixed choice of monomials $\Phi_i \in \mathcal{V}_{\text{class}}$, we get a multilinear functional $(f_1, \dots, f_n) \to \mathscr{T}(\prod^n f_j\Phi_j)$ mapping test functions on M to the algebra $\mathcal{W}$. In the following, we will sometimes use the more suggestive informal integral notation[5]

$$\mathscr{T}\left(\prod_{i=1}^{n} f_i\Phi_i\right) = \int \mathscr{T}(\Phi_1(x_1)\cdots\Phi_n(x_n))f_1(x_1)\cdots f_n(x_n) \tag{22}$$

for this multi-linear map. Note that this notation is exactly analogous to the usual informal integral notation for distributions $u(f) = \int u(x)f(x)$ acting on test densities f. The Wick monomials are simply time-ordered products with a single factor, and we will use the notation

$$\mathscr{T}(f\Phi) = \Phi(f) = \int \Phi(x)f(x). \tag{23}$$

for these objects. Note, however, we will *not* use the much more standard notation $\mathscr{T}(\prod^n \Phi_i(f_i))$ for time-ordered products, since this would suggest that the time-ordered products are functions of the Wick monomials $\Phi_j(f_j)$ rather than of the classical functionals $f_j\Phi_j$ of the field φ.

We turn now to a review of the properties satisfied by time-ordered products.

2.2 Properties of time ordered products: Axioms T1-T9

In [14], we imposed a list of requirements on time-ordered products. Since a time-ordered product in a single factor is just a Wick polynomial, these requirements on time-ordered products also apply to Wick polynomials. In addition, Wick polynomials are further restricted by the requirement that if $A \in \mathcal{F}_{\rm class}$ is independent of φ, i.e., if A is of the form

$$A = (\nabla)^m f C \boldsymbol{\epsilon} \tag{24}$$

for some test tensor field f and some monomial C in the Riemann tensor and its derivatives, then the corresponding Wick polynomial is given by

$$\mathscr{T}(A) = \int_M (\nabla)^m f C\boldsymbol{\epsilon} \cdot \mathbb{1}, \tag{25}$$

where $\mathbb{1}$ is the identity element in $\mathcal{W}$. Similarly, if $A = f\varphi$, then we require that

$$\mathscr{T}(f\varphi) = \varphi(f), \tag{26}$$

where $\varphi(f)$ is the free quantum field, i.e., the algebra element in $\mathcal{W}$ obeying the relations (i)–(iv) above.

For the convenience of the reader, we now provide the list of axioms given in [14]. We refer the reader to [13] and [14] for further discussion of the motivation for these conditions as well as further discussion of their meaning and implications.

[5] Note that we do not need to specify an integration element in the formula below since the quantities $f_i\Phi_i$ already have the character of a density.

T1 Locality/Covariance. The time ordered products are local, covariant fields, in the following sense. Consider an isometric embedding χ of a spacetime $(M', \mathbf{g}')$ into a spacetime $(M, \mathbf{g})$ (i.e., $\mathbf{g}' = \chi^*\mathbf{g}$) preserving the causality structure, and let $\alpha_\chi : \mathcal{W}(M', \mathbf{g}') \to \mathcal{W}(M, \mathbf{g})$ be the corresponding algebra homomorphism. Then time ordered products are required to satisfy

$$\alpha_\chi \left[\mathscr{T}_{\mathbf{g}'} \left(\prod f_i \Phi_i \right) \right] = \mathscr{T}_{\mathbf{g}} \left(\prod (\chi_* f_i) \Phi_i \right). \tag{27}$$

Here, $\chi_* f$ denotes the compactly supported tensor field on M obtained by pushing forward the compactly supported tensor f field on N via the map χ. [For example, $\chi_* f(x) = f(\chi^{-1}(x))$ if f is scalar and x in the image of χ.] In particular, for the (scalar) Wick products, the requirement reads

$$\alpha_\chi \left[\Phi_{\mathbf{g}'}(x) \right] = \Phi_{\mathbf{g}}(\chi(x)) \quad \text{for all } x \in M'. \tag{28}$$

T2 Scaling. The time ordered products scale "almost homogeneously" under rescalings $\mathbf{g} \to \lambda^{-2}\mathbf{g}$ of the spacetime metric in the following sense. Let $\mathscr{T}_{\mathbf{g}}$ be a local, covariant time ordered product with n factors, and let $\mathcal{S}_\lambda \mathscr{T}_{\mathbf{g}}$ be the rescaled local, covariant field given by $\mathcal{S}_\lambda \mathscr{T}_{\mathbf{g}} \equiv \lambda^{-Dn} \sigma_\lambda T_{\lambda^{-2}\mathbf{g}}$, where $\sigma_\lambda : \mathcal{W}(M, \lambda^{-2}\mathbf{g}) \to \mathcal{W}(M, \mathbf{g})$ is the canonical isomorphism defined in lemma 4.2 of [13]. The scaling requirement on the time ordered product is then that there is some N such that

$$\frac{\partial^N}{\partial^N \ln \lambda} \lambda^{-d_T} \mathcal{S}_\lambda \mathscr{T}_{\mathbf{g}} = 0. \tag{29}$$

Here, d_T is the engineering dimension of the time-ordered product, defined as[6] $d_T = \sum d_{\Phi_i}$, with

$$\begin{aligned} d_\Phi \quad = \quad & \frac{(D-2)}{2} \times \#(\text{factors of } \varphi) + \#(\text{derivatives}) + 2 \times \#(\text{factors of curvature}) \\ & + \#(\text{“up” indices}) - \#(\text{“down” indices}), \end{aligned} \tag{30}$$

where D is the dimension of the spacetime M.

T3 Microlocal Spectrum condition. Let ω be any continuous state on $\mathcal{W}(M, \mathbf{g})$, so that, as shown in [12], ω has smooth truncated n-point functions for $n \neq 2$ and a two-point function $\omega_2(f_1, f_2) = \omega(\varphi(f_1)\varphi(f_2))$ of Hadamard from, i.e., $\mathrm{WF}(\omega_2) \subset \mathcal{C}_+(M, \mathbf{g})$, where

$$\mathcal{C}_+(M, \mathbf{g}) = \{(x_1, k_1; x_2, -k_2) \in T^*M^2 \setminus \{0\} \mid (x_1, k_1) \sim (x_2, k_2); k_1 \in (V^+)_{x_1}\}. \tag{31}$$

[6] The rule for assigning an engineering dimension to a field is obtained by requiring that the classical action be invariant under scaling. Formula (30) holds only for scalar field theory, i.e., in other theories, the dimension of the basic field(s) may be different from $(D-2)/2$.

Here the notation $(x_1, k_1) \sim (x_2, k_2)$ means that x_1 and x_2 can be joined by a null-geodesic and that k_1 and k_2 are cotangent and coparallel to that null-geodesic. $(V^+)_x$ is the future lightcone at x. Furthermore, let

$$\omega_{\mathscr{T}}(x_1, \dots, x_n) = \omega \left[\mathscr{T} \left(\prod_{i=1}^{n} \Phi_i(x_i) \right) \right]. \tag{32}$$

Then we require that

$$\mathrm{WF}(\omega_{\mathscr{T}}) \subset \mathcal{C}_{\mathscr{T}}(M, \mathbf{g}), \tag{33}$$

where the set $\mathcal{C}_{\mathscr{T}}(M, \mathbf{g}) \subset T^*M^n \setminus \{0\}$ is described as follows (we use the graphological notation introduced in [4, 5]): Let $G(p)$ be a "decorated embedded graph" in $(M, \mathbf{g})$. By this we mean an embedded graph $\subset M$ whose vertices are points $x_1, \dots, x_n \in M$ and whose edges, e, are oriented null-geodesic curves. Each such null geodesic is equipped with a coparallel, cotangent covectorfield p_e. If e is an edge in $G(p)$ connecting the points x_i and x_j with $i < j$, then $s(e) = i$ is its source and $t(e) = j$ its target. It is required that p_e is future/past directed if $x_{s(e)} \notin J^\pm(x_{t(e)})$. With this notation, we define

$$\begin{aligned} \mathcal{C}_{\mathscr{T}}(M, \mathbf{g}) \; = \; & \Big\{ (x_1, k_1; \dots; x_n, k_n) \in T^*M^n \setminus \{0\} \mid \exists \text{ decorated graph } G(p) \text{ with vertices} \\ & x_1, \dots, x_n \text{ such that } k_i = \sum_{e: s(e) = i} p_e - \sum_{e: t(e) = i} p_e \quad \forall i \Big\}. \end{aligned} \tag{34}$$

T4 Smoothness. The functional dependence of the time ordered products on the spacetime metric, $\mathbf{g}$, is such that if the metric is varied smoothly, then the time ordered products vary smoothly, in the following sense. Consider a family of metrics $\mathbf{g}^{(s)}$ depending smoothly upon a set of parameters s in a parameter space $\mathcal{P}$. Furthermore, let $\omega^{(s)}$ be a family of Hadamard states with smooth truncated n-point functions ($n \neq 2$) depending smoothly on s and with two-point functions $\omega_2^{(s)}$ depending smoothly on s in the sense that, when viewed as a distribution jointly in (s, x_1, x_2), we have

$$\mathrm{WF}(\omega_2^{(s)}) \subset \{(s, \rho; x_1, k_1; x_2, k_2) \in T^*(\mathcal{P} \times M^2) \setminus \{0\} \mid (x_1, k_1; x_2, k_2) \in \mathcal{C}_+(M, \mathbf{g}^{(s)})\}, \tag{35}$$

where the family of cones $\mathcal{C}_+(M, \mathbf{g}^{(s)})$ is defined by eq. (31) in terms of the family $\mathbf{g}^{(s)}$. Then we require that the family of distributions given by

$$\omega_{\mathscr{T}}^{(s)}(x_1, \dots, x_n) = \omega^{(s)} \left[\mathscr{T}_{\mathbf{g}^{(s)}} \left(\prod_{i=1}^{n} \Phi_i(x_i) \right) \right] \tag{36}$$

(viewed as distributions in the variables $(s, x_1, \dots, x_n)$) depends smoothly on s with respect to the sets $\mathcal{C}_{\mathscr{T}}(M, \mathbf{g}^{(s)})$ defined in eq. (34), in the sense that

$$\begin{aligned} \mathrm{WF}(\omega_{\mathscr{T}}^{(s)}) \subset \{ & (s, \rho; x_1, k_1; \dots; x_n, k_n) \in T^*(\mathcal{P} \times M^n) \setminus \{0\} \mid \\ & (x_1, k_1; \dots; x_n, k_n) \in \mathcal{C}_{\mathscr{T}}(M, \mathbf{g}^{(s)})\}. \end{aligned} \tag{37}$$

We similarly demand that the time ordered products also have a smooth dependence upon the parameters m^2, ξ in the free theory.

T5 Analyticity. Similarly, we require that, for an analytic family of analytic metrics (depending analytically upon a set of parameters), the expectation value of the time-ordered products in an analytic family of states[7] varies analytically in the same sense as in T4, but with the smooth wave front set replaced by the analytic wave front set. We similarly demand an analytic dependence upon the the parameters m^2, ξ.

T6 Symmetry. The time ordered products are symmetric under a permutation of the factors.

T7 Unitarity. Let $\bar{\mathscr{T}}(\prod f_i \Phi_i) = [\mathscr{T}(\prod \bar{f}_i \Phi_i)]^*$, $\Phi_i \in \mathcal{V}_{\rm class}$, be the "anti-time-ordered" product. Then we require

$$\bar{\mathscr{T}}(f_1\Phi_1 \dots f_n\Phi_n) = \sum_{I_1 \sqcup \dots \sqcup I_j = \{1,\dots,n\}} (-1)^{n+j} \mathscr{T}\left(\prod_{i \in I_1} f_i \Phi_i\right) \dots \mathscr{T}\left(\prod_{j \in I_j} f_j \Phi_j\right), \tag{38}$$

where the sum runs over all partitions of the set $\{1, \dots, n\}$ into pairwise disjoint subsets $I_1, \dots, I_j$.

T8 Causal Factorization. For time ordered products with more than one factor, we require the following causal factorization rule, which reflects the time-ordering of the factors. Consider a set of test functions $(f_1, \dots, f_n)$ and a partition of $\{1, \dots, n\}$ into two non-empty disjoint subsets I and I^c, with the property that no point $x_i \in \operatorname{supp} f_i$ with $i \in I$ is in the past of any of the points $x_j \in \operatorname{supp} f_j$ with $j \in I^c$, that is, $x_i \notin J^-(x_j)$ for all $i \in I$ and $j \in I^c$. Then the corresponding time ordered product factorizes in the following way:

$$\mathscr{T}\left(\prod_{k=1}^{n} f_k \Phi_k\right) = \mathscr{T}\left(\prod_{i \in I} f_i \Phi_i\right) \mathscr{T}\left(\prod_{j \in I^c} f_j \Phi_j\right). \tag{39}$$

In the case of 2 factors, this requirement reads (in the informal notation introduced above)

$$\mathscr{T}(\Phi(x)\Psi(y)) = \begin{cases} \Phi(x)\Psi(y) & \text{when } x \notin J^+(y); \\ \Psi(y)\Phi(x) & \text{when } y \notin J^-(x). \end{cases} \tag{40}$$

[7] As explained in remark (2) on P. 311 of [13], it suffices to consider a suitable analytic family of linear functionals on $\mathcal{W}$ that do not necessarily satisfy the positivity condition required for states.

T9 Commutator. The commutator of a time-ordered product with a free field is given by lower order time-ordered products times suitable commutator functions, namely

$$\left[\mathscr{T}\left(\prod^{n} f_i\Phi_i\right), \varphi(F)\right] = \mathrm{i}\sum_{i=1}^{n}\mathscr{T}\left(f_1\Phi_1\dots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\dots f_n\Phi_n\right), \tag{41}$$

where $\Delta = \Delta^{\text{adv}} - \Delta^{\text{ret}}$ is the causal propagator (commutator function), and where we are using the notation $(\Delta F)(x) = \int_M \Delta(x,y)F(y)$ for the action of the causal propagator on a smooth *density* F of compact support[8]. Here, the functional derivative, $\delta A/\delta\varphi \in \mathcal{F}_{\text{class}}$, of an arbitrary element of $A \in \mathcal{F}_{\text{class}}$ is given by

$$\frac{\delta A}{\delta\varphi} = \sum_r (-1)^r \nabla_{(a_1}\cdots\nabla_{a_r)}\frac{\partial A}{\partial(\nabla_{(a_1}\cdots\nabla_{a_r)}\varphi)}. \tag{42}$$

This formula corresponds to the usual "Euler-Lagrange"-type expression familiar from the calculus of variations; see appendix B for further discussion.

Remark: In [14], condition T9 was explicitly stated only for the case where each Φ_i has no dependence on derivatives of φ. Equation (41) is the appropriate generalization to arbitrary Φ_i. For the case of a Wick power (i.e., a time-ordered product in one argument), eq. (41) can be motivated by the requirement of maintaining the desired relationship between Poisson-brackets and commutators.

The main results of [13] and [14] are that there exists a definition of time-ordered products that satisfies conditions T1-T9 and that, furthermore, this definition is unique up to the expected renormalization ambiguites. Our goal now is to impose additional conditions appropriate to time-ordered products whose factors Φ_i depend upon derivatives of φ, and to then prove the corresponding existence and uniqueness theorems. These additional conditions will arise from the following basic principle already stated in the introduction:

Principle of Perturbative Agreement: *If the interaction Lagrangian $L_1 = \sum_i f_i\Phi_i$ (where each f_i is smooth and of compact support and each $\Phi_i \in \mathcal{V}_{\text{class}}$) is such that the quantum field theory defined by the full Lagrangian $L_0 + L_1$ can be solved exactly, then the perturbative construction of the quantum field theory as defined by the Bogoliubov formula must agree with the exact construction.*

[8] As previously noted at the beginning of this section, when writing expressions like ΔF or likewise $\Delta^{\text{adv/ret}}F$, we take the point of view that the Green's functions are linear maps from smooth compactly supported *densities* on M to smooth *scalar* functions on M.

3 The Leibniz rule

3.1 Formulation of the Leibniz rule, T10, and proof of consistency with axioms T1-T9

Our first new requirement arises from considering a classical functional $A \in \mathcal{F}_{\text{class}}$ of the form

$$A = \mathrm{d}\, B, \tag{43}$$

where B is in the analog of the space $\mathcal{F}_{\text{class}}$ (see eq. (14)) but with "D-form" replaced by "$(D-1)$-form", and where d is the exterior differential (mapping $(D-1)$-forms to D-forms). An example of such a B is

$$B_{a_1 \dots a_{D-1}} = f^b \epsilon_{b a_1 \dots a_{D-1}} \Phi \tag{44}$$

where f^c is a test vector field and Φ is a scalar element of $\mathcal{V}_{\text{class}}$. The general such B would be of a similar form, except that Φ and f could have additional tensor indices, derivatives could act on f, and $\boldsymbol{\epsilon}$ could be contracted with an index of Φ rather than an index of f. For B of the form eq.(44), A would take the explicit form.

$$A = (\nabla^c f_c)\Phi \boldsymbol{\epsilon} + f_c \nabla^c \Phi \boldsymbol{\epsilon}, \tag{45}$$

Classically, the Lagrangian $L = L_0 + A$ defines the same theory as the Lagrangian L_0. Consequently, the "interacting" quantum field theory defined by the interaction Lagrangian $L_1 = A$ should coincide with the free quantum field theory, i.e., all of the perturbative corrections should vanish for an interaction Lagrangian of this form. To ensure this, we shall now add the following condition to our list of axioms of the previous section:

T10 Leibniz Rule. Let $A \in \mathcal{F}_{\text{class}}$ be any classical functional of the form eq. (43). Then for all $f_i \Phi_i \in \mathcal{F}_{\text{class}}$, we require that

$$\mathscr{T}(A f_1 \Phi_1 \cdots f_n \Phi_n) = 0, \tag{46}$$

i.e., any time-ordered product containing a factor of $A = \mathrm{d}\, B$ must vanish.

Remark: Condition T10 has previously been proposed (in the context of quantum field theory in flat spacetime) in [18] and [9, 10] and is referred to as the "action Ward identity" in these references.

Condition T10 for time-ordered products with two or more factors is clearly necessary and sufficient for the vanishing of *all* perturbative corrections to the interacting fields (including the interacting time-ordered products). However, causal factorization (T8) then implies that condition T10 must hold for Wick powers as well. Thus, condition T10 is necessary and sufficient to guarantee that the theory defined perturbatively by the interaction Lagrangian $L_1 = \mathrm{d}\, B$ yields exactly the free theory.

However, it may not be obvious what, if anything, condition T10 has to do with the "Leibniz rule", so we shall now explain the relationship of this condition to more usual formulations of the Leibniz rule. By doing so, we will also clarify our notation and further elucidate the viewpoint on time-ordered products introduced in the previous section.

Consider, first, the case of time-ordered products in one factor, i.e., Wick powers, in which case condition T10 simply states that for all B,

$$\mathscr{T}(\mathrm{d}\, B) = 0. \tag{47}$$

Therefore, for the case in which B is given by eq. (44)—and hence A is given by eq. (45)—we obtain

$$\mathscr{T}((\nabla_a f^a)\boldsymbol{\epsilon}\Phi + f^a \boldsymbol{\epsilon}\nabla_a \Phi) = 0. \tag{48}$$

for all scalar $\Phi \in \mathcal{V}_{\text{class}}$ and all test vector fields f^a. It should be understood here that $\nabla_a \Phi$ represents the classical expression corresponding to taking the derivative of Φ. For example, if $\Phi = \varphi^\alpha$ for some natural number α, then $\nabla_a \Phi = \alpha\varphi^{\alpha-1}\nabla_a\varphi$. But $\mathscr{T}((\nabla_a f^a)\boldsymbol{\epsilon}\Phi)$ is the same thing as the distributional derivative of $-\mathscr{T}(\Phi)$ smeared with $f^a\boldsymbol{\epsilon}$. Hence, using our notation $\mathscr{T}(f\Phi) = \Phi(f)$ for Wick powers, we may re-write eq. (48) as

$$\nabla_a \Phi(f^a \boldsymbol{\epsilon}) = (\nabla_a \Phi)(f^a \boldsymbol{\epsilon}). \tag{49}$$

Here, the quantity $\nabla_a \Phi$, appearing on the left side of this equation represents the distributional derivative of the algebra valued distribution Φ, whereas the quantity $(\nabla_a \Phi)$ appearing on the right side of this equation represents the Wick polynomial associated with the classical quantity $\nabla_a \Phi$. (Note that since these logically distinct quantities look the same except for the parentheses, our notation $\Phi(f)$ for Wick powers would be unacceptable if eq. (48) was not imposed!) Thus, in the above example where $\Phi = \varphi^\alpha$, eq. (49) takes the form

$$\nabla_a \varphi^\alpha(f_a \boldsymbol{\epsilon}) = \alpha(\varphi^{\alpha-1}\nabla_a\varphi)(\boldsymbol{\epsilon} f^a), \tag{50}$$

or, in the more common, informal notation

$$\nabla_a[\varphi^\alpha(x)] = \alpha(\varphi^{\alpha-1}\nabla_a\varphi)(x). \tag{51}$$

Again, the left side of this equation denotes the distributional derivative of φ^α, so this equation does indeed correspond to the usual notion of the Leibniz rule. Analogous results hold for the relations for Wick powers arising from T10 for general forms of B.

The meaning of requirement T10 for time ordered products with more than one factor can be seen as follows. Again, for simplicity, let B be of the form eq. (44). Condition T10 states that for all $h_i \Psi_i \in \mathcal{F}_{\text{class}}$, we have

$$-\mathscr{T}(\boldsymbol{\epsilon}(\nabla_c f^c)\Phi \prod \boldsymbol{\epsilon} h_j \Psi_j) = \mathscr{T}(\boldsymbol{\epsilon} f^c (\nabla_c \Phi) \prod \boldsymbol{\epsilon} h_j \Psi_j). \tag{52}$$

In the more common, informal notation this equation can be re-written as

$$\nabla_y^a[\mathscr{T}(\Phi(y)\Psi_1(x_1)\cdots\Psi_n(x_n))] = \mathscr{T}((\nabla^a\Phi)(y)\Psi_1(x_1)\cdots\Psi_n(x_n))\,. \tag{53}$$

Here, the left side denotes the distributional derivative of $\mathscr{T}(\Phi(y)\Psi_1(x_1)\cdots\Psi_n(x_n))$ with respect to the variable y, whereas the factor $(\nabla_a\Phi)$ appearing on the right side denotes the classical field expression obtained by taking the derivative of Φ. In other words, for time-ordered products with more than one factor, the operational meaning of T10 is simply that derivatives can be "freely commuted" through $\mathscr{T}$. Since the arguments of time-ordered products are classical field expressions, the Leibniz rule, of course, holds for the expressions hit by the derivative inside of $\mathscr{T}$.

It is useful to further illustrate the meaning of condition T10—and the extent to which it differs from conventional viewpoints on time-ordered products—with a simple example. Let us attempt to calculate $\mathscr{T}(\varphi(x)\varphi(y))$ according to our axiom scheme. By causal factorization (T8), $\mathscr{T}(\varphi(x)\varphi(y))$ must satisfy

$$\mathscr{T}(\varphi(x)\varphi(y)) = \begin{cases}\varphi(x)\varphi(y) & \text{if } x \notin J^+(y), \\ \varphi(y)\varphi(x) & \text{if } y \notin J^+(x),\end{cases} \tag{54}$$

which determines $\mathscr{T}(\varphi(x)\varphi(y))$ except on the "diagonal" $x = y$. However, since there do not exist any local and covariant distributions (T1) with support on the diagonal that have the correct scaling behavior (T2) as well as the desired smooth and analytic dependence upon the spacetime metric T4 and T5, it follows that $\mathscr{T}(\varphi(x)\varphi(y))$ is unique. This unique extension of the distribution defined by eq. (54) to the diagonal is

$$\mathscr{T}(\varphi(x)\varphi(y)) = \vartheta(x^0 - y^0)\varphi(x)\varphi(y) + \vartheta(y^0 - x^0)\varphi(y)\varphi(x) \tag{55}$$

where ϑ denotes the step function. (The right side of this equation is mathematically well defined on account of the wavefront set properties of $\varphi(x)\varphi(y)$; as already noted in section 1, the corresponding expression for general Wick monomials (see eq. (7)) is not well defined.) If we apply the Klein-Gordon operator P to the variable x of this distribution, we obtain

$$(P \otimes 1)\mathscr{T}(\varphi(x)\varphi(y)) = i\delta(x,y)\mathbb{1} \tag{56}$$

Consider, now, the time-ordered product $\mathscr{T}((P\varphi)(x)\varphi(y))$. By causal factorization (T8), this distribution satisfies

$$\mathscr{T}((P\varphi)(x)\varphi(y)) = 0 \quad \text{if } x \neq y \tag{57}$$

The most obvious extension of this distribution to the diagonal is, of course, to put $\mathscr{T}((P\varphi)(x)\varphi(y)) = 0$ for all x, y, including the diagonal. This is the conventional assumption. However, since $\mathscr{T}((P\varphi)(x)\varphi(y))$ has dimension length^{-D}, there *does* exist a distribution with support on the diagonal that satisfies the above required properties, namely $\delta(x,y)\mathbb{1}$. Consequently, within the scheme of axioms T1-T9, we have the freedom to add a "contact term" and define $\mathscr{T}((P\varphi)(x)\varphi(y))$ to be an arbitrary multiple of $\delta(x,y)\mathbb{1}$. Axiom T10 together with eq.(56) requires, in fact, that we make use of this freedom to define $\mathscr{T}((P\varphi)(x)\varphi(y))$ to be given by

$$\mathscr{T}((P\varphi)(x)\varphi(y)) = \mathrm{i}\delta(x,y)\mathbb{1}. \tag{58}$$

Since the Wick power $P\varphi$ vanishes identically, this explicitly shows that it is inconsistent with axioms T1-T10 to view a time-ordered product as a multilinear map on Wick polynomials rather than as a multilinear map on elements of $\mathcal{F}_{\text{class}}$.

We now prove that, for arbitrary Wick powers and time-ordered products, it is consistent to impose the Leibniz rule T10 in addition to our previous axioms T1-T9. In essence, the following proposition provides a generalization to curved spacetime of the proof of the "action Ward identity" given in [10].

Proposition 3.1. There exists a prescription for defining time ordered products satisfying our requirements T1–T10.

Proof. As in [14], we will proceed by an inductive argument on the number of factors, N_T, appearing in the time ordered product. Consider, first, the case of Wick monomials, i.e., $N_T = 1$. We previously showed [13] that the following prescription of "local Hadamard normal ordering" (i.e., "covariant point-splitting regularization") satisfies conditions T1-T9: Let $H(x,y)$ be a symmetric, locally constructed Hadamard parametrix.[9] We define [13]

$$:\varphi(x_1)\dots\varphi(x_k):_H = \frac{\delta^k}{\mathrm{i}^k \delta f(x_1)\dots\delta f(x_k)} \exp\left[\frac{1}{2}H(f\otimes f) + \mathrm{i}\varphi(f)\right]\Bigg|_{f=0} \tag{59}$$

For an arbitrary $\Phi = C(\nabla)^{r_1}\varphi\cdots(\nabla)^{r_k}\varphi \in \mathcal{V}_{\text{class}}$ (where C denotes a curvature term and all tensor indices have been suppressed), we define the corresponding Wick monomial by [13]

$$\begin{aligned}\mathscr{T}(f\Phi) = \Phi(f) &= \int C(y) :\varphi(x_1)\dots\varphi(x_k):_H F(y; x_1, \dots, x_k) \\ &= \int C(y) : \prod_{i=1}^{k} (\nabla)^{r_i}\varphi(y) :_H \ f(y)\boldsymbol{\epsilon}(y) \end{aligned} \tag{60}$$

[9] See e.g. eqs. (7) and (8) and Appendix A of [17] for the explicit form of H in D dimensions. Note that reference [17] uses a parametrix, Z_n, that is "truncated" at nth order, which will give an acceptable prescription only when the total number of derivatives, N_∇, appearing in the Wick power is sufficiently small. In order to give a prescription that is valid for arbitrary N_∇, one must define H by the procedure explained below eq. (69) of [13].

where

$$F(y; x_1, \ldots, x_k) = f(y)(\nabla_{x_1})^{r_1} \cdots (\nabla_{x_k})^{r_k} \delta(y, x_1, \ldots, x_k) \prod_i^k \boldsymbol{\epsilon}(x_i). \tag{61}$$

(Note that for the definition of general Wick powers with derivatives, it is essential for this prescription to be well defined that $H(x, y)$ be symmetric in x and y, so that it does not matter which of the variables $(x_1, \ldots, x_k)$ we select to apply derivatives to.) The arguments of [13] can now be straightforwardly generalized to show that this prescription satisfies not only conditions T1-T9 but also satisfies T10. Thus, there is no difficulty in adding condition T10 to the list of properties that we require for Wick powers.

However, since our previous existence proof for time-ordered products [14] does not provide a correspondingly explicit prescription for their definition, we cannot give a similar, direct proof that condition T10 can be imposed on time-ordered products. Instead, we must proceed by re-proving the existence theorem of [14], where we now explicitly allow the factors appearing in the time-ordered products to contain derivatives of φ and where we now add condition T10 to the list of requirements.

We inductively assume that the construction of the time-ordered products satisfying T1–T10 has been performed up to $< N_T$ factors. Our task is to construct the time-ordered products with N_T factors. However, as in [14], given the time-ordered products with $< N_T$ factors, the time ordered products, $\mathscr{T}$, with N_T factors are determined by causal factorization as distributions, $\mathscr{T}^0$, on $M^{N_T} \setminus \Delta_{N_T}$, where

$$\Delta_n \equiv \{(x, x, \ldots, x) \in M^n \mid x \in M\} \tag{62}$$

denotes the total diagonal. Furthermore, it is easily verified that $\mathscr{T}^0$ satisfies T1–T10 when acting on test functions supported away from the total diagonal. Consequently, our task is to extend $\mathscr{T}^0$ to a distribution in $\mathcal{D}'(M^{N_T})$, i.e., to a distribution defined everywhere, in such way that T1–T7 and T9–T10 are preserved in the extension process. (T8 has already been satisfied by the requirement that $\mathscr{T}$ be an extension of $\mathscr{T}^0$.) In fact, we need only show that an extension can be chosen so as to preserve T1–T5 and T9–T10, since the symmetry property, T6, and unitarity property, T7, can always be satisfied by a simple re-definition of $\mathscr{T}$ if all of the other properties have been satisfied [14].

As in [14], we can reduce this task to a much more manageable one by the use of a "local Wick expansion" for $\mathscr{T}^0$. The appropriate form of this local Wick expansion in the case where the arguments of $\mathscr{T}^0$ are general elements[10] of $\mathcal{F}_{\text{class}}$ is

$$\mathscr{T}^0\left(\prod_{i=1}^{N_T} f_i\Phi_i\right) = \sum_{\alpha_1,\alpha_2,\dots} \frac{1}{\alpha_1!\dots\alpha_{N_T}!}\int\prod_j \boldsymbol{\epsilon}(y_j)$$
$$t^0\left[\delta^{\alpha_1}\Phi_1\otimes\dots\otimes\delta^{\alpha_{N_T}}\Phi_{N_T}\right](y_1,\dots,y_{N_T})$$
$$f_1(y_1)\dots f_{N_T}(y_{N_T}) : \prod_{i=1}^{N_T}\prod_j[(\nabla)^j\varphi(y_j)]^{\alpha_{ij}} :_H \quad . \tag{63}$$

Here, we are using the following notation: The t^0 are multilinear mappings

$$t^0 : \bigotimes^{N_T}\mathcal{V}_{\text{class}} \quad\rightarrow\quad \mathcal{D}'(M^{N_T}\setminus\Delta_{N_T}) \tag{64}$$
$$\otimes_i\Phi_i \quad\rightarrow\quad t^0[\otimes_i\Phi_i](y_1,\dots,y_{N_T}) \tag{65}$$

from classical field expressions to c-number distributions in the product manifold minus its total diagonal[11]. Each α_i is a multi-index $(\alpha_{i1},\alpha_{i2},\dots)$, and we are using the shorthand $\alpha_i! = \prod_j \alpha_{ij}!$ for such a multi-index. If $\Phi\in\mathcal{V}_{\text{class}}$ and α is a multi-index, we are using the notation

$$\delta^\alpha\Phi = \left\{\prod_i\left(\frac{\partial}{\partial(\nabla)^i\varphi}\right)^{\alpha_i}\right\}\Phi. \tag{66}$$

As in [14], eq. (63) can be proved by induction in N_φ, using the commutator property, T9. By use of the local Wick expansion, we reduce the problem of extending $\mathscr{T}^0$ to the problem of extending the expansion coefficients t^0. The time-ordered product defined via eq. (63) from the extension of t^0 will automatically satisfy the commutator requirement T9. Thus, we need only show that the expansion coefficients t^0 can be extended so as to satisfy T1-T5 and T10.

It follows directly from the assumed properties T1–T10 of the time ordered products for $< N_T$ factors that the t^0 are distributions that are locally and covariantly constructed out of the metric, that they satisfy a microlocal spectrum condition, that they depend smoothly and analytically on the metric, that they have an "almost homogeneous scaling behavior", and that they satisfy the Leibniz rule in the sense that

$$(1\otimes\cdots\underbrace{\nabla}_{i\text{-th slot}}\otimes\dots 1)t^0[\otimes_i\Phi_i] = t^0[\Phi_1\otimes\cdots\nabla\Phi_i\otimes\cdots\Phi_{N_T}]. \tag{67}$$

[10] Since the Hadamard parametrix $H(x,y)$ is only defined when x,y are in a convex normal neighborhood of each other, it follows that the local Wick expansion is only defined if $F=\otimes_i f_i$ is supported in a sufficiently small neighborhood of the total diagonal. Note that this does not cause any problems in the present context since we are only interested in an arbitrarily small neighborhood of the total diagonal for the extension problem.

[11] More precisely, the t^0 are distributions that are defined on a suitable neighborhood of the total diagonal, minus the total diagonal itself; see the previous footnote.

In parallel with the arguments of [14], properties T1-T5 and T10 will hold for all time-ordered products with N_T factors if and only if each t^0 can be extended to a distribution t defined on all of M^{N_T} in such a way that the above properties are preserved in the extension process.

The methods of [14] already provide an extension t of t^0 that satisfies all of the required properties except that it is not guaranteed to satisfy the Leibniz relation

$$(1 \otimes \cdots \underbrace{\nabla}_{i\text{-th slot}} \otimes \dots 1) t[\otimes_i \Phi_i] = t[\Phi_1 \otimes \cdots \nabla \Phi_i \otimes \cdots \Phi_{N_T}]. \tag{68}$$

We will now complete the proof by showing how this relation can be satisfied.

Let $\mathcal{V}_{\text{class}}$ denote the space of classical field expressions, eq. (13). Let $\mathcal{V}_{\text{class}}(N_\varphi, N_\nabla)$ denote the subspace of $\mathcal{V}_{\text{class}}$ spanned by the monomial expressions in the curvature, in φ, and in symmetrized derivatives of φ that have a total number of precisely N_φ powers of φ and a total number of precisely N_∇ derivatives acting on the factors of φ. Let

$$Q_\nabla : \mathcal{V}_{\text{class}}(N_\varphi, N_\nabla - 1) \to \mathcal{V}_{\text{class}}(N_\varphi, N_\nabla) \tag{69}$$

denote the map whose action[12] on an element $\Phi \in \mathcal{V}_{\text{class}}(N_\varphi, N_\nabla - 1)$ is defined by first applying ∇_a to Φ, then dropping all terms where ∇_a acts on factors of curvature rather than factors of φ and, finally, symmetrizing over all derivatives acting on any given factor of φ.

We note, first, that for $N_\varphi > 0$, the map Q_∇ has vanishing kernel, i.e., in essence, the derivative of any nonvanishing expression with a nontrivial dependence on φ cannot vanish. To see this explicitly, choose an arbitrary but fixed point $x \in M$, a coordinate basis $x^\mu = (x^0, x^1, \dots, x^{D-1})$, and consider the coordinate components

$$\Phi_{\underline{\nu}}(x) = \sum_{\underline{\mu}_1 \cdots \underline{\mu}_n} C^{\underline{\mu}_1 \cdots \underline{\mu}_n}{}_{\underline{\nu}}(x) \prod_{i=1}^{n} \nabla_{\underline{\mu}_i} \varphi(x) \tag{70}$$

of a $\Phi \in \mathcal{V}_{\text{class}}(N_\varphi = n, N_\nabla)$, where $\underline{\nu}$ etc. is a shorthand for a symmetrized combination $(\nu_1 \dots \nu_k)$ of components. With each such coordinate component (70), we assign a unique element $p_\Phi \in \mathbb{C}[P_1, \dots, P_n]$, the ring of polynomials in the indeterminates $P_i^\mu, i = 1, \dots, n, \mu = 0, \dots, D-1$ which are symmetric under exchange of P_i and P_j, by the following rule: With the i-th factor of φ in expression (70), we associate the monomial in $P_i = (P_i^0, \dots, P_i^{D-1})$ obtained by replacing each derivative operator by the corresponding component of P_i. We then multiply the resulting monomials in P_i for all $i = 1, \dots, n$, we multiply by the corresponding real constants $C^{\cdots}{}_{\dots}(x)$ and we symmetrize in i. It is then

[12] Note that the definition of Q_∇ appears more natural in a framework in which one views $\mathcal{V}_{\text{class}}$ not as a vector space over the reals, but instead as a module over the ring of polynomial curvature expressions, $\mathcal{R}_{\text{class}}$. In this context, Q_∇ is simply defined to act as the derivative followed by symmetrization on monomials in $\mathcal{V}_{\text{class}}$ without curvature coefficients, and then extended to all of $\mathcal{V}_{\text{class}}$ by $\mathcal{R}_{\text{class}}$-linearity.

clear that the components of $Q_\nabla \Phi$ correspond to the polynomials $(\sum_i P_i^\mu) p_\Phi$, and it is clear that $Q_\nabla \Phi$ for $\Phi \in \mathcal{V}_{\rm class}(N_\varphi = n, N_\nabla)$ will be zero if and only if all these polynomials are zero. It is easy to see (e.g., by the arguments given on p. 22 of [10]) that this can only happen if in fact $p_\Phi = 0$, and hence that $\Phi = 0$, as we desired to show.

Let $\mathcal{V}^0_{\rm class}(N_\varphi, N_\nabla)$ denote the subspace of $\mathcal{V}_{\rm class}(N_\varphi, N_\nabla)$ spanned by expressions in the image of $\mathcal{V}_{\rm class}(N_\varphi, N_\nabla - 1)$ under the map Q_∇, multiplied by arbitrary curvature tensors. Let $\mathcal{V}^1_{\rm class}(N_\varphi, N_\nabla)$ be a complementary subspace, so that

$$\mathcal{V}_{\rm class}(N_\varphi, N_\nabla) = \mathcal{V}^0_{\rm class}(N_\varphi, N_\nabla) \oplus \mathcal{V}^1_{\rm class}(N_\varphi, N_\nabla). \tag{71}$$

Note that $\mathcal{V}^0_{\rm class}(N_\varphi, N_\nabla)$ is uniquely defined by our construction, but there are, of course, many possible choices[13] of complementary subspace $\mathcal{V}^1_{\rm class}(N_\varphi, N_\nabla)$. The key point is that if we fix all of the arguments of t except for the i-th and if we know the action of t on all $\Phi_i \in \mathcal{V}_{\rm class}(N_\varphi, N_\nabla - 1)$, then — because Q_∇ has vanishing kernel — the Leibniz rule eq. (68) uniquely determines the action of t for $\Phi_i \in \mathcal{V}^0_{\rm class}(N_\varphi, N_\nabla)$. On the other hand, the Leibniz rule imposes no constraints whatsoever on the action of t for $\Phi_i \in \mathcal{V}^1_{\rm class}(N_\varphi, N_\nabla)$. We will therefore refer to $\mathcal{V}^0_{\rm class}(N_\varphi, N_\nabla)$ as the "Leibniz dependent" subspace of $\mathcal{V}_{\rm class}(N_\varphi, N_\nabla)$, and will refer to $\mathcal{V}^1_{\rm class}(N_\varphi, N_\nabla)$ as the subspace of "Leibniz independent" expressions.

We now fix N_T and fix the number, N^i_φ, of powers of φ in each factor of the argument of t, and proceed by induction on $\{N^1_\nabla, \dots, N^{N_T}_\nabla\}$. The proof of [14] already directly establishes existence of the desired extension of t when $N^1_\nabla = \cdots = N^{N_T}_\nabla = 0$, since the Leibniz rule clearly imposes no additional restrictions in this case. We now inductively assume existence has been proven for all $N^i_\nabla < n_i$, where $i = 1, ..., N_T$. The inductive proof will be completed if we can show that for any j, existence continues to hold whenever $N^j_\nabla = n_j$ and $N^i_\nabla < n_i$ for $i \neq j$. To prove existence for $N^j_\nabla = n_j$, we decompose $\Phi_j \in \mathcal{V}_{\rm class}(N^j_\varphi, N^j_\nabla = n_j)$ into its "Leibniz dependent" and "Leibniz independent" pieces, eq. (71). On $\mathcal{V}^1_{\rm class}(N^j_\varphi, N^j_\nabla = n_j)$, we define the extension of t as in [14], whereas on $\mathcal{V}^0_{\rm class}(N^j_\varphi, N^j_\nabla = n_j)$ we simply *define* the extension of t so as to satisfy eq. (68), i.e., we use the left side of that equation to define the right side. It is clear that defining t in this way yields a local and covariant distribution that depends smoothly and analytically on the metric, that has an almost homogeneous scaling behavior, and that satisfies the desired microlocal properties, since taking covariant derivatives preserves these properties. Consequently, an extension of t satisfying all of the desired properties (including the Leibniz rule) exists.

□

[13] A particular choice of $\mathcal{V}^1_{\rm class}(N_\varphi, N_\nabla)$ in the context of flat spacetime theories was made in [10]. It is worth noting that when $N_\varphi = 2$, we have $\mathcal{V}_{\rm class}(2, N_\nabla) = \mathcal{V}^0_{\rm class}(2, N_\nabla)$ when N_∇ is odd, i.e., there are no "Leibniz independent" expressions when N_∇ is odd; when N_∇ is even, a convenient choice of $\mathcal{V}^1_{\rm class}(2, N_\nabla)$ are the expressions of the form of local curvature terms times $\varphi \nabla_{(a_1} \dots \nabla_{a_{N_\nabla})} \varphi$.

3.2 Anomalies with respect to the equations of motion

We conclude this section by elucidating the difficulties (i.e., "anomalies") that arise when one attempts to impose further "reasonable" conditions concerning the equations of motion in addition to T1-T10 on Wick powers containing derivatives. Specifically, we shall show that in two spacetime dimensions, it is impossible to require the vanishing of $(\nabla_a \varphi) P \varphi$, where $P = \nabla^a \nabla_a - m^2 - \xi R$ is the Klein-Gordon operator. We also shall show that in four spacetime dimensions, it is impossible to require the vanishing of both $\varphi P \varphi$ and $(\nabla_a \varphi) P \varphi$. These difficulties are closely related to the well-known trace anomaly property for a conformally invariant field in these dimensions. However, in contrast to previous discussions, in our framework the relation $T^a{}_a = 0$ holds as a classical algebraic identity (not requiring the field equations) for the conformally invariant field in $D = 2$ spacetime dimensions. Consequently, in our framework, there cannot be a trace anomaly for the conformally invariant scalar field in two spacetime dimensions; rather, in two dimensions there is necessarily an anomaly in the conservation of T_{ab}.

Consider a prescription (such as the local Hadamard normal ordering defined above in eq. (60)) for defining Wick polynomials in D spacetime dimensions that satisfies T1-T10. Using the Leibniz rule, T10, the stress-tensor T_{ab}, eq. (6), may be re-written entirely in terms of the Wick monomials

$$\Psi \equiv \varphi^2, \quad \Psi_{ab} \equiv \varphi \nabla_a \nabla_b \varphi \tag{72}$$

as follows:

$$T_{ab} = \frac{1}{2} \nabla_a \nabla_b \Psi - \Psi_{ab} - \frac{1}{2} g_{ab} \left(\frac{1}{2} \nabla^c \nabla_c \Psi + m^2 \Psi - \Psi^c{}_c\right) + \xi [G_{ab} \Psi - \nabla_a \nabla_b \Psi + g_{ab} \nabla^c \nabla_c \Psi]. \tag{73}$$

The divergence of T_{ab} is straightforwardly calculated (again using the Leibniz rule) to be given by

$$\nabla^a T_{ab} = (\nabla_b \varphi) P \varphi. \tag{74}$$

On the other hand, we also have the obvious relation

$$\Psi^a{}_a - (m^2 + \xi R) \Psi = \varphi P \varphi. \tag{75}$$

The above equations hold for any prescription satisfying T1-T10. Now let us calculate $\varphi P \varphi$ and $(\nabla_a \varphi) P \varphi$ by the local Hadamard normal ordering prescription. In odd dimensions, these quantities vanish, but in even dimensions the computations reported in Lemma 2.1 of [17] yield[14]

$$\varphi P \varphi = Q \mathbb{1} \tag{76}$$

[14] The difference between the behavior occurring in even and odd dimensions can be understood as arising from the following fact: In odd dimensions, one can construct a local and covariant Hadamard

$$(\nabla_a\varphi)P\varphi = \frac{D}{2(D+2)}\nabla_a Q \mathbb{1} \tag{77}$$

where Q is a nonvanishing local curvature scalar of dimension (length)$^{-D}$ that can be computed explicitly from the Hadamard recursion relations.

If we wish to require the vanishing of $\varphi P\varphi$ and $(\nabla_a\varphi)P\varphi$, our task is to modify—in a manner consistent with axioms T1-T10—the definitions of the Wick powers, $\Psi = \varphi^2$ and $\Psi_{ab} = \varphi\nabla_a\nabla_b\varphi$, so that the left sides of eqs. (74) and (75) vanish. However, since Ψ and Ψ_{ab} are each quadratic in φ, our previous uniqueness theorem [13] establishes that the allowed freedom in the definition of these quantities consists of local curvature terms of the correct dimension times the identity, $\mathbb{1}$. More precisely, the allowed freedom to modify the definition of these quantities is[15]

$$\Psi \to \Psi + C\mathbb{1} \tag{78}$$

$$\Psi_{ab} \to \Psi_{ab} + C_{ab}\mathbb{1} \tag{79}$$

where C is any scalar constructed out of the metric, curvature, derivatives of the curvature, m^2 and ξ, with dimension (length)$^{-(D-2)}$ and C_{ab} is any tensor (symmetric in a and b) that is constructed out of the metric, curvature, derivatives of the curvature, and m^2 and has dimension (length)$^{-D}$. Therefore, in order to modify the local Hadamard normal ordering prescription so as to preserve T1-T10 and also make the right sides of eqs. (74) and (75) vanish, we must solve the following equations

$$-(\nabla^a C_{ab} - \frac{1}{2}\nabla_b C^a{}_a) + \frac{1}{4}\nabla_b\nabla^a\nabla_a C + \frac{1}{2}R_b{}^c\nabla_c C + \frac{1}{2}(m^2+\xi R)\nabla_b C = -\nabla_b Q \tag{80}$$

$$C^a{}_a - m^2 C - \xi R C = -\frac{D}{2(D+2)}Q \tag{81}$$

parametrix $H(x,y)$ that satisfies the wave equation in each variable up to arbitrarily high order in the geodesic distance between x and y. As a result, the "local Hadamard normal ordering" prescription for Wick powers satisfies T1-T10 *and* also satisfies the property that any Wick power containing a factor of the wave operator must vanish. By contrast, in even dimensions, it is impossible to construct a local and covariant Hadamard parametrix $H(x,y)$, that is symmetric in x and y and satisfies the wave equation to arbitrarily high order in the geodesic distance between x and y. Consequently, if one requires $H(x,y)$ to be symmetric (as is necessary for the prescription for defining general Wick monomials involving derivatives to be well defined), then it will fail to satisfy the wave equation, and "anomalies" will occur for the regularized quantities.

[15] Condition T10, of course, was not imposed in [13]. However, it is worth noting that the subspace of classical field expressions spanned by φ^2 and $\varphi\nabla_a\nabla_b\varphi$ does not intersect the "Leibniz dependent" subspace $\mathcal{V}^0_{\rm class}$ (see footnote 13), so condition T10 actually imposes no extra conditions on these quantities, i.e., the full ambiguity given by eqs. (78) and (79) is present even when we impose T10.

Let us specialize, now, to the case of two spacetime dimensions, $D = 2$. Since C has dimension zero, the most general choice of C is simply $C = \alpha$, where α is a constant that is independent of m^2 but may have arbitrary analytic dependence on ξ. However, since C appears in eq. (80) only in the form $\nabla_b C$, it cannot contribute to that equation. Similarly, since C_{ab} has dimension (length)$^{-2}$, it must take the form $C_{ab} = \beta_1 R_{ab} + \beta_2 R g_{ab} + \beta_3 m^2 g_{ab}$, where $\beta_1, \beta_2, \beta_3$ are constants that are independent of m^2 but may have arbitrary analytic dependence on ξ. However, in two spacetime dimensions, we have $R_{ab} = \frac{1}{2} R g_{ab}$, and since C_{ab} appears in eq. (80) only in the combination $C_{ab} - \frac{1}{2} C^c{}_c g_{ab}$, it follows immediately that C_{ab} also cannot contribute to eq. (80). Since $\nabla_a Q$ is nonvanishing, it is therefore impossible to solve eq. (80). Consequently, in two spacetime dimensions, there does not exist a prescription for defining Wick powers that satisfies axioms T1-T10 and also satisfies $(\nabla_a \varphi) P \varphi = 0$. Since $\nabla^a T_{ab} = (\nabla_b \varphi) P \varphi$ by eq. (74) above, this means, equivalently, that it is impossible to satisfy conservation of stress-energy in two spacetime dimensions within our axiomatic framework.

By contrast, in spacetime dimension $D > 2$, no difficulty arises in satisfying eq. (80) alone (in addition to axioms T1-T10), since we may always solve this equation by choosing $C = 0$ and taking

$$C_{ab} = -\frac{2}{D-2} Q g_{ab} \tag{82}$$

Thus, in all spacetime dimensions except $D = 2$, there is no obstacle to imposing $(\nabla_a \varphi) P \varphi = 0$—or, equivalently, conservation of stress-energy—within our axiom scheme. However, difficulties do arise if, in addition, we attempt to impose $\varphi P \varphi = 0$ as well. For example, when $D = 4$, the general form of C is

$$C = \alpha_0 R + \alpha_1 m^2, \tag{83}$$

where α_0, α_1 are constants. If one substitutes this general form of C into eq. (80), it turns out that it is still always possible to solve eq. (80) for C_{ab}. The general solution of eq. (80) is most conveniently expressed in terms of the quantity $\bar{C}_{ab} \equiv C_{ab} - \frac{1}{2} C^c{}_c g_{ab}$, and takes the explicit form

$$\begin{aligned} \bar{C}_{ab} \;\; = \;\; & \left(Q + \frac{\alpha_0}{4} \nabla^c \nabla_c R + \frac{1}{2} \alpha_0 m^2 R + \frac{1}{8} \alpha_0 (2\xi + 1) R^2 \right) g_{ab} + \frac{1}{2} \alpha_0 R G_{ab} \\ & + \bar{\beta}_1 I_{ab} + \bar{\beta}_2 J_{ab} + \bar{\beta}_3 m^2 G_{ab} + \bar{\beta}_4 m^4 g_{ab} \end{aligned} \tag{84}$$

where $\bar{\beta}_1, \dots, \bar{\beta}_4$ are arbitrary constants, and I_{ab} and J_{ab} are the two independent conserved local curvature tensors of dimension (length)$^{-4}$. We now substitute the general form, eq. (83), of C and this general solution, eq. (84), for C_{ab} into eq. (81). Since both I_{ab} and J_{ab} have trace proportional to $\nabla^a \nabla_a R$, we obtain an equation of the form

$$Q = \gamma_1 \nabla^a \nabla_a R + \gamma_2 R^2 + \gamma_3 m^2 R + \gamma_4 m^4. \tag{85}$$

However, by explicit calculation, Q contains terms of the form $C^{abcd}C_{abcd}$ and $R^{ab}R_{ab}$, which cannot be expressed as a sum of the curvature terms on the right side. Consequently, there are no solutions to eq. (81) when $D = 4$. Similar results presumably hold in all higher even dimensions, but a proof of this would require both a calculation of Q and an analysis of the conserved local curvature terms of dimension $(\text{length})^{-D}$.

Finally, we note that our viewpoint with respect to the definition of the stress-energy tensor differs in two significant aspects with that of Moretti [17] and others. First, we take the free field quantum stress-energy tensor, T_{ab}, to be defined in terms of Wick monomials by eq. (6) and we do not allow any modifications of this formula. It is natural that we take this viewpoint, because it is precisely the quantity defined by eq. (6) that will directly enter condition T11b of the next section. Furthermore, if condition T11b is imposed—as is possible except in 2 spacetime dimensions, as will be proven in section 6—then, as we shall show in section 5, one obtains not only the conservation of the stress energy tensor T_{ab} in the free theory, but one also obtains conservation of the interacting stress-energy tensor Θ_{ab} in an arbitrary interacting theory. By contrast, Moretti [17] allows modifications to the formula for the stress-energy tensor that are proportional to $\varphi P \varphi$ and thus vanish classically. If one were only interested in considering the free field theory and were seeking a definition of its stress-energy tensor that is conserved and that corresponds to the classical expression in the classical limit, we see no argument against allowing such a re-definition[16]. However, it seems unlikely that this approach could naturally lead to a conserved stress-energy tensor in interacting theories.

Second, Moretti [17] takes the Wick monomials appearing in his (modified) formula for T_{ab} to be defined by a particular, fixed prescription, namely local Hadamard normal ordering (see eq. (60) above). By contrast, we allow an arbitrary prescription for defining Wick products satisfying T1-T10. However, it turns out that—with the exception of one case—the freedom (78) and (79) allowed by T1-T10 in the definition of the relevant Wick products is sufficient to encompass the modifications to T_{ab} obtained by Moretti by adding terms proportional to $\varphi P \varphi$ but keeping the prescription for defining Wick products fixed. In other words—with one exception—we achieve the same final result for T_{ab} as an element of $\mathcal{W}$ by modifying the prescription for defining Wick products rather than by modifying the formula for T_{ab} in terms of Wick products. The exception is the case of 2 spacetime dimensions. Indeed, it can be seen directly from eq. (73) that when $D = 2$ and when $m = 0$, the allowed freedom (78) and (79) does not permit any modification whatsoever to T_{ab}. Thus, while our results agree with those of Moretti when $D \neq 2$, they differ when $D = 2$.

[16] Indeed, this was the philosophy taken in the prior work of one of us [20] on the stress-energy tensor, before the general theory of Wick products in curved spacetime had been developed.

4 Quadratic interaction Lagrangians and retarded response

4.1 Formulation of the general condition T11

In this section, we formulate the new requirement, T11, that arises from our Principle of Perturbative Agreement when the perturbation, L_1, of the free Lagrangian, L_0, is at most quadratic in the field φ and contains at most 2 derivatives of φ. The most general such nontrivial interaction Lagrangian for a real scalar field is

$$L_1 = \frac{1}{2}[j(x)\varphi + w^{ab}(x)\nabla_a\varphi\nabla_b\varphi + v(x)\varphi^2]\boldsymbol{\epsilon} \tag{86}$$

where j, w^{ab}, and v are smooth. Without loss of generality, we will assume that j, w^{ab}, and v are of compact support on M, since the conditions that we derive are local conditions that will not depend on their support properties, and it is simpler to consider the compact support case. The term $j\varphi\boldsymbol{\epsilon}$ in eq. (86) corresponds to the addition of an external current; the term $v\varphi^2\boldsymbol{\epsilon}$ corresponds to the presence of an external potential (or, equivalently, a spacetime variable mass); finally, the change in L produced by a changing the spacetime metric from g_{ab} to g'_{ab} corresponds to taking $w^{ab}\boldsymbol{\epsilon} = g'^{ab}\boldsymbol{\epsilon}' - g^{ab}\boldsymbol{\epsilon}$ and $v\boldsymbol{\epsilon} = m^2(\boldsymbol{\epsilon}' - \boldsymbol{\epsilon}) + \xi(R'\boldsymbol{\epsilon}' - R\boldsymbol{\epsilon})$. Note that we have not included a term of the form $A^a\varphi\nabla_a\varphi\boldsymbol{\epsilon}$ in L_1, since such a term is Leibniz equivalent to $v\varphi^2\boldsymbol{\epsilon}$ with $v = -\nabla_a A^a$. However, if we were considering a complex scalar field, then we would have an additional term in L_1 of the form $\mathrm{i}A^a(\bar{\varphi}\nabla_a\varphi - \varphi\nabla_a\bar{\varphi})\boldsymbol{\epsilon}$.

The quantum field theory of a scalar field φ with Lagrangian $L = L_0 + L_1$ can be constructed in the following two independent ways. First, it can be constructed perturbatively about L_0 by means of the Bogoliubov formula. This formula is most conveniently expressed in terms of retarded products, so we first recall the definition of retarded and advanced products, $\mathscr{R}$ and $\mathscr{A}$, in terms of time-ordered products. If $A, B \in \mathcal{F}_{\text{class}}$, we define

$$\mathscr{R}(e^{\mathrm{i}A}; e^{\mathrm{i}B}) = \mathcal{S}(B)^{-1}\mathcal{S}(A+B), \quad \mathscr{A}(e^{\mathrm{i}A}; e^{\mathrm{i}B}) = \mathcal{S}(A+B)\mathcal{S}(B)^{-1}, \tag{87}$$

where $\mathcal{S}$ and $\mathcal{S}^{-1}$ are given by the formal series expressions

$$\mathcal{S}(A) = \mathscr{T}(e^{\mathrm{i}A}), \quad \mathcal{S}(A)^{-1} = \bar{\mathscr{T}}(e^{\mathrm{i}A}), \tag{88}$$

and where $\bar{\mathscr{T}}$ denotes the "anti-time-ordered" product given by eq. (38). Equation (87) is to be interpreted as an infinite sequence of well defined equations obtained by formally expanding the exponentials on the left side, formally substituting eq. (88) for $\mathcal{S}$ and $\mathcal{S}^{-1}$ on the right side, and then equating the terms with the same number of powers of A and B. For example, if we set $A = \sum f_i\Phi_i$ and $B = h\Psi$ and expand to first order in B, we get the formula

$$\mathscr{R}\left(\prod f_i\Phi_i; h\Psi\right) = -\Psi(h)\mathscr{T}\left(\prod f_i\Phi_i\right) + \mathscr{T}\left(h\Psi\prod f_i\Phi_i\right) \tag{89}$$

as well as a similar formula for the advanced products. The retarded and advanced products have the important support property

$$\begin{aligned}&\operatorname{supp} \mathscr{A}/\mathscr{R}(\prod \Phi_i(x_i); \prod \Psi_j(y_j)) \subset \\ &\qquad\qquad \{(x_1, \dots, x_n; y_1, \dots, y_m) \mid \text{some } x_i \in J^{-/+}(y_j) \text{ for at least one } j.\}. \quad (90)\end{aligned}$$

which follows from the causal factorization property, T8, of the time ordered products.

Now let L_1 be any compactly supported interaction Lagrangian density that is polynomial in φ and its derivatives. Let $\Phi_i \in \mathcal{V}_{\text{class}}$. Then the Bogoliubov formula defines the *interacting* time-ordered product $\mathscr{T}_{L_1}(\prod f_i \Phi_i)$ as an element of the non-interacting algebra $\mathcal{W}(M, \mathbf{g})$ by the power series expression

$$\mathscr{T}_{L_1}\left(\prod_{i=1}^m f_i \Phi_i\right) = \mathscr{R}\left(\prod_{i=1}^m f_i \Phi_i; e^{\mathrm{i}L_1}\right) = \sum_n \frac{\mathrm{i}^n}{n!} \mathscr{R}\left(\prod_{i=1}^m f_i \Phi_i; \underbrace{L_1 \cdots L_1}_{n \text{ factors}}\right). \quad (91)$$

This definition of time-ordered products for the interacting quantum field corresponds to the boundary condition that the interacting field be equal to the corresponding non-interacting field outside the causal future of the support of the interaction Lagrangian L_1. The interacting field corresponding to the opposite boundary condition (with the future of the support of L_1 replaced by the past) is given by the analogous formula involving advanced products. As is well known, the perturbation series (91) is expected not to converge[17] for general L_1, so this relation is, in general, only a formal one.

The Bogoliubov formula (91) holds for an arbitrary interaction Lagrangian. However, if L_1 takes the simple form (86), then there is a second means of constructing "interacting" time-ordered products: We simply construct them directly for the theory given by the Lagrangian $L_0' = L_0 + L_1$. As already indicated, the Lagrangian L_0' corresponds to a free scalar field in a curved spacetime with metric $\mathbf{g}'$ in the presence of an external potential V' and an external source J'. We have already constructed the quantum field theory of φ in an arbitrary, globally hyperbolic spacetime $(M, \mathbf{g})$. The generalization of this construction to include an external potential, V, is accomplished in an entirely straightforward manner as follows: In the construction of the algebras $\mathcal{A}(M, \mathbf{g}, V)$ and $\mathcal{W}(M, \mathbf{g}, V)$, we simply replace the original Klein-Gordon operator $P = \nabla^a \nabla_a - \xi R - m^2$ by $\nabla^a \nabla_a - \xi R - m^2 - V$. In the definition of the classical field algebra, $\mathcal{V}_{\text{class}}$, we must now also allow arbitrary factors of V and its symmetrized covariant derivatives. In the axioms for time-ordered products, we simply make the obvious modifications to T1, T2, T4, and T5 to allow for the presence of V. The proof of existence of a prescription for defining time-ordered products satisfying T1-T10 then goes through without any substantive changes.

Given the theory of the real scalar field φ in the absence of an external current, J, the corresponding theory in the presence of an external current may be uniquely constructed

[17] However, see the remarks at the end of section 7.

as follows (where, for simplicity, we assume $V = 0$ in the following discussion): First, the CCR algebra, $\mathcal{A}(M, \mathbf{g}, J)$, is constructed by starting with the free algebra generated by symbols $\varphi_J(f)$ and $\varphi_J(h)^*$, and factoring by the relations (i), (ii) and (iv) of section 2, together with the relation (iii')

$$\varphi_J(Pf) = \int fJ\boldsymbol{\epsilon} \cdot \mathbb{1}, \tag{92}$$

where P is the Klein-Gordon operator, eq. (9). Thus, the only modified relation compared to the case of vanishing source is (iii'), which ensures that the field φ_J satisfies the Klein-Gordon equation with source J in the distributional sense. Note that the commutation relations (iv) of the field with source are identical to the commutation relations of the field without source. To construct $\mathcal{W}(M, \mathbf{g}, J)$, we define the generators $W_n(u)$ by eq. (8) with φ_J replacing φ but with ω_2 taken to be a Hadamard state of the theory with vanishing source, so that ω_2 still satisfies the homogeneous equation in each entry.

The Wick monomials may now be defined for the theory with external source by exactly the same formula, eq. (60), as used in the theory without source, with the only difference being that the normal ordered expressions of the field without source that appear on the right side of (60) must be replaced by the local Hadamard normal ordered expressions $:\varphi_J(x_1)\cdots\varphi_J(x_k):_H$ of the field φ_J with source. The latter are defined exactly as for the case of a vanishing source by eq. (59), where H is the same local Hadamard parametrix for the Klein-Gordon operator P as used in the theory without a source. It then follows from causal factorization, T8, and the commutator property, T9, that a local Wick expansion of the form eq. (63) holds for time-ordered products, $\mathscr{T}_J^0(\Phi_1(x_1)\cdots\Phi_n(x_n))$ when $x_i \neq x_j$ for all i, j, where the expansion coeficients, $t^0[\otimes\Phi_i]$, are identical to those of the theory without source. We may therefore *define* time-ordered products in the theory with source by choosing the extension, $t[\otimes\Phi_i]$, to be *independent* of the source J. The resulting definition of time-ordered products satisfies axioms T1-T10, with the obvious modifications to T1, T2, T4, and T5 to allow for the presence of J. This construction of the theory of a real scalar field in the presence of an external source, J, in terms of the theory defined when $J = 0$ corresponds to demanding that the renormalization prescription be independent[18] of J.

Our Principle of Perturbative Agreement demands that for L_1 given by eq. (86), the perturbative theory defined by the Bogoliubov formula (91) must agree with the exact theory for the Lagrangian $L_0' = L_0 + L_1$. However, we cannot yet easily compare these constructions, since the Bogoliubov formula expresses the interacting time-ordered products as elements of the algebra $\mathcal{W}(M, \mathbf{g})$, whereas the exact construction yields time-ordered

[18] J-dependent renormalization prescriptions that satisfy the appropriate versions of T1-T10 could be defined by choosing a local Hadamard parametrix for the Klein-Gordon operator P that depends nontrivially on J in a local and covariant manner (e.g., choosing $H'(x, y) = H(x, y) + J(x)J(y)$) and/or by choosing the extension, t, of t^0 to depend nontrivially on J in a local and covariant manner.

products as elements of a different algebra, $\mathcal{W}(M, \mathbf{g}', V', J')$. Therefore, in order to compare these two expressions for the time-ordered products, we must map $\mathcal{W}(M, \mathbf{g}', V', J')$ into $\mathcal{W}(M, \mathbf{g})$ in such a way that, in the past (i.e., outside the future of the supports of $\mathbf{g} - \mathbf{g}'$, V', and J'), the interacting time-ordered products in $\mathcal{W}(M, \mathbf{g}', V', J')$ are mapped into the corresponding time-ordered products in $\mathcal{W}(M, \mathbf{g})$. The desired map, denoted $\tau^{\rm ret}$, was constructed in lemma 4.1 of [13] in the case where $V' = J' = 0$. We now briefly review its construction and generalize it to the case of nonvanishing external potential and current.

Let $(M, \mathbf{g})$ be a globally hyperbolic spacetime and $(M, \mathbf{g}', V', J')$ be such that $(M, \mathbf{g}')$ also is globally hyperbolic and outside some compact set $K \subset M$, we have $\mathbf{g}' = \mathbf{g}$, $V = 0$, and $J = 0$. Let Σ_t be a foliation of $(M, \mathbf{g})$ by Cauchy surfaces. Choose t_1 such that Σ_{t_1} does not intersect the causal future of K and choose $t_0 < t_1$, so that $\Sigma_{t_0} \subset I^-(\Sigma_{t_1})$. (It follows automatically that Σ_{t_0} and Σ_{t_1} are also Cauchy surfaces for $(M, \mathbf{g}')$.) Let ψ be a smooth function on M such that $\psi(x) = 0$ for x in the future of Σ_{t_1} and $\psi(x) = 1$ for x in the past of Σ_{t_0}. The action of $\tau^{\rm ret}$ on $\varphi_{(\mathbf{g}', V', J')}$ may now be defined as follows: Let f be a test function on M. We define

$$F = \Delta_{(\mathbf{g}', V')} f \tag{93}$$

and we define

$$f' = P'(\psi F) \tag{94}$$

with $P' = \nabla'^a \nabla'_a - \xi R' - m^2 - V'$ and with $\Delta_{(\mathbf{g}', V')}$ being the advanced minus retarded Green's function associated with P'. Then f' is a test function with support lying between Σ_{t_0} and Σ_{t_1}. Furthermore, it is easily checked that $\Delta_{(\mathbf{g}', V')}(f - f') = 0$, which implies that $f - f' = P'h$ where $h \equiv \Delta^{\rm adv}_{(\mathbf{g}', V')}(f - f')$ is of compact support [20], and hence is a test function. Consequently, by eq. (92), we have

$$\varphi_{(\mathbf{g}', V', J')}(f) = \varphi_{(\mathbf{g}', V', J')}(f') + \int h J' \boldsymbol{\epsilon}' \cdot \mathbb{1} \tag{95}$$

Since the supports of $\Delta^{\rm adv}_{(\mathbf{g}', V')} f'$ and J' do not overlap, and since $\Delta^{\rm adv}_{(\mathbf{g}', V')}(x, y) = \Delta^{\rm ret}_{(\mathbf{g}', V')}(y, x)$ (up to factors of $\boldsymbol{\epsilon}'$) we may re-write this equation as

$$\varphi_{(\mathbf{g}', V', J')}(f) = \varphi_{(\mathbf{g}', V', J')}(f') + \int f \Delta^{\rm ret}_{(\mathbf{g}', V')} J' \boldsymbol{\epsilon}' \cdot \mathbb{1} \tag{96}$$

All of the above equations are relations in the algebra $\mathcal{W}(M, \mathbf{g}', V', J')$. We want to define the map $\tau^{\rm ret} : \mathcal{W}(M, \mathbf{g}', V', J') \to \mathcal{W}(M, \mathbf{g})$ to be such that it maps $\varphi_{(\mathbf{g}', V', J')}(f')$ to $\varphi_{\mathbf{g}}(f')$ when the support of f' lies outside the future of K and to be such that $\tau^{\rm ret}(\mathbb{1}) = \mathbb{1}$. Therefore, for arbitrary f, we define

$$\tau^{\rm ret}[\varphi_{(\mathbf{g}', V', J')}(f)] = \varphi_{\mathbf{g}}(f') + \int f \Delta^{\rm ret}_{(\mathbf{g}', V')} J' \boldsymbol{\epsilon}' \cdot \mathbb{1} \tag{97}$$

The above formula for the action of $\tau^{\rm ret}$ on $\varphi_{(\mathbf{g}',V',J')}$ can be rewritten in a more useful form as follows. Let $S : \mathcal{D}(M) \to \mathcal{D}'(M)$ be the map defined by its distributional kernel,

$$S(f_1, f_2) = \int_{\Sigma_-} (F_1 \nabla_a F_2 - F_2 \nabla_a F_1)\, \mathrm{d}\,\sigma^a, \tag{98}$$

where $F_1 = \Delta_{\mathbf{g}} f_1$, $F_2 = \Delta_{(\mathbf{g}',V')} f_2$, and Σ_- is any Cauchy surface that does not intersect the future of K. Define $A^{\rm ret} : \mathcal{D}(M) \to \mathcal{D}'(M)$ by

$$A^{\rm ret} f = -P'(\psi S f). \tag{99}$$

Then we have

$$\tau^{\rm ret}[\varphi_{(\mathbf{g}',V',J')}(f)] = \varphi_{\mathbf{g}}(A^{\rm ret} f) + \int f \Delta^{\rm ret}_{(\mathbf{g}',V')} J' \boldsymbol{\epsilon}' \cdot 1\!\!1 \tag{100}$$

The map $\tau^{\rm ret}$ can be uniquely extended to all of $\mathcal{A}(M, \mathbf{g}', V', J')$ as a *-isomorphism and, thereby, to $W_n(u)$ when u is smooth. The further extension of $\tau^{\rm ret}$ to $W_n(u)$ for u a distribution in the space eq. (12) then can be accomplished as in lemma 4.1 of [13], with the trivial modifications resulting from the presence of V and the straightforward modifications resulting from the presence of J.

Our Principle of Perturbative Agreement now leads to the following requirement:

T11 Quadratic interaction Lagrangians. Let $(M, \mathbf{g})$ and $(M, \mathbf{g}')$ be globally hyperbolic spacetimes such that $\mathbf{g}' = \mathbf{g}$ outside of a compact set K. Let V' and J' have support in K. Then for all $\Phi_i \in \mathcal{V}_{\rm class}$ we have

$$\tau^{\rm ret}\left[\mathscr{T}_{(\mathbf{g}',V',J')}\left(\prod_{i=1}^m f_i \Phi_i\right)\right] = \sum_n \frac{\mathrm{i}^n}{n!} \mathscr{R}_{\mathbf{g}}\left(\prod_{i=1}^m f_i \Phi_i; \underbrace{L_1 \cdots L_1}_{n \text{ factors}}\right). \tag{101}$$

where L_1 is the interaction Lagrangian of the form eq. (86) given by $L_1 = L_0 - L_0'$.

In order to express this condition in a more explicit and useful form, we consider separately the subcases of (a) external source variation, (b) metric variation, and (c) external potential variation. These will lead to sub-requirements T11a, T11b, and T11c.

4.2 External source variation: Axiom T11a

We now apply condition T11 to the case of an interaction Lagrangian of the form $L_1 = J\varphi\boldsymbol{\epsilon}$, where J is a compactly supported smooth function ("external current"). In this case, condition T11 reduces to

$$\tau^{\rm ret}\left[\mathscr{T}_J\left(\prod_{i=1}^m f_i \Phi_i\right)\right] = \sum_n \frac{\mathrm{i}^n}{n!} \mathscr{R}_{J=0}\left(\prod_{i=1}^m f_i \Phi_i; \underbrace{J\varphi\boldsymbol{\epsilon} \cdots J\varphi\boldsymbol{\epsilon}}_{n \text{ factors}}\right), \tag{102}$$

However, if only an external current is present, eq. (97) becomes simply

$$\tau^{\mathrm{ret}}[\varphi_J(f)] = \varphi_{J=0}(f) - \int f \Delta^{\mathrm{ret}} J \boldsymbol{\epsilon} \cdot \mathbb{1}. \tag{103}$$

More generally, for $A_i \in \mathcal{F}_{\mathrm{class}}$, we have

$$\tau^{\mathrm{ret}} \left[\mathscr{T}_J \left(\prod_i A_i(\varphi) \right) \right] = \mathscr{T}_{J=0} \left(\prod_i A_i(\varphi - \Delta^{\mathrm{ret}} J \boldsymbol{\epsilon}) \right), \quad A_i \in \mathcal{F}_{\mathrm{class}}, \tag{104}$$

which can be proved by induction the number of factors of the time ordered product, making use of the fact that the c-number coefficients in the Wick expansion of $\mathscr{T}_J$ are independent of J. Expanding eq. (102) to first order in J and using eq. (104), we obtain

T11a Free field factor. We have

$$\mathscr{R}(\prod f_j \Phi_j; J\varphi\boldsymbol{\epsilon}) = \mathrm{i} \sum_j \mathscr{T} \left(f_1 \Phi_1 \dots (\Delta^{\mathrm{ret}} J \boldsymbol{\epsilon}) \frac{\delta(f_j \Phi_j)}{\delta \varphi} \dots f_n \Phi_n \right). \tag{105}$$

Remarks: **(1)** Condition T11a corresponds to condition N4 of [7] in the context of QED in flat spacetime.

(2) We can use eq. (89) to re-write eq. (105) purely in terms of time-ordered products as

$$\mathscr{T}(J\varphi\boldsymbol{\epsilon} \prod f_j \Phi_j) = \varphi(J\boldsymbol{\epsilon}) \mathscr{T}(\prod f_j \Phi_j) + \mathrm{i} \sum_j \mathscr{T} \left(f_1 \Phi_1 \dots (\Delta^{\mathrm{ret}} J \boldsymbol{\epsilon}) \frac{\delta(f_j \Phi_j)}{\delta \varphi} \dots f_n \Phi_n \right). \tag{106}$$

Hence, condition T11a implies that a time-ordered product with $n+1$ factors such that at least one of the factors is φ can be expressed in terms of time-ordered products with fewer factors. Using this fact, one may show that condition T11a implies all of the relations obtained by expanding eq. (102) to any order in J. Thus, condition T11a is equivalent to eq. (102) and contains the full content of condition T11 in the case of an external current.

(3) The requirement T11a could also have be formulated in terms of advanced products by replacing "$\mathscr{R}$" by "$\mathscr{A}$" on the left side of eq. (105) and by replacing the retarded propagator Δ^{ret} by the advanced propagator Δ^{adv} on the right side. It is not difficult to show (using the commutator property T9) that this would yield an equivalent requirement.

(4) If we choose $J = (\nabla^a \nabla_a - m^2 - \xi R) h$ and use the Leibniz rule T10 as well as $(\nabla^a \nabla_a - m^2 - \xi R) \Delta^{\mathrm{ret}} = \delta$, eq. (106) yields

$$\mathscr{T} \left(\boldsymbol{\epsilon} h (\nabla^a \nabla_a - m^2 - \xi R) \varphi \prod f_i \Phi_i \right) = \mathrm{i} \sum_i \mathscr{T} \left(f_1 \Phi_1 \cdots h \frac{\delta(f_i \Phi_i)}{\delta \varphi} \dots f_n \Phi_n \right), \tag{107}$$

In theorem 5.3 in the next section, we will see that eq. (107) is necessary and sufficient for the interacting field to satisfy the interacting equations of motion.

(5) In the simple case of two free-field factors, eq. (106) reduces (in unsmeared form) to simply

$$\mathscr{T}(\varphi(x)\varphi(y)) = \varphi(x)\varphi(y) + \mathrm{i}\Delta^{\mathrm{ret}}(x,y)\mathbb{1}. \tag{108}$$

This agrees with eq. (7), which was deduced from axioms T1-T9. Similarly, condition T11a directly yields

$$\mathscr{T}(P\varphi(x)\varphi(y)) = i\delta(x,y)\mathbb{1}, \tag{109}$$

which agrees with eq. (58), which was deduced from the Leibniz rule. These agreements are comforting, but they illustrate that many nontrivial consistency checks will arise when we attempt to impose condition T11a along with T1-T10. A proof that T1-T10, T11a, and T11b (see below) can all be consistently imposed will be given in section 6.

4.3 Metric variation: Axiom T11b

We now apply condition T11 to the case where the interaction Lagrangian corresponds to a variation in the spacetime metric, i.e., $L_1 = L_0(\mathbf{g}) - L_0(\mathbf{g}')$, where $\mathbf{g}$ and $\mathbf{g}'$ are both globally hyperbolic and differ only in a compact subset K. In this case, condition T11 becomes

$$\tau^{\mathrm{ret}}\left[\mathscr{T}_{\mathbf{g}'}\left(\prod_{i=1}^{m} f_i\Phi_i\right)\right] = \sum_n \frac{\mathrm{i}^n}{n!}\mathscr{R}_{\mathbf{g}}\left(\prod_{i=1}^{m} f_i\Phi_i; \underbrace{L_1\cdots L_1}_{n\text{ factors}}\right). \tag{110}$$

As in the case of an external current considered in the previous subsection, it is useful to pass to an infinitesimal version of this equation. To accomplish this, we introduce a smooth 1-parameter family of metrics $\mathbf{g}^{(s)}$ differing from $\mathbf{g} = \mathbf{g}^{(0)}$ only within K. To first order in s, the interaction Lagrangian density is then given by $L_1 = (s/2)\boldsymbol{\epsilon} h_{ab}T^{ab}$, where $h_{ab} = \frac{\partial}{\partial s}g^{(s)}_{ab}$, and where T_{ab} is the stress energy tensor (6). For all $f_i\Phi_i \in \mathcal{F}_{\mathrm{class}}$ we define

$$\delta^{\mathrm{ret}}_{\mathbf{g}}\left[\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right)\right] = \frac{\partial}{\partial s}\tau^{\mathrm{ret}}_{\mathbf{g}^{(s)}}\left[\mathscr{T}_{\mathbf{g}^{(s)}}\left(\prod f_i\Phi_i\right)\right]\Bigg|_{s=0}. \tag{111}$$

In appendix A, we show that the right side of this equation exists as a well defined element of $\mathcal{W}(M,\mathbf{g})$. By differentiating eq. (110) with respect to s and setting $s=0$, we obtain the following infinitesimal version of condition T11 in the case of metric variations:

T11b Stress-energy factor: Let $\mathscr{T}_{\mathbf{g}^{(s)}}$ be the 1-parameter family of time-ordered products associated with a smooth 1-parameter family of globally hyperbolic metrics $\mathbf{g}^{(s)}$ on M that vary only within some compact subset K, and such that $\mathbf{g} \equiv \mathbf{g}^{(0)}$. Then we require that for all $f_i\Phi_i \in \mathcal{F}_{\rm class}$,

$$
\begin{aligned}
\delta^{\rm ret}_{\mathbf{g}}\left[\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right)\right] &= \frac{\rm i}{2}\mathscr{R}_{\mathbf{g}}\left(\prod f_i\Phi_i; \boldsymbol{\epsilon} h_{ab}T^{ab}\right) \\
&+ \sum_i \mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\cdots h_{ab}\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\cdots f_n\Phi_n\right), \qquad (112)
\end{aligned}
$$

where h_{ab} is the compactly supported tensor field given by

$$
h_{ab} = \frac{\partial}{\partial s} g^{(s)}_{ab}\bigg|_{s=0}, \qquad (113)
$$

and the functional derivative, $\delta A/\delta g_{ab}$, of a classical functional $A \in \mathcal{F}_{\rm class}$ with respect to the metric, $\mathbf{g}$, is defined in appendix B and is explicitly given by the formula

$$
\frac{\delta A}{\delta g_{ab}} = \sum_r (-1)^r \, \mathring{\nabla}_{(c_1}\cdots\mathring{\nabla}_{c_r)} \, \frac{\partial A}{\partial(\mathring{\nabla}_{(c_1}\cdots\mathring{\nabla}_{c_r)}\, g_{ab})}. \qquad (114)
$$

In this formula, $\mathring{\nabla}_a$ is an arbitrary fixed, background derivative operator, and it is understood that we have re-written the dependence of A on ∇_a and the curvature in terms of $\mathring{\nabla}_a$ and $\mathring{\nabla}_a$-derivatives of $\mathbf{g}$. Note that when none of the functionals $f_i\Phi_i$ explicitly depend upon the metric (including dependence on ∇_a or curvature terms), then the term in the second line of eq. (112) is absent.

Remarks: **(1)** We are not aware of condition T11b having been proposed previously.

(2) Condition T11b represents only the "first order" part of the identity (110), so one might wonder if one would get any new requirements by expanding eq. (110) to higher orders. However, it can be checked by an explicit calculation that this is not the case, i.e., that all of the higher order relations implicit in eq. (110) already follow from the first order condition stated as T11b. This is not surprising since condition T11b is required to hold for metric variations about *all* (globally hyperbolic) spacetimes.

(3) Using eq. (89) we can re-write condition T11b purely in terms of time-ordered products as

$$
\begin{aligned}
\delta^{\rm ret}_{\mathbf{g}}\left[\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right)\right] &= \frac{\rm i}{2}\mathscr{T}_{\mathbf{g}}\left(\boldsymbol{\epsilon} h_{ab}T^{ab}\prod f_i\Phi_i\right) - \frac{\rm i}{2}T^{ab}(\boldsymbol{\epsilon} h_{ab})\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right) \\
&+ \sum_i \mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\cdots h_{ab}\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\cdots f_n\Phi_n\right). \qquad (115)
\end{aligned}
$$

(4) In Euclidean field theory for the action (2) on a complete Riemannian manifold there will, in general, be a unique Green's function for the (now elliptic) operator P. Hence, there would be no distinction between retarded and advanced variations, nor between retarded and advanced products. There also would be a unique, preferred vacuum state, $\langle\ \rangle_0$. The Euclidean version of condition T11b would be:

$$\begin{aligned} \delta_{\mathbf{g}}\langle\Phi_1(f_1)\cdots\Phi_n(f_n)\rangle_0 &= \frac{1}{2}\langle\Phi_1(f_1)\cdots\Phi_n(f_n)T^{ab}(\boldsymbol{\epsilon}h_{ab})\rangle_0 \\ &+ \sum_i\left\langle\Phi_1(f_1)\cdots\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}(h_{ab})\cdots\Phi_n(f_n)\right\rangle_0 . \end{aligned} \tag{116}$$

This corresponds to the formula that one would formally obtain by assuming that the correlation functions $\langle\Phi_1(f_1)\cdots\Phi_n(f_n)\rangle_0$ can be defined by a path integral

$$\langle\Phi_1(f_1)\cdots\Phi_n(f_n)\rangle_0 = \int [D\varphi]\,\Phi_1(f_1)\cdots\Phi_n(f_n)e^{-S(\varphi,\mathbf{g})} . \tag{117}$$

Of course, in curved spacetime, there is no direct relationship between the formulations of the Euclidean and Lorentzian versions of quantum field theory, since a (non-static) Lorentzian spacetime will not, in general, be a real section of a complex analytic manifold with complex analytic metric that also admits a real Riemannian section. Nevertheless, we may view condition T11b as a mathematically precise formulation—applicable in the Lorentzian case—of a relation that can be formally derived from the Euclidean path integral.

(5) The requirement T11b could also have be formulated in terms of advanced variations and advanced products by replacing $\delta^{\rm ret}_{\mathbf{g}}$ by $\delta^{\rm adv}_{\mathbf{g}}$ on the left side of eq. (112) and replacing "$\mathscr{R}$" by "$\mathscr{A}$" on the right side of that equation, i.e.,

$$\begin{aligned} \delta^{\rm adv}_{\mathbf{g}}\left[\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right)\right] &= \frac{\rm i}{2}\mathscr{A}_{\mathbf{g}}\left(\prod f_i\Phi_i;\boldsymbol{\epsilon}h_{ab}T^{ab}\right) \\ &+ \sum_i \mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\cdots h_{ab}\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\cdots f_n\Phi_n\right), \end{aligned} \tag{118}$$

However, this formulation of condition T11b can be seen to be equivalent to eq. (112) as follows. If $\mathbf{g}^{(s)}$ is the one-parameter family of metrics appearing in eq. (112), then

$$\beta_s \equiv \tau^{\rm adv}_{\mathbf{g}^{(s)}}\circ(\tau^{\rm ret}_{\mathbf{g}^{(s)}})^{-1}, \tag{119}$$

is an automorphism of $\mathcal{W}(M,\mathbf{g})$ for all s with the property that $\beta_0 = id$. It was proven in [6], that, for all $a\in\mathcal{W}$, we have

$$\left.\frac{\partial}{\partial s}\beta_s(a)\right|_{s=0} = \frac{\rm i}{2}[T^{ab}(\boldsymbol{\epsilon}h_{ab}),a]\,, \tag{120}$$

where T^{ab} is the stress-energy tensor[19]. In particular, for any time-ordered product, we have[20]

$$\delta^{\rm adv}(\mathscr{T}) - \delta^{\rm ret}(\mathscr{T}) = \frac{\rm i}{2}[T^{ab}(\boldsymbol{\epsilon} h_{ab}), \mathscr{T}]. \tag{121}$$

Equivalence of eqs. (112) and (118) then follows from this equation and the definitions of advanced and retarded products.

4.4 External potential variation

Finally, for completeness, we state the infinitesimal version of condition T11 for the case of a variation of the external potential:

T11c φ^2 factor. Let $(M, \mathbf{g})$ be globally hyperbolic and let $V^{(s)}$ be a smooth one-parameter family of smooth functions which vary only in a fixed compact set K. Write $V = V^{(0)}$ and write $U = (\partial V^{(s)}/\partial s)|_{s=0}$. Then we require that for all $f_i\Phi_i \in \mathcal{F}_{\rm class}$,

$$\begin{aligned} \delta^{\rm ret}_V \left[\mathscr{T}_{(\mathbf{g},V)}\left(\prod f_i\Phi_i\right)\right] &= \frac{\rm i}{2}\mathscr{R}_{(\mathbf{g},V)}\left(\prod f_i\Phi_i; \boldsymbol{\epsilon} U\varphi^2\right) \\ &+ \sum_i \mathscr{T}_{(\mathbf{g},V)}\left(f_1\Phi_1 \cdots U\frac{\delta(f_i\Phi_i)}{\delta V}\cdots f_n\Phi_n\right). \end{aligned} \tag{122}$$

Remarks: **(1)** In writing condition T11c, we have generalized the definition of $\tau^{\rm ret}$ in the obvious way so that it now maps $\mathcal{W}(M, \mathbf{g}', V', J')$ to $\mathcal{W}(M, \mathbf{g}, V)$. The second term on the right side of eq. (122) is present in this formula because, as mentioned above, in the construction of the theory with an external potential, elements of $\mathcal{V}_{\rm class}$ are allowed to depend explicitly upon V.

(2) For the most part, condition T11c imposes restrictions on the definition of time-ordered products only if one has defined the exact theory in an arbitrary external potential. However, even if one considers only the theory defined by the action (2) (which does not include an external potential), condition T11c does impose a restriction on the definition of time-ordered products in the case where U is constant on the union of the supports of the f_i. For simplicity, we shall not consider this or any other consequences of condition T11c in the remainder of this paper. However, it should be straightforward to generalize the proof of section 6 to show that condition T11c can be consistently imposed for quantum field theory in curved spacetime with an arbitrary external potential.

[19] Equation (120) holds for any valid prescription for defining Wick powers satisfying T1–T10, since the ambiguity in T_{ab} is proportional to $\mathbb{1}$.

[20] Note that the advanced and retarded variations are only defined on local covariant field quantities such as the time-ordered products. By contrast, eq. (120) holds for an arbitrary element $a \in \mathcal{W}$.

(3) As mentioned at the beginning of this section, if we considered a complex scalar field, then we could also have a term in L_1 of the form $\mathrm{i}A^a(\bar{\varphi}\nabla_a\varphi - \varphi\nabla_a\bar{\varphi})\boldsymbol{\epsilon}$, corresponding to the presence of an external electromagnetic field. Our Principle of Perturbative Agreement would then lead to a corresponding additional condition ("T11d") on time-ordered products. We expect that this additional condition can also be consistently imposed (in addition to the analogs of all of our other conditions) for a complex scalar field. We also expect that the imposition of this condition will imply current conservation for the free and interacting fields in analogy with Theorems 5.1 and 5.3 below.

5 Some key consequences of our new requirements

In this section, we will derive some important consequences of our new requirements for both the free field theory and the interacting field theory. The demonstration that our requirements can, in fact, be imposed (except in two spacetime dimensions) will be given in section 6.

5.1 Consequences for the free field

In this subsection, we will derive some key consequences of condition T11b for the stress-energy tensor T_{ab} associated with the free field Lagrangian L_0.

Theorem 5.1. Suppose that the prescription for defining Wick products and time ordered products satisfies conditions T1–T10 together with condition T11b. Then the stress tensor T_{ab} defined via that prescription is automatically conserved

$$\nabla_a T^{ab}(x) = 0. \tag{123}$$

More generally, we have the following free field "Ward identity" for T_{ab}:

$$\begin{aligned} 0 &= \mathscr{T}\left((\boldsymbol{\epsilon}\nabla^a\xi^b)T_{ab}\prod^n f_i\Phi_i\right) \\ &+ \mathrm{i}\sum_i \mathscr{T}\left(f_1\Phi_1\cdots\frac{\delta(f_i\Phi_i)}{\delta\varphi}\pounds_\xi\varphi\cdots f_n\Phi_n\right). \end{aligned} \tag{124}$$

Proof. We first show that the divergence of the stress tensor is a c-number, i.e., proportional to the identity operator. Let F be a density of compact support, and let ξ^a be a compactly supported vector field. Then $(\nabla_a T^{ab})(\boldsymbol{\epsilon}\xi_b) = -(1/2)T_{ab}(\boldsymbol{\epsilon}\pounds_\xi g^{ab})$, and the commutator property, T9, yields

$$[T^{ab}(\boldsymbol{\epsilon}\pounds_\xi g_{ab}), \varphi(F)] = \mathrm{i}\mathscr{T}\left((\Delta F)\frac{\delta}{\delta\varphi}\boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab}\right). \tag{125}$$

We want to show that the right side of this equation is, in fact, equal to 0. To see this, we write $\boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab} = 2(\pounds_\xi g_{ab})\,\delta L_0/\delta g_{ab}$ and use the fact, proven in appendix B, that functional derivatives of L_0 with respect to φ and $\mathbf{g}$ commute modulo exact forms in the sense of eq. (268). We therefore obtain

$$\begin{aligned}(\Delta F)\frac{\delta}{\delta\varphi}\boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab} &= 2(\pounds_\xi g_{ab})\frac{\delta}{\delta g_{ab}}\left((\Delta F)\frac{\delta L_0}{\delta\varphi}\right) + \mathrm{d}\,B_0 \\ &= 2(\pounds_\xi g_{ab})\frac{\delta}{\delta g_{ab}}\Big((\Delta F)\boldsymbol{\epsilon}P\varphi\Big) + \mathrm{d}\,B_0\,, \end{aligned} \tag{126}$$

where in this equation ΔF is viewed as being evaluated at the metric $\mathbf{g}$ about which the variations are being taken (i.e., the $\delta/\delta g_{ab}$ does not act on Δ). However, we have

$$\begin{aligned}(\pounds_\xi g_{ab})\frac{\delta}{\delta g_{ab}}\Big((\Delta F)\boldsymbol{\epsilon}P\varphi\Big) &= \pounds_\xi\Big((\Delta F)\boldsymbol{\epsilon}P\varphi\Big) - \Big(\pounds_\xi(\Delta F)\Big)\boldsymbol{\epsilon}P\varphi - (\Delta F)\boldsymbol{\epsilon}P(\pounds_\xi\varphi) \\ &= -\Big(\pounds_\xi(\Delta F)\Big)\boldsymbol{\epsilon}P\varphi - P(\Delta F)\pounds_\xi\varphi + \mathrm{d}\,B_1 \\ &= -\Big(\pounds_\xi(\Delta F)\Big)\boldsymbol{\epsilon}P\varphi + \mathrm{d}\,B_1\,, \end{aligned} \tag{127}$$

where in the second line we used the facts that $\pounds_\xi$ applied to any D-form is exact and that P is self-adjoint, whereas in the last line we used the fact that $P(\Delta F) = 0$. Using the Leibniz rule, T10, we see that the right side of eq. (125) is equal to $-2\mathrm{i}\varphi[\boldsymbol{\epsilon}P(\pounds_\xi\Delta F)]$, which indeed vanishes since the quantum field φ satisfies the Klein-Gordon equation. Thus, $T^{ab}(\boldsymbol{\epsilon}\pounds_\xi g_{ab})$ commutes with $\varphi(F)$ for all compactly supported F. By Proposition 2.1 of [13], every element of $\mathcal{W}$ with this property has to be proportional to $\mathbb{1}$. Since $\nabla^a T_{ab}$ is locally and covariantly constructed out of the metric by T1, we must therefore have that

$$T^{ab}(\boldsymbol{\epsilon}\pounds_\xi g_{ab}) = \int_M C_a\xi^a\boldsymbol{\epsilon}\cdot\mathbb{1} \tag{128}$$

for some local curvature term C_a. Furthermore, by our scaling axiom T2, C_a must be a polynomial in the Riemann tensor and its covariant derivatives of dimension length^{-D-1}. We will now show that if condition T11b holds, then C_a, in fact, has to vanish.

To prove this, we consider the retarded variation of the local covariant field $T^{ab}(\boldsymbol{\epsilon}\pounds_\xi g_{ab})$ with the metric variation taken to be of the "pure gauge" form $h_{ab} = \pounds_\eta g_{ab}$, where η^a is a compactly supported vector field. Condition T11b in the simple case of only one factor $f_1\Phi_1 = \boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab}$ yields

$$\delta^{\mathrm{ret}}(T^{ab}(\boldsymbol{\epsilon}\pounds_\xi g_{ab})) = \frac{\mathrm{i}}{2}\mathscr{R}(\boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab}; \boldsymbol{\epsilon}(\pounds_\eta g_{cd})T^{cd}) + \mathscr{T}\left((\pounds_\eta g_{cd})\frac{\delta}{\delta g_{cd}}(\boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab})\right). \tag{129}$$

By eq. (128), the left side of this equation is just

$$\delta^{\mathrm{ret}}(T^{ab}(\boldsymbol{\epsilon}\pounds_\xi g_{ab}) = \int_M \xi^a \pounds_\eta (C_a \boldsymbol{\epsilon}) \cdot \mathbb{1} = -\int_M [\eta, \xi]^a C_a \boldsymbol{\epsilon} \cdot \mathbb{1}\,, \tag{130}$$

where a partial integration was done in the last step. Now subtract from eq. (129) the same equation with η^a and ξ^a interchanged. We obtain

$$\begin{aligned} -2\int_M [\eta,\xi]^a C_a \boldsymbol{\epsilon} \cdot \mathbb{1} &= \frac{\mathrm{i}}{2}\mathscr{R}\left(\boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab}; \boldsymbol{\epsilon}(\pounds_\eta g_{cd})T^{cd}\right) - \frac{\mathrm{i}}{2}\mathscr{R}\left(\boldsymbol{\epsilon}(\pounds_\eta g_{cd})T^{cd}; \boldsymbol{\epsilon}(\pounds_\xi g_{ab})T^{ab}\right) \\ &+ 2\mathscr{T}\left((\pounds_\eta g_{cd})\frac{\delta}{\delta g_{cd}}\left\{(\pounds_\xi g_{ab})\frac{\delta}{\delta g_{ab}}L_0\right\} - (\pounds_\xi g_{cd})\frac{\delta}{\delta g_{cd}}\left\{(\pounds_\eta g_{ab})\frac{\delta}{\delta g_{ab}}L_0\right\}\right)\,, \end{aligned} \tag{131}$$

where we again substituted $\boldsymbol{\epsilon}T^{ab} = 2\delta L_0/\delta g_{ab}$. The terms on the right side can be simplified as follows: For the retarded products, we use the identity $\mathscr{R}(f\Phi, h\Psi) - \mathscr{R}(h\Psi, f\Phi) = [\Psi(h), \Phi(f)]$, which holds for any Wick products Φ, Ψ. In the case at hand, Φ and Ψ are equal to the divergence of the stress tensor and therefore have a vanishing commutator by eq. (128). Hence, there is no contribution from the terms in eq. (131) involving retarded products. The last term on the right side can be simplified using the identity

$$(D_\xi D_\eta - D_\eta D_\xi)A = D_{[\eta,\xi]}A + \mathrm{d}\,C \tag{132}$$

holding for the "derivative operator"

$$D_\xi A = (\pounds_\xi g_{ab})\frac{\delta A}{\delta g_{ab}} \tag{133}$$

on classical functionals A of the metric such as L_0. A proof of this identity is given in appendix B. Inserting this relation (with $A = L_0$) and using again eq. (128), we find that the last term in eq. (131) is just $-\int_M [\eta,\xi]^a C_a \boldsymbol{\epsilon} \cdot \mathbb{1}$. Thus, we obtain

$$\int_M C_a [\xi, \eta]^a \boldsymbol{\epsilon} = 0. \tag{134}$$

This equation holds for all smooth compactly supported vector fields ξ^a, η^a. Variation with respect to ξ^a yields

$$(\nabla_a \eta^b)C_b + (\nabla_b \eta^b)C_a + \eta^b \nabla_b C_a = 0 \tag{135}$$

for all η^a, at every point in M. Now focus on an arbitrary, but fixed point $x \in M$. At x, the quantities η^a and ${K_a}^b = \nabla_a \eta^b$ can be chosen independently to be arbitrary tensors. Choosing first ${K_a}^b = 0$ and η^a arbitrary, we conclude that $\nabla_b C_a = 0$ at x. Thus, at any $x \in M$ we must have

$$({K_a}^b + {K_c}^c {\delta_a}^b)C_b = 0 \tag{136}$$

for all $K_a{}^b$, which is possible only when $C_b = 0$. This completes the proof of stress-tensor conservation, eq. (123).

To prove the more general Ward identity, eq. (124), we again consider condition T11b for the case of a "pure gauge" metric variation $h_{ab} = \pounds_\xi g_{ab} = 2\nabla_{(a}\xi_{b)}$, but we now consider arbitrary factors of $f_i\Phi_i$. We obtain

$$\begin{aligned}
\delta^{\rm ret}\left[\mathscr{T}\left(\prod f_i\Phi_i\right)\right] &= \mathrm{i}\mathscr{R}\left(\prod^n f_i\Phi_i;(\boldsymbol{\epsilon}\nabla^a\xi^b)T_{ab}\right) \\
&+ \sum_i \mathscr{T}\left(f_1\Phi_1\cdots(\pounds_\xi g_{ab})\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\cdots f_n\Phi_n\right). \qquad (137)
\end{aligned}$$

But, for our "pure gauge" metric variation, we have[21]

$$\begin{aligned}
\delta^{\rm ret}_{\mathbf{g}}\left(\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right)\right) &= \frac{\partial}{\partial s}\mathscr{T}_{\mathbf{g}}((\chi_{s\,*}f_1)\Phi_1\cdots(\chi_{s\,*}f_n)\Phi_n)\Big|_{s=0} \\
&= -\sum_i \mathscr{T}_{\mathbf{g}}(f_1\Phi_1\cdots(\pounds_\xi f_i)\Phi_i\cdots f_n\Phi_n), \qquad (138)
\end{aligned}$$

since the time ordered products are local, covariant fields. Moreover, writing the retarded product on the right side of eq. (137) in terms of time ordered products and using the relation $T_{ab}(\boldsymbol{\epsilon}\nabla^a\xi^b) = 0$ which we just proved above, we find

$$\begin{aligned}
\text{right side of eq. (137)} &= \mathrm{i}\mathscr{T}\left((\boldsymbol{\epsilon}\nabla^a\xi^b)T_{ab}\prod^n f_i\Phi_i\right) \\
&+ \sum_i \mathscr{T}\left(f_1\Phi_1\cdots(\pounds_\xi g_{ab})\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\cdots f_n\Phi_n\right). \qquad (139)
\end{aligned}$$

We now use the fact—proven in appendix B—that for any classical field D-form $f_i\Phi_i \in \mathcal{F}_{\rm class}$, we have

$$(\pounds_\xi f_i)\Phi_i + \frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\pounds_\xi g_{ab} + \frac{\delta(f_i\Phi_i)}{\delta\varphi}\pounds_\xi\varphi = \mathrm{d}\,H \qquad (140)$$

for some $(D-1)$-form H that is locally constructed out of g_{ab}, φ, f_i, and ξ^a. Inserting this relation into eq. (138) and (139), and using T10, we get the desired relation eq. (124). $\square$

Remarks: **(1)** There exist completely reasonable classical field theories for which T_{ab} in the quantum field theory cannot be made divergence free within our axiom scheme. As we have seen in subsection 3.2 above, one example of such a theory is the free scalar

[21]Note that the Lie derivative of a tensor field $f = f_{a\ldots c}{}^{b\ldots d}$ is defined by $\pounds_\xi f = \frac{\partial}{\partial s}\chi_s^* f$, which in turn is equal to $-\frac{\partial}{\partial s}\chi_{s\,*}f$, since $\chi_s^* = (\chi_s^{-1})_* = \chi_{-s\,*}$.

field in $D = 2$ spacetime dimensions. Hence Theorem 5.1 implies that T11b cannot be satisfied in addition to conditions T1-T10 for scalar field theory for $D = 2$.

(2) There appear to be two independent possible obstructions to the imposition of the analog of condition T11b in a general free quantum field theory. First, there may exist algebraic identities (i.e., relations that do not involve the field equations) satisfied by the classical stress-energy tensor. Within our axiom scheme, these identities must be respected by the quantum stress-energy tensor, and, consequently, the freedom to modify the definition of Wick powers by arbitrary local curvature terms of the correct dimension does not translate into a similar ability to modify the definition of T_{ab} so as to make it conserved, as is necessary for T11b to hold. As we have seen in subsection 3.2 above, this occurs for the free scalar field in $D = 2$ spacetime dimensions. However, we will see in the course of our analysis in section 6.2.6 below that, in principle, there also can exist a "cohomological obstruction" to the imposition of condition T11b. Although such a cohomological obstruction does not occur in scalar field theory, it can occur in parity violating theories, and it appears to be the cause of the failure of conservation of T_{ab} for the theories described in [1] in $D = 4k + 2$ spacetime dimensions. (In these theories, one finds that $\nabla^a T_{ab} = A_b \mathbb{1}$, where A_b (the "gravitational anomaly") is a curvature polynomial that does not arise as the divergence of a symmetric curvature tensor, i.e., $A_b \neq \nabla^a A_{ab}$ for any symmetric A_{ab}.) Thus, the analog of condition T11b also cannot be satisfied in theories analyzed in [1], but the root cause of the failure of condition T11b for these theories appears to be different in nature from the root cause of the failure of condition T11b for a scalar field in $D = 2$ dimensions.

(3) Note that our Ward identity, eq. (124), is a relation between elements in the free field algebra $\mathcal{W}(M, \mathbf{g})$, rather than an relation between correlation functions, which is the more conventional way to express Ward identities.

A similar type of argument to that used in the first part of the above proof can be applied in the context of a conformally coupled massless field to yield the following nontrivial consistency (or "cocycle") relation for the trace of the stress-energy tensor:

Theorem 5.2. Suppose that conditions T1–T10 and T11b are satisfied. Then, for the case of a massless, conformally coupled scalar field [i.e., $m = 0, \xi = (D-2)/4(D-1)$], we have $T^a{}_a(x) = C(x)\mathbb{1}$, where $C(x)$ is a local curvature term of mass dimension D that satisfies the "cocycle condition"

$$\int_M [k(\delta_f C) - f(\delta_k C)]\boldsymbol{\epsilon} = 0, \tag{141}$$

for any smooth compactly supported functions f, k on M, where

$$\delta_f C(\mathbf{g}) = \frac{\partial}{\partial s} C(e^{sf}\mathbf{g})\Big|_{s=0} \tag{142}$$

denotes the infinitesimal variation of a curvature term under a change in the conformal factor.

Proof. That the trace of the quantum stress tensor in the massless, conformally coupled case is proportional to the identity, $T^a{}_a = C\mathbb{1}$, follows, as in the proof of the previous theorem, from the fact that $[T^a{}_a(\boldsymbol{\epsilon} f), \varphi(F)] = 0$, which is an immediate consequence of the commutator property, T9, and the field equation for φ. By the scaling property T2, C must be a curvature polynomial of dimension length^{-D}. To show that T11b implies that this curvature polynomial satisfies the cocycle condition eq. (141), we consider the retarded variation of the field $T^a{}_a(\boldsymbol{\epsilon} f)$ with respect to the metric perturbation $h_{ab} = kg_{ab}$, where k is some smooth, compactly supported function (i.e., we consider an infinitesimal change k in the conformal factor of the metric g_{ab}). Condition T11b in the simple case where only the single factor $f_1\Phi_1 = \boldsymbol{\epsilon} f T^a{}_a$ is present now yields

$$\delta^{\rm ret}(T^a{}_a(\boldsymbol{\epsilon} f)) = \frac{\mathrm{i}}{2}\mathscr{R}(\boldsymbol{\epsilon} f T^a{}_a; \boldsymbol{\epsilon} k T^b{}_b) + \mathscr{T}\left((kg_{cd})\frac{\delta}{\delta g_{cd}}(\boldsymbol{\epsilon} f T^a{}_a)\right). \tag{143}$$

For the left side we use the fact that $T^a{}_a(\boldsymbol{\epsilon} f) = \int fC\boldsymbol{\epsilon}\cdot\mathbb{1}$, so the retarded variation with respect to $h_{ab} = kg_{ab}$ yields $\int f\delta_k(C\boldsymbol{\epsilon})\cdot\mathbb{1}$. Now antisymmetrize the above equation in k and f. We obtain

$$\begin{aligned}\int_M [k(\delta_f C) - f(\delta_k C)]\boldsymbol{\epsilon}\cdot\mathbb{1} &= \frac{\mathrm{i}}{2}\mathscr{R}\left(\boldsymbol{\epsilon} f T^a{}_a; \boldsymbol{\epsilon} k T^b{}_b\right) - \frac{\mathrm{i}}{2}\mathscr{R}\left(\boldsymbol{\epsilon} k T^b{}_b; \boldsymbol{\epsilon} f T^a{}_a\right) \\ &+ 2\mathscr{T}\left((fg_{cd})\frac{\delta}{\delta g_{cd}}\left\{(kg_{ab})\frac{\delta}{\delta g_{ab}}L_0\right\} - (kg_{ab})\frac{\delta}{\delta g_{ab}}\left\{(fg_{cd})\frac{\delta}{\delta g_{cd}}L_0\right\}\right). \end{aligned}\tag{144}$$

As in the proof of Theorem 5.1, the two retarded products on the right side combine to yield the commutator $(\mathrm{i}/2)[T^a{}_a(f\boldsymbol{\epsilon}), T^b{}_b(k\boldsymbol{\epsilon})]$, which in turn vanishes because the trace of the stress tensor is proportional to $\mathbb{1}$ (note that the retarded products individually might be non-vanishing). The last term on the right side also vanishes since taking the variation of L_0 with respect to the conformal factors f and k clearly does not depend on the order in which they are taken. Consequently, the right side vanishes, and we obtain the desired cocycle property (141) for the trace of the stress tensor, C. □

Remarks: **(1)** The cocycle condition on the conformal anomaly that we have derived here from axioms T1-T10 and T11b is the same condition as would be formally derived by assuming that the (expectation value of the) quantum stress-energy tensor can be calculated by taking the variation of some "effective action" with respect to the metric. Conditions of this nature are known in the literature under the name "Wess-Zumino consistency conditions" [21].

(2) The method of proof of the above theorem only relies upon properties T1–T10 and T11b, and therefore can be generalized to arbitrary field theories that satisfy suitable analogs of these conditions, and whose stress energy tensor has a c-number trace. We shall consider such "non-perturbative" results elsewhere.

(3) In odd spacetime dimensions, there simply are no scalar polynomials in the curvature of dimension length^{-D}, so there is no trace anomaly. By contrast, in even dimensions, there always exist curvature scalars C of dimension length^{-D} satisfying the cocycle condition. For example, any term scaling as $C \to \Omega^D C$ under a conformal transformation $g_{ab} \to \Omega^2 g_{ab}$ is a solution to the cocycle condition (141), so when $D = 2k$ with $k > 1$, any monomial expression in the Weyl tensor which contains k factors of the Weyl tensor is a solution. In $D = 4$ spacetime dimensions, there are 3 linearly independent local, covariant scalars with dimension (length)$^{-4}$ which solve the cocycle condition[22], namely, $C_1 = C_{abcd}C^{abcd}$, $C_2 = R_{abcd}R^{abcd} - 4R_{ab}R^{ab} + R^2$ (the Euler density), and $C_3 = \nabla^a \nabla_a R$. Since there are 4 linearly independent local covariant curvature terms with that dimension (namely, R^2 in addition to the above 3 terms), this shows explicitly that the cocycle condition is non-trivial, and thus is potentially useful for restricting the form of the trace anomaly. Of course, the existence of solutions to the cocycle condition does not automatically imply that there is actually a trace anomaly, as the coefficients of these terms might be zero. However, for the massless, conformally coupled scalar field in $D = 4$ dimensions, the arguments given in subsection 3.2 can be used to show that the coeficients of C_1 and C_2 must be nonvanishing for any prescription satisfying axioms T1-T10 and T11b. (The coeficient of C_3 can be set to zero using the renormalization freedom allowed by these axioms.) By the same type of arguments, it can presumably be established that C cannot be zero in any even dimension $D > 2$, although the calculations that must be carried out to show this rapidly become very complicated as the number of dimensions D of the spacetime increases. All solutions to the cocycle condition in $D = 6$ have been found in ref. [3]. We are not aware of an efficient algorithm to determine the general solution to the cocycle condition in arbitrary dimensions, and this appears to be an interesting mathematical problem.

5.2 Consequences for interacting fields

In this subsection, we will derive some important consequences of our requirements with regard to perturbatively defined interacting field theories. (Other consequences such as the existence of the renormalization group are derived in [15].) We will consider interacting theories described by a classical Lagrangian of the form

$$L = L_0 + L_1 \tag{145}$$

[22]If our axioms were weakened so as to require the locality and covariance condition T1 only for orientation preserving isometries, then the "parity violating" curvature term $C_4 = \epsilon_{abcd}R^{ab}{}_{pq}R^{pqcd}$ would be allowed and would also satisfy the cocycle condition.

where L_0 is given by eq. (2) and where the interaction Lagrangian is of the form

$$L_1 = \frac{1}{2} \sum \kappa_i \Phi_i. \tag{146}$$

The κ_i denote coupling parameters and each $\Phi_i \in \mathcal{V}_{\mathrm{class}}$ is any polynomial in the field φ and its derivatives as well as the Riemann tensor and its derivatives. In particular, we do not require that L_1 be renormalizable. Associated with the Lagrangian L is the classical stress-energy tensor Θ_{ab} given by

$$\Theta^{ab} = 2\boldsymbol{\epsilon}^{-1} \frac{\delta L}{\delta g_{ab}} = T^{ab} + 2\boldsymbol{\epsilon}^{-1} \frac{\delta L_1}{\delta g_{ab}}, \tag{147}$$

where T_{ab} is the stress tensor (6) associated with the free Lagrangian L_0.

As reviewed in subsection 4.1 above, if θ is a smooth function of compact support, interacting fields in the quantum field theory associated with the interaction Lagrangian θL_1 can be defined in perturbation theory in terms of time-ordered products of the free theory by the Bogoliubov formula, eq. (91). As shown in [5] and in section 3.1 of [15], one may always then take the limit as $\theta \to 1$ in a suitable way so as to (perturbatively) define the interacting theory with interaction Lagrangian L_1. (No restrictions on the asymptotic properties of the spacetime $(M, \mathbf{g})$ are needed in order to take this limit.) As explained in [15], the resulting interacting fields—denoted $\Phi_{L_1}(x)$—and interacting time-ordered products—denoted $\mathscr{T}_{L_1}(\prod f_i \Phi_i)$—live (after smearing with a smooth compactly supported test functions) in an suitable abstract algebra $\mathcal{B}_{L_1}(M, \mathbf{g})$ of formal power series of elements of $\mathcal{W}(M, \mathbf{g})$.

The classical stress tensor Θ^{ab} is conserved when the classical field equations associated with the Lagrangian, L, hold for φ. However, it is a priori far from clear that the quantized interacting field operator φ_{L_1} satisfies the interacting field equations, and, even if it does, it is far from clear that the interacting stress-energy operator $\Theta^{ab}_{L_1}$ is conserved. The following theorem—which constitutes one of the main results of this paper—establishes that if axioms T1-T10 hold, then condition T11a guarantees that φ_{L_1} satisfies the interacting field equations, and condition T11b guarantees that the interacting stress-energy operator $\Theta^{ab}_{L_1}$ is conserved.

Theorem 5.3. Suppose that the prescription for defining time-ordered products in the free theory with Lagrangian L_0 satisfies axioms T1-T10. Let L_1 be any interaction Lagrangian of the form eq. (146). Then the following properties hold for the interacting theory:

(1) Let B be a $(D-1)$-form on M depending polynomially on the classical field φ and its derivatives and the Riemann tensor and its derivatives. Then the map $\Phi_{L_1 + \mathrm{d}B}(f) \to \Phi_{L_1}(f)$ defines an isomorphism

$$\mathcal{B}_{L_1 + \mathrm{d}B}(M, \mathbf{g}) \cong \mathcal{B}_{L_1}(M, \mathbf{g}), \tag{148}$$

i.e., the theory is unchanged if a total divergence is added to the Lagrangian.

(2) The Leibniz rule holds for the interacting fields in the sense that

$$\nabla_a[\Phi_{L_1}(x)] = (\nabla_a\Phi)_{L_1}(x), \tag{149}$$

where the expression $(\nabla_a\Phi)$ on the right denotes the field expression obtained by applying the Leibniz rule. More generally, the Leibniz rule also holds for the interacting time-ordered products.

(3) If, in addition to T1-T10, axiom T11a also holds, then the equations of motion are satisfied in the interacting theory, i.e.,

$$(\nabla^a\nabla_a - m^2 - \xi R)\varphi_{L_1}(x) = -(\delta L_1/\delta\varphi)_{L_1}(x) \tag{150}$$

in the sense of distributions valued in $\mathcal{B}_{L_1}(M, \mathbf{g})$. Here, the variation on the right is the usual Euler-Lagrange type variation defined in eq. (42) above.

(4) If, in addition to T1-T10, axiom T11b also holds, then the interacting stress-energy tensor is conserved

$$\nabla_a\Theta^{ab}_{L_1}(x) = 0. \tag{151}$$

More generally, for all $J_i\Psi_i \in \mathcal{F}_{\text{class}}$, and all vector fields ξ^a of compact support, the following interacting field Ward identity holds:

$$\begin{aligned} 0 &= \mathscr{T}_{L_1}\left((\boldsymbol{\epsilon}\nabla^a\xi^b)\Theta_{ab}\prod^n J_i\Psi_i\right) \\ &+ \mathrm{i}\sum_i \mathscr{T}_{L_1}\left(J_1\Psi_1\cdots\frac{\delta(J_i\Psi_i)}{\delta\varphi}\pounds_\xi\varphi\cdots J_n\Psi_n\right). \end{aligned} \tag{152}$$

Proof. From the construction of the interacting fields given in section 3.1 of [15], it is clear that it suffices to prove the statements in the theorem for a cutoff interaction θL_1, where θ is a smooth function of compact support which is equal to 1 in the spacetime region under consideration. Statements (1) and (2) of the theorem are seen to be an immediate consequence of the Leibniz rule T10 applied to the individual terms in the formula

$$\Phi_{\theta L_1}(f) \equiv \sum_{n\geq 0}\frac{\mathrm{i}^n}{n!}\mathscr{R}\left(f\Phi; (\theta L_1)^n\right), \tag{153}$$

where $\theta = 1$ on the support of f.

In order to prove statement (3), we must show that for any smooth function f of compact support, we have

$$\varphi_{\theta L_1}(\boldsymbol{\epsilon}(\nabla^a\nabla_a - m^2 - \xi R)f) = -(\delta L_1/\delta\varphi)_{\theta L_1}(f), \tag{154}$$

where, again, $\theta = 1$ on the support of f. In terms of retarded products, we need to show that

$$0 = \mathscr{R}\left(\boldsymbol{\epsilon} f(\nabla^a\nabla_a - m^2 - \xi R)\varphi; e^{\mathrm{i}\theta L_1}\right) + \mathscr{R}\left(f\frac{\delta L_1}{\delta\varphi}; e^{\mathrm{i}\theta L_1}\right), \tag{155}$$

However, using the definition of the retarded products in terms of time-ordered products [see eq. (87)], and using the fact that $\theta \equiv 1$ on the support of f, we see that eq. (155) is equivalent to

$$\mathscr{T}\left(\boldsymbol{\epsilon} f(\nabla^a\nabla_a - m^2 - \xi R)\varphi\prod^n \theta L_1\right) = \mathrm{i}n\mathscr{T}\left(f\frac{\delta(\theta L_1)}{\delta\varphi}\prod^{n-1}\theta L_1\right) \tag{156}$$

for all natural numbers n. But this equation is equivalent to (107) above, which was previously shown to hold as a direct consequence of condition T11a. Thus, we have succeeded in showing that the equations of motion (150) hold in the interacting theory.

To prove eq. (151) of statement (4), we must show that for any smooth vector field ξ^a of compact support, we have

$$(\Theta_{ab})_{\theta L_1}(\boldsymbol{\epsilon}\nabla^a\xi^b) = 0. \tag{157}$$

where $\theta = 1$ on the support of ξ^a. In terms of retarded products, we need to show that

$$0 = \mathscr{R}\left((\boldsymbol{\epsilon}\nabla^a\xi^b)T_{ab}; e^{\mathrm{i}\theta L_1}\right) + 2\mathscr{R}\left((\nabla^a\xi^b)\frac{\delta L_1}{\delta g^{ab}}; e^{\mathrm{i}\theta L_1}\right). \tag{158}$$

Equation (158) is seen to be equivalent to

$$\mathscr{T}\left((\boldsymbol{\epsilon}\nabla^a\xi^b)T_{ab}\prod^n\theta L_1\right) \quad = \quad \mathrm{i}n\mathscr{T}\left((\pounds_\xi g_{ab})\frac{\delta(\theta L_1)}{\delta g^{ab}}\prod^{n-1}\theta L_1\right) \tag{159}$$

for all natural numbers n. Now, if we apply eq. (140) to the case $f_i = \theta$, $\Phi_i = L_1$ and use the fact that $\theta = 1$ on the support of ξ^a, we obtain

$$\frac{\delta(\theta L_1)}{\delta g_{ab}}\pounds_\xi g_{ab} + \frac{\delta(\theta L_1)}{\delta\varphi}\pounds_\xi\varphi = \mathrm{d}\, B. \tag{160}$$

Therefore, by the Leibniz rule T10, we can rewrite eq. (159) in the equivalent form

$$\mathscr{T}\left((\boldsymbol{\epsilon}\nabla^a\xi^b)T_{ab}\prod^n\theta L_1\right) \quad = \quad -\mathrm{i}n\mathscr{T}\left(\frac{\delta(\theta L_1)}{\delta\varphi}\pounds_\xi\varphi\prod^{n-1}\theta L_1\right). \tag{161}$$

But this equation holds as a consequence of the free field Ward identity eq. (124), which was proven to hold when condition T11b is satisfied. Thus, we have shown that eq. (151) holds, i.e., the interacting stress-energy is conserved in the interacting theory.

To prove the interacting Ward identity, eq. (152), we will need the generalization of eq. (124) for the case where L_1 may also depend upon an external source $J_{ab\dots c}$,

$$L_1 = L_1(g_{ab}, (\nabla)^k\varphi, J_{ab\dots c}). \tag{162}$$

We assume the source to be a smooth compactly supported tensor field on M although certain distributional sources would also be admissible[23]. The generalization of the conservation law eq. (151) appropriate to this case is[24]

$$\Theta^{ab}_{L_1}(\pounds_\xi g_{ab}) + 2\left(\frac{\delta L_1}{\delta J_{ab\dots c}}\right)_{L_1}(\pounds_\xi J_{ab\dots c}) = 0 \tag{163}$$

for any compactly supported test vector field ξ^a. In unsmeared form, this equation can be written as

$$\begin{aligned}\nabla_q\Bigg[\Theta^{qr}_{L_1}(x) + \left(J^r{}_{ab\dots c}\frac{\delta L_1}{\delta J_{qab\dots c}}\right)_{L_1}(x)\\ + \left(J_a{}^r{}_{b\dots c}\frac{\delta L_1}{\delta J_{aqb\dots c}}\right)_{L_1}(x) + \dots + \left(J_{ab\dots c}{}^r\frac{\delta L_1}{\delta J_{ab\dots cq}}\right)_{L_1}(x)\Bigg]\\ = \left((\nabla^r J_{ab\dots c})\frac{\delta L_1}{\delta J_{ab\dots c}}\right)_{L_1}(x).\end{aligned} \tag{164}$$

A similar formula holds when there is any finite number of external sources.

Now consider, for a given Φ, the m-parameter family of interaction Lagrangians $K_1 = L_1 + \sum\lambda_j J_j\Psi_j$. We differentiate the interacting field Φ_{K_1} with respect to the parameters λ_i—identifying at the same time Φ_{K_1} with an element in $\mathcal{B}_{L_1}(M,\mathbf{g})$ via a suitably defined isomorphism $\tau^{\rm ret}: \mathcal{B}_{K_1}(M,\mathbf{g}) \to \mathcal{B}_{L_1}(M,\mathbf{g})$ associated with the respective algebras of interacting fields. We thereby obtain the retarded products[25] in the interacting field theory associated with L_1,

$$\frac{\partial^m}{\partial\lambda_1\dots\partial\lambda_m}\tau^{\rm ret}\left[\Phi_{L_1+\sum\lambda_j J_j\Psi_j}(F)\right]\Bigg|_{\lambda_i=0} = \mathscr{R}_{L_1}\left(F\Phi;\prod_j J_j\Psi_j\right). \tag{165}$$

[23]It can be shown as a consequence of the microlocal spectrum condition that any distributional source with spacelike WF(J) would be admissible, i.e., lead to well defined interacting field expressions. For example J given by the delta distribution supported on a timelike smooth submanifold S, $\delta_S(f) = \int_S fn\cdot\boldsymbol{\epsilon}$, (with n^a the normal to S) is acceptable.

[24]The factor of 2 in front of the second term arises because Θ_{ab} is twice the metric variation.

[25]In a similar way, we could write the advanced products in the interacting field theory considering instead the corresponding *-isomorphism $\tau^{\rm adv}: \mathcal{B}_{K_1}(M,\mathbf{g}) \to \mathcal{B}_{L_1}(M,\mathbf{g})$, but this would make no difference in the argument.

Now consider the special case in which Φ is the stress energy tensor associated with the Lagrangian density $L_0 + K_1$, i.e., we choose

$$\Phi^{ab} = \Theta^{ab} + 2\boldsymbol{\epsilon}^{-1} \sum \lambda_j \frac{\delta(J_j \Psi_j)}{\delta g_{ab}}, \tag{166}$$

where Θ_{ab} is the stress-energy tensor eq. (147) associated with $L_0 + L_1$. We also choose the "F" in eq. (165) to be $F_{ab} = \boldsymbol{\epsilon} \nabla_a \xi_b$, where ξ^a is a smooth, compactly supported vector field. We use formula (163) (with L_1 replaced by K_1) to calculate $\Phi^{ab}_{K_1}(F_{ab})$, and differentiate the resulting identity with respect to the parameters λ_i. This gives

$$\begin{aligned} &\mathrm{i}\mathscr{R}_{L_1}\left(\boldsymbol{\epsilon}(\nabla_a \xi_b)\Theta^{ab}; \prod_j J_j \Psi_j\right) = \\ &\qquad \sum_j \mathscr{R}_{L_1}\left(\frac{\delta(J_j\Psi_j)}{\delta g_{ab}} \pounds_\xi g_{ab}; \prod_{i \neq j} J_i \Psi_i\right) + \sum_j \mathscr{R}_{L_1}\left(\Psi_j \pounds_\xi J_j; \prod_{i\neq j} J_i \Psi_i\right). \end{aligned} \tag{167}$$

We now again apply eq. (140), this time with $f_i \Phi_i = J_j \Psi_j$, to obtain

$$\frac{\delta(J_j\Psi_j)}{\delta g_{ab}} \pounds_\xi g_{ab} + \Psi_j \pounds_\xi J_j + \frac{\delta(J_j \Psi_j)}{\delta \varphi} \pounds_\xi \varphi = \mathrm{d}\, B, \tag{168}$$

and we apply the Leibniz rule to the retarded products in (167) (which also holds for the interacting quantities, since these are expressible in terms of the time ordered products in the free theory). Finally, we express the retarded products $\mathscr{R}_{L_1}$ in the interacting theory in terms of time ordered products $\mathscr{T}_{L_1}$ in the interacting theory (using a formula completely analogous to eq. (112)). When this is done, we arrive at the Ward identity, eq. (152), for the interacting field theory associated with the interaction Lagrangian L_1. $\square$

Remarks **(1)** We note explicitly that Theorem 5.3 does *not* say that an interacting field Φ_{L_1} vanishes when the classical field expression Φ is of the form $\Phi = \Psi \frac{\delta L}{\delta \varphi}$, with Ψ containing factors of φ. In other words, the theorem does not say that a general interacting field Φ_{L_1} vanishes if it would vanish in the classical interacting theory associated with L by the classical equations of motion. Rather, the theorem asserts only that this is true in the special cases $\Phi = \frac{\delta L}{\delta \varphi}$ and $\Phi_b = \nabla^a \Theta_{ab}$. Indeed, we have already seen in subsection 3.2 above that even in the free theory, field expressions of the form $\Psi \frac{\delta L_0}{\delta \varphi}$ will, in general be nonvanishing.

(2) Note that as in the case of the free theory, the interacting Ward identity, eq. (152), is a relation between elements in the algebra $\mathcal{B}_{L_1}(M, \mathbf{g})$ of interacting fields, rather than a relation between correlation functions associated with a state. Note also that the interacting Ward identity has the same form as the Ward identity (124) in the free quantum field theory, except that the free stress-energy tensor T_{ab} is replaced by the interacting stress-energy tensor Θ_{ab}. Note, however, that the Ward identity in the free theory is an operator identity between elements in the algebra $\mathcal{W}(M, \mathbf{g})$, whereas the interacting Ward identity is an identity in the interacting field algebra $\mathcal{B}_{L_1}(M, \mathbf{g})$.

(3) In our informal distribution notation (22) for the time-ordered products, the Ward identity (152) takes the form

$$\nabla_a^y \mathscr{T}_{L_1}\left(\Theta^{ab}(y) \prod^n \Psi_i(x_i)\right) = \mathrm{i} \sum_i \delta(y, x_i)\, \mathscr{T}_{L_1}\left(\Psi_1(x_1) \cdots \left((\nabla^b \varphi) \frac{\delta}{\delta \varphi} \Psi_i\right)(x_i) \cdots \Psi_n(x_n)\right). \quad (169)$$

6 Proof that there exists a prescription for time-ordered products satisfying T11a and T11b in addition to T1-T10

Our remaining task is to prove that requirements T11a and—in $D > 2$ dimensions—T11b can be consistently imposed in addition to requirements T1-T10. Specifically, we shall prove the following:

Theorem 6.1. In all spacetime dimensions $D > 2$, there exists a prescription for defining time-ordered products of the quantum scalar field with Lagrangian L_0, eq. (2), that satisfies conditions T1-T10, T11a, and T11b. When $D = 2$, there exists a prescription satisfying T1-T10 and T11a, but condition T11b cannot be imposed in addition to T1-T10.

We have already proven that condition T11b cannot be satisfied in addition to T1-T10 in $D = 2$ spacetime dimensions (see remark (1) following Theorem 5.1 above), so we need only prove the existence statements here.

We have already proved in proposition 3.1 above that T1–T10 always can be satisfied. Our strategy will therefore be to use the remaining "renormalization freedom" to additionally satisfy T11a and T11b. This remaining renormalization freedom may be precisely characterized as follows: In our previous work [13] (see also [15]) we proved a uniqueness theorem for time-ordered products satisfying T1–T9 whose factors do not contain derivatives of the fields. This result can be straightforwardly generalized to the case when derivatives are present and the prescription also satisfies T10. The generalized result is as follows: Let $\mathscr{T}$ and $\mathscr{T}'$ be arbitrary prescriptions for defining time-ordered products satisfying T1–T10. Then they must be related in the following way:

$$\mathscr{T}'\left(\prod_{i=1}^{n} A_i\right) = \mathscr{T}\left(\prod_{i=1}^{n} A_i\right) + \sum_{I_0\cup I_1\cup\cdots\cup I_k=\{1,\dots,n\}} \mathscr{T}\left(\prod_{k>0} \mathcal{O}_{|I_k|}\left(\bigotimes_{j\in I_k} A_j\right) \prod_{i\in I_0} A_i\right). \quad (170)$$

Here the $\mathcal{O}_r$ are linear maps (essentially the "counterterms", see eq. (175) below) $\mathcal{O}_r : \otimes^r \mathcal{F}_{\text{class}} \to \mathcal{F}_{\text{class}}$ that can be written in the following form:

$$\begin{aligned}\mathcal{O}_r(\otimes f_i \Phi_i)(x) = \sum_{\alpha_1,\alpha_2,\dots} \frac{1}{\alpha_1!\dots\alpha_r!} \int \prod_j \boldsymbol{\epsilon}(y_j) \\ c\left[\delta^{\alpha_1}\Phi_1 \otimes \cdots \otimes \delta^{\alpha_r}\Phi_r\right](x; y_1, \dots, y_r) \\ f_1(y_1)\dots f_{N_T}(y_r) \prod_{i=1}^{r} \prod_j [(\nabla)^j \varphi(y_i)]^{\alpha_{ij}}, \quad (171)\end{aligned}$$

where we are using the same notation as in the Wick expansion (63). The c are linear maps on $\otimes^r \mathcal{V}_{\text{class}}$ taking values in the distributions over M^{r+1}. These distributions are always writable as a sum of derivatives of the delta function $\delta(x; y_1, \dots, y_r)$, times polynomials in the Riemann tensor and its covariant derivatives and m^2. The engineering dimension of each such term appearing in $c[\otimes_i \Phi_i]$ (with the dimension of the delta function counted as rD) must be equal precisely to the sum of the engineering dimensions of the Φ_i, defined as in the scaling requirement, T2. The c must satisfy the reality condition

$$\overline{c\left[\otimes_{i=1}^n \Phi_i\right]} = (-1)^{n+1} c\left[\otimes_{i=1}^n \Phi_i\right] \quad (172)$$

as a consequence of the unitarity property satisfied by $\mathscr{T}$ and $\mathscr{T}'$, and they must satisfy the symmetry condition

$$c\left[\otimes_{i=1}^n \Phi_i\right](y; x_1, \dots, x_n) = c[\otimes_{i=1}^n \Phi_{\pi i}](y; x_{\pi 1}, \dots, x_{\pi n}) \quad \forall \text{ permutations } \pi, \quad (173)$$

as a consequence of the symmetry of the time ordered products. Finally, the imposition of the Leibniz rule, T10, on the time ordered products $\mathscr{T}$ and $\mathscr{T}'$ yields the following additional constraint on the c:

$$c\left[\Phi_1 \otimes \dots \nabla\Phi_i \otimes \dots \Phi_n\right] = (1 \otimes \cdots \underbrace{\nabla}_{i\text{-th slot}} \otimes \dots 1) c\left[\otimes_i \Phi_i\right]. \quad (174)$$

Formula eq. (170) can be restated more compactly using the generating functional $\mathcal{S}(A)$ for the time ordered products defined in eq. (88):

$$\mathcal{S}'(A) = \mathcal{S}(A + \frac{1}{\mathrm{i}}\mathcal{O}(e^{\mathrm{i}A})), \quad (175)$$

where

$$\mathcal{O}(e^{\mathrm{i}A}) = \sum_{n\geq 0} \frac{\mathrm{i}^n}{n!} \mathcal{O}_n \left(\bigotimes^n A \right) \tag{176}$$

is a formal power series in $\mathcal{F}_{\mathrm{class}}$. In other words, if $L_1 = A$ is the interaction Lagrangian, then $L_2 \equiv (1/\mathrm{i})\mathcal{O}(e^{\mathrm{i}L_1})$ corresponds precisely to the (finite) counterterms that must be added to L_1 in order to compensate for the change in the renormalization prescription from $\mathscr{T}$ to $\mathscr{T}'$.

Our task is to show that T11a and T11b can be satisfied by making changes within the allowed class of changes that we have just characterized in terms of the c.

6.1 Proof that T11a can be satisfied

It is not difficult to prove that T11a can always be satisfied in any dimension D, including $D = 2$. In fact, T11a automatically holds for the Wick powers (i.e., time-ordered products with one factor) when the latter are defined via the local normal ordering prescription given in eq. (60). To show that T1–T10 together with T11a can be satisfied for arbitrary time-ordered products, we proceed inductively in the number of powers of φ as follows. We assume that we are given a prescription which satisfies T1-T10 for arbitrary time-ordered products, and we assume, inductively, that T11a also holds for all time-ordered products $\mathscr{T}(f_1\Phi_1 \dots f_n\Phi_n)$ that contain a total number $N_\varphi < k$ powers of φ. From the identity $\mathscr{R}(\boldsymbol{\epsilon} J_1\varphi; \boldsymbol{\epsilon} J_2\varphi) = \mathrm{i}\Delta^{\mathrm{ret}}(\boldsymbol{\epsilon} J_1, \boldsymbol{\epsilon} J_2)$, we easily see that T11a is satisfied when $N_\varphi = 1$, which case occurs only when $n = 1$ and Φ_1 is linear in φ.

Consider now a set of fields $\Phi_1, \dots, \Phi_n$ with $N_\varphi = k$, and let $G_n(J; f_1, \dots, f_n)$ be the difference between the left and right sides of T11a (see eq. (105)). We wish to show that it is possible to change our prescription, if necessary, so that $G'_n = 0$ for the new prescription $\mathscr{T}'$, while maintaining T1–T10 on all time-ordered products and maintaining T11a on the time-ordered products with $N_\varphi < k$. It can easily be seen, from the causal factorization property and the definition of the retarded products, that $G_n(J; f_1, \dots, f_n) = 0$ for test functions $J, f_1, \dots, f_n$ supported off the total diagonal Δ_{n+1} in the product manifold M^{n+1}. Furthermore, using the inductive assumption and T9, one can verify by an explicit calculation that the commutator $[G_n(J; f_1, \dots, f_n), \varphi(F)]$ vanishes for any compactly supported F. Thus, by prop. 2.1 of [13], G_n must be proportional to the identity operator and can therefore be identified with a multilinear functional taking valuese in the complex numbers. By conditions T1-T5, this functional must actually be a distribution (i.e., it must be continuous in the appropriate sense) which is local and covariantly constructed from the metric, with a smooth/analytic dependence upon the metric and m^2, ξ, and with an almost homogeneous scaling behavior. Therefore, by the arguments in [13], G_n has to be a sum of covariant derivatives of the delta-distribution on M^{n+1}, multiplied by polynomials in m^2, covariant derivatives of the Riemann tensor, and analytic functions of ξ, of the appropriate dimension. It follows from unitarity T7 that G_n satisfies the reality condition $\bar{G}_n = (-1)^{n+1} G_n$.

We now set $c[\varphi \otimes (\otimes_i \Phi_i)] = -\mathrm{i} G_n$, and define $c[(\nabla)^k \varphi \otimes (\otimes_i \Phi_i)]$ via eq. (174). We use these c to define a new prescription $\mathscr{T}'$ via eqs. (170) and (171). It is clear that the new prescription satisfies $G'_n = 0$ and hence satisfies T11a for $N_\varphi = k$. Thus, our inductive proof will be complete if we can show that the c satisfy all of the properties that are necessary for the new prescription to satisfy T1-T10 on all time-ordered products. However, it is clear from its definition that c satisfies all of these properties, with the possible exception of the symmetry property (173). We now complete the proof by showing that c also satisfies this symmetry property. The symmetry property of $c[\varphi \otimes (\otimes_i \Phi_i)]$ holds trivially except in the case where we have a factor, say Φ_1, of the form $\Phi_1 = \varphi$ and we consider the interchange of Φ_1 and φ. Thus, let us consider the difference between the left and right sides of eq. (105) with free field factor $\boldsymbol{\epsilon} J_2 \varphi$, in the case when $f_1 \Phi_1 = \boldsymbol{\epsilon} J_1 \varphi$. Antisymmetrizing in J_1 and J_2, we get

$$
\begin{aligned}
& G_n(J_1; J_2, f_2, \dots, f_n) - G_n(J_2; J_1, f_2, \dots, f_n) \\
= \;& \left(\mathrm{i}\Delta^{\mathrm{ret}}(\boldsymbol{\epsilon} J_2, \boldsymbol{\epsilon} J_1) - \mathrm{i}\Delta^{\mathrm{ret}}(\boldsymbol{\epsilon} J_1, \boldsymbol{\epsilon} J_2) - [\varphi(\boldsymbol{\epsilon} J_1), \varphi(\boldsymbol{\epsilon} J_2)] \right) \mathscr{T}\left(\prod_{i=2}^{n} f_i \Phi_i \right) \\
+ \;& \sum_{i,j=2}^{n} \left[\mathscr{T}\left(\cdots (\Delta^{\mathrm{ret}} J_1 \boldsymbol{\epsilon}) \frac{\delta(f_i \Phi_i)}{\delta \varphi} \cdots (\Delta^{\mathrm{ret}} J_2 \boldsymbol{\epsilon}) \frac{\delta(f_j \Phi_j)}{\delta \varphi} \cdots \right) - (J_1 \leftrightarrow J_2) \right] \\
+ \;& \text{other terms,}
\end{aligned}
\tag{177}
$$

where "other terms" stand for expressions that vanish under the inductive assumption that T11a is true for $N_\varphi < k$. The first expression on the right side vanishes, because the commutator of φ with itself is given by $\mathrm{i}\Delta$ [see eq.(5)], and because $\Delta^{\mathrm{ret}}(\boldsymbol{\epsilon} J_2, \boldsymbol{\epsilon} J_1) = \Delta^{\mathrm{adv}}(\boldsymbol{\epsilon} J_1, \boldsymbol{\epsilon} J_2)$. The second expression on the right side vanishes because the time ordered products are symmetric. This shows that $G_n(J_1; J_2, f_2, \dots, f_n)$ is symmetric in J_1, J_2, implying that $c[\varphi \otimes \varphi \otimes \Phi_2 \otimes \dots \Phi_n]$ is symmetric in the spacetime arguments associated with the factors of φ, as we desired to show. This completes the proof.

We have therefore obtained a construction of time-ordered products satisfying T1–T10 and T11a. We will work with such a prescription in everything that follows. Any other prescription satisfying these properties will differ from the given one by formulas (170) and (171), where the distributions c must now satisfy the additional constraint

$$
c[\varphi \otimes (\otimes_i \Phi_i)] = 0 \tag{178}
$$

due to the imposition of the further requirement T11a.

6.2 Proof that T11b can be satisfied when $D > 2$

For the remainder of this section, we restrict consideration to spacetimes of dimension $D > 2$, and we will prove that the remaining requirement, T11b, can be satisfied together with all other requirements T1–T10, T11a.

Condition T11b is far from obvious even for the Wick products, and it is not satisfied by our local normal ordering prescription (60) (which satisfies T1–T10, T11a), as can be seen from the fact that the stress tensor T_{ab} when defined via the local normal ordering prescription fails to be conserved (see subsection 3.2), whereas any prescription satisfying T11b automatically gives rise to a conserved stress tensor by thm. 5.1. Thus, in order to construct a prescription satisfying T11b together with all other requirements, we have to reconsider even the definition of Wick powers.

For these reasons, it is not surprising that our proof of T11b is technically much more complex than the proof of T10 or T11a given in the previous sections. Nevertheless, the basic logic underlying the proof is actually rather simple and transparent. We now outline this basic logic, leaving the details to the following six subsections 6.2.1–6.2.6. As with many other constructions in this paper, it is convenient not to attempt to construct the time ordered products satisfying T11b in one stroke for an arbitrary number N_φ of factors of φ, but to proceed inductively in the number of factors. Starting off with the trivial case, we therefore assume that a prescription satisfying T11b has been give up to less than k factors. At $N_\varphi = k$ factors we consider the algebra valued map D_n which is precisely the failure of T11b to be satisfied: For a given collection of $f_i \Phi_i \in \mathcal{F}_{\rm class}$ with a total number of k factors of φ, and any smooth, compactly supported variation h_{ab} of the metric, this is given by

$$\begin{aligned} D_n^{ab}(h_{ab}; f_1, \dots, f_n) \quad \equiv \quad & \delta^{\rm ret}\left[\mathscr{T}\left(\prod_{i=1}^n f_i \Phi_i\right)\right] \\ - \quad & \frac{\mathrm{i}}{2}\mathscr{R}\left(\prod_{i=1}^n f_i\Phi_i; \boldsymbol{\epsilon} h_{ab} T^{ab}\right) \\ - \quad & \sum_i \mathscr{T}\left(f_1\Phi_1 \cdots h_{ab}\frac{\delta(f_i\Phi_i)}{\delta g_{ab}} \cdots f_n\Phi_n\right), \end{aligned} \tag{179}$$

where the retarded variation is taken with respect to the infinitesimal variation h_{ab} of the metric. (Note that D_n involves time ordered products with $N_T = n+1$ factors.) The basic idea of the proof is to show that the given prescription $\mathscr{T}$ for the time ordered products can be adjusted, if necessary, to a new prescription $\mathscr{T}'$—related to the original one by eq. (170)—in such a way that $D'_n = 0$ for this new prescription, and so that the coefficient distributions c implicit in eq. (170) obey the constraints described above. This then would show that T1–T10, T11a, and T11b will hold for the modified prescription for time ordered products with up to k factors of φ.

The obvious strategy for doing this is, of course, to absorb D_n into a redefinition of the appropriate time ordered products involving a stress energy factor by simply subtracting it from the given prescription, and we will indeed follow this basic strategy. However, while it is straightforward to show that subtracting D_n from the corresponding time ordered products $\mathscr{T}$ with a stress energy factor will automatically produce a new prescription $\mathscr{T}'$ satisfying $D'_n = 0$, it is not at all obvious that $\mathscr{T}'$ will continue to satisfy the other requirements T1–T10 and T11a. In order to demonstrate that this is indeed the case, we proceed by establishing a number of properties about D_n in the following subsections. The upshot is that D_n is 'sufficiently harmless', in the sense that subtracting it from the given prescription $\mathscr{T}$ will produce a $\mathscr{T}'$ which continues to have the desired properties T1–T10 and T11a.

In more detail, we proceed as follows:

(1) In subsection 6.2.1, we first show that D_n is a functional of $h_{ab}, f_1, \dots, f_n$ that is supported on the total diagonal.

(2) In subsection 6.2.2, we then establish that, at the induction order considered, D_n is a c-number.

(3) In subsection 6.2.3, we show that D_n is local and covariant, with an appropriate scaling behavior.

(4) In subsection 6.2.4, we show that $D_n = 0$ if one of the field factors is equal to φ.

(5) In subsection 6.2.5., we establish that D_n is not merely a linear functional, but in fact a distribution (i.e., continuous in the appropriate sense) with a smooth dependence upon the metric and with an appropriate scaling behavior under scaling of the metric.

(6) In subsection 6.2.6., we show that D_n has the appropriate symmetry property when one of the factors Φ_i is equal to a stress energy tensor T_{cd}.

These properties imply that D_n is, in fact, a delta function, multiplied by appropriate curvature polynomials (with appropriate symmetry properties). Since the freedom to redefine time-ordered products consists precisely in adding such delta function expressions, we can absorb D_n into a redefinition of time ordered products (here it is used that $D > 2$), while preserving T1–T10 and T11a. This is described in detail in subsection 6.2.7.

We now elaborate these arguments. As for the induction start, when there are no factors of φ in the fields $f_1\Phi_1, \dots, f_n\Phi_n$ on which D_n depends, we obviously must have $n = 0$. In this case, $D_0^{ab}(h_{ab}) = -(\mathrm{i}/2)\mathscr{R}(\boldsymbol{\epsilon} h_{ab} T^{ab})$, since $\delta^{\mathrm{ret}}(\mathbb{1}) = 0$. But any retarded product with only one factor vanishes by definition, so there is nothing to show for $N_\varphi = 0$. Let us therefore inductively assume that $D_n = 0$ for any set of $f_1\Phi_1, \dots, f_n\Phi_n$, with a total number N_φ of φ less than k.

6.2.1 Proof that D_n is supported on the total diagonal

First, we will show that D_n is supported on the total diagonal Δ_{n+1} in the product manifold M^{n+1}. For this, choose a test function $h_{ab} \otimes f_1 \otimes \cdots \otimes f_n$ whose support does not intersect Δ_{n+1}. Then, without loss of generality, we can assume that one of the following cases occurs:

(1) There is a Cauchy surface Σ in M such that $\operatorname{supp} h_{ab} \subset J^+(\Sigma)$ and $\operatorname{supp} f_i \subset J^-(\Sigma)$ for all $i = 1, \dots, n$.

(2) The same as the previous one, but with "+" and "−" interchanged.

(3) There is a Cauchy surface Σ, and a proper, non-empty subset $I \subset \{1, \dots, n\}$ with the property that $\operatorname{supp} h_{ab}, \operatorname{supp} f_i \subset J^+(\Sigma)$ for all $i \in I$, and such that $\operatorname{supp} f_j \subset J^-(\Sigma)$ for all j in the complement J of I.

(4) The same as the previous one, but with "+" and "−" interchanged.

We now analyze these cases one-by-one. To simplify the notation, let us use the shorthand

$$A_i = f_i \Phi_i \in \mathcal{F}_{\text{class}}. \tag{180}$$

In case (1), the support of infinitesimal variation h_{ab} is outside the causal past of the support of the A_i, and we consequently have that $\delta^{\text{ret}}[\mathscr{T}(\prod A_i)] = 0$. Thus, the first term in D_n vanishes. But the other terms also vanish: The second because of the support properties of the retarded products, eq. (90), and the third one because $\operatorname{supp} f_i \cap \operatorname{supp} h_{ab}$ is empty.

In case (2), it follows that $\delta^{\text{adv}}[\mathscr{T}(\prod A_i)] = 0$ by the same argument as above. Thus, the first term in D_n is equal to

$$\begin{aligned} \delta^{\text{ret}}\left[\mathscr{T}\left(\prod A_i\right)\right] &= \delta^{\text{ret}}\left[\mathscr{T}\left(\prod A_i\right)\right] - \delta^{\text{adv}}\left[\mathscr{T}\left(\prod A_i\right)\right] \\ &= -\frac{\mathrm{i}}{2}\left[T^{ab}(\boldsymbol{\epsilon} h_{ab}), \mathscr{T}\left(\prod A_i\right)\right] \\ &= \frac{\mathrm{i}}{2}\mathscr{R}\left(\prod A_i; \boldsymbol{\epsilon} h_{ab} T^{ab}\right) - \frac{\mathrm{i}}{2}\mathscr{A}\left(\prod A_i; \boldsymbol{\epsilon} h_{ab} T^{ab}\right) \\ &= \frac{\mathrm{i}}{2}\mathscr{R}\left(\prod A_i; \boldsymbol{\epsilon} h_{ab} T^{ab}\right) \end{aligned} \tag{181}$$

where in the second line we have used eqs. (119) and (120), where in the third line we have used an identity for retarded and advanced products, and where in the fourth line we used that $\operatorname{supp} f_i \subset J^+(\operatorname{supp} h_{ab})$ and the support property of the advanced products. The calculation shows that the first term and the second term in D_n cancel. But the third term vanishes, because $\operatorname{supp} f_i \cap \operatorname{supp} h_{ab}$ is empty, showing that $D_n = 0$ in case (2).

In case (3), we use the causal factorization property T8 of the time ordered products and the homomorphism property of $\tau^{\rm ret}$ (that is, $\tau^{\rm ret}(ab) = \tau^{\rm ret}(a)\tau^{\rm ret}(b)$) to write

$$\begin{aligned}
\text{first term in eq. (179)} \quad &= \quad \delta^{\rm ret}\left[\mathscr{T}\left(\prod_{i\in I} A_i\right)\mathscr{T}\left(\prod_{j\in J} A_j\right)\right] \qquad (182)\\
&= \quad \delta^{\rm ret}\left[\mathscr{T}\left(\prod_{i\in I} A_i\right)\right]\mathscr{T}\left(\prod_{j\in J} A_j\right) + \mathscr{T}\left(\prod_{i\in I} A_i\right)\delta^{\rm ret}\left[\mathscr{T}\left(\prod_{j\in J} A_j\right)\right].
\end{aligned}$$

Since neither I nor J are empty by assumption, and since $A_1, \dots, A_n$ together have at most a total of $N_\varphi = k$ factors of φ, it follows that $A_i, i \in I$ as well as $A_j, j \in J$ each have strictly less than k factors of φ. Hence we can use our inductive assumption which gives $D_{|I|} = D_{|J|} = 0$. It follows that

$$\begin{aligned}
&\text{first term in eq. (179)} = \\
&\frac{\rm i}{2}\mathscr{R}\left(\prod_{i\in I} A_i; \boldsymbol{\epsilon} h_{ab}T^{ab}\right)\mathscr{T}\left(\prod_{j\in J} A_j\right) + \frac{\rm i}{2}\mathscr{T}\left(\prod_{i\in I} A_i\right)\mathscr{R}\left(\prod_{j\in J} A_j; \boldsymbol{\epsilon} h_{ab}T^{ab}\right)\\
&\qquad + \sum_{k\in I}\mathscr{T}\left(\frac{\delta A_k}{\delta\varphi}\prod_{i\in I, i\neq k} A_i\right)\mathscr{T}\left(\prod_{j\in J} A_j\right)\\
&\qquad\qquad + \mathscr{T}\left(\prod_{i\in I} A_i\right)\sum_{l\in J}\mathscr{T}\left(\frac{\delta A_l}{\delta\varphi}\prod_{j\in J, j\neq l} A_j\right). \qquad (183)
\end{aligned}$$

For the second and third term in eq. (179), we likewise use the causal factorization property and the definition of the retarded product. It is then seen that these terms precisely cancel the first term in eq. (179), showing that $D_n = 0$ in case (3).

Case (4) can be treated in the same way as the previous one.

6.2.2 Proof that D_n is a c-number

We next want to show that the algebra element $D_n \in \mathcal{W}$ is in fact proportional to the identity operator. By [13, prop. 2.1], an element $a \in \mathcal{W}$ is proportional to the identity if and only if $[a, \varphi(F)] = 0$ for all smooth, compactly supported densities F. Thus, we will be done if we can show that

$$[D_n^{ab}(h_{ab}; f_1, \dots, f_n), \varphi(F)] = 0. \qquad (184)$$

Inductively, we know this is true when $N_\varphi < k$ since D_n itself vanishes then. We now prove that it is also true when $N_\varphi = k$.

We begin by calculating the commutator with the first term in D_n [see eq. (179)], which, using the homomorphism property of τ^{ret} is equal to

$$\left[\delta^{\mathrm{ret}}\left\{\mathscr{T}\left(\prod f_i\Phi_i\right)\right\},\varphi(F)\right] = \\ \delta^{\mathrm{ret}}\left\{\left[\mathscr{T}\left(\prod f_i\Phi_i\right),\varphi(F)\right]\right\} - \left[\mathscr{T}\left(\prod f_i\Phi_i\right),\delta^{\mathrm{ret}}\left\{\varphi(F)\right\}\right]. \quad (185)$$

We now simplify the first term on the right side of this expression using the commutator property of the time ordered products, T9, and we simplify the second term on the right side using that

$$\delta^{\mathrm{ret}}[\varphi(F)] = -\varphi(\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{adv}}F), \quad (186)$$

which follows from a direct calculation using the definition of τ^{ret} (see [6]). Here, $\delta(\boldsymbol{\epsilon}P)$ is the infinitesimal variation of the densitized Klein-Gordon operator under a change in the metric,

$$\delta(\boldsymbol{\epsilon}P)_{\mathbf{g}}f = \frac{\partial}{\partial s}(\boldsymbol{\epsilon}P)_{\mathbf{g}+s\mathbf{h}}f\bigg|_{s=0}. \quad (187)$$

(Note that $\delta(\boldsymbol{\epsilon}P)$ is a second order differential operator mapping smooth scalar functions to densities.) Substituting eq. (186) into eq. (185) gives

$$\left[\delta^{\mathrm{ret}}_{\mathbf{g}}\left\{\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right)\right\},\varphi_{\mathbf{g}}(F)\right] = \\ \mathrm{i}\frac{\partial}{\partial s}\tau^{\mathrm{ret}}_{\mathbf{g}^{(s)}}\left(\sum_{i=1}^{n}\mathscr{T}_{\mathbf{g}^{(s)}}\left(f_1\Phi_1\dots(\Delta_{\mathbf{g}^{(s)}}F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\dots f_n\Phi_n\right)\right)\bigg|_{s=0} \\ + \left[\mathscr{T}_{\mathbf{g}}\left(\prod f_i\Phi_i\right),\varphi_{\mathbf{g}}(\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{adv}}F)\right]. \quad (188)$$

The first term on the right side involves only $N_\varphi = k-1$ factors of φ, and therefore can be simplified using the inductive assumption that $D_n = 0$ in that case. The second term on the right side can again be simplified using the commutator property. This gives[26]

$$
\begin{aligned}
\Big[\delta_{\mathbf{g}}^{\mathrm{ret}}\Big\{\mathscr{T}_{\mathbf{g}}\Big(\prod f_i\Phi_i\Big)\Big\}, \varphi_{\mathbf{g}}(F)\Big] = \\
& -\frac{1}{2}\sum_{i=1}^{n}\mathscr{R}_{\mathbf{g}}\left(f_1\Phi_1\dots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\dots f_n\Phi_n;\boldsymbol{\epsilon}h_{ab}T^{ab}\right) \\
& +\mathrm{i}\sum_{i=1}^{n}\mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\dots h_{ab}\frac{\delta}{\delta g_{ab}}\left\{(\Delta F)\frac{\delta}{\delta\varphi}(f_i\Phi_i)\right\}\dots f_n\Phi_n\right) \\
& +\mathrm{i}\sum_{i=1}^{n}\mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\dots\frac{\partial}{\partial s}\Delta_{\mathbf{g}(s)}F\Big|_{s=0}\frac{\delta(f_i\Phi_i)}{\delta\varphi}\dots f_n\Phi_n\right) \\
& +\mathrm{i}\sum_{i=1}^{n}\sum_{k\neq i}\mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\dots h_{ab}\frac{\delta(f_k\Phi_k)}{\delta g_{ab}}\dots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\dots f_n\Phi_n\right) \\
& +\mathrm{i}\sum_{i=1}^{n}\mathscr{T}_{\mathbf{g}}\left(f_1\Phi_1\dots(\Delta\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{adv}}F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\dots f_n\Phi_n\right). \qquad (189)
\end{aligned}
$$

We next calculate the commutator of the second term in D_n [see eq. (179)] with $\varphi(F)$, by expanding the retarded product in terms of time-ordered products and using, for each of the resulting terms the commutator property of the time-ordered products,

$$
\begin{aligned}
-\frac{\mathrm{i}}{2}\left[\mathscr{R}\left(\prod f_i\Phi_i;\boldsymbol{\epsilon}h_{ab}T^{ab}\right),\varphi(F)\right] &= \frac{1}{2}\mathscr{R}\left(\prod f_i\Phi_i;(\Delta F)\frac{\delta(\boldsymbol{\epsilon}h_{ab}T^{ab})}{\delta\varphi}\right) \\
&+\frac{1}{2}\sum_{i=1}^{n}\mathscr{R}\left(f_1\Phi_1\cdots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\cdots f_n\Phi_n;\boldsymbol{\epsilon}h_{ab}T^{ab}\right). \qquad (190)
\end{aligned}
$$

Using that the variational derivatives $\delta/\delta g_{ab}$ and $\delta/\delta\varphi$ commute up to an exact form (see eq. (268)), and using eq. (266) of appendix B, we have

$$
\begin{aligned}
\frac{1}{2}(\Delta F)\frac{\delta(\boldsymbol{\epsilon}h_{ab}T^{ab})}{\delta\varphi} &= h_{ab}\frac{\delta}{\delta g_{ab}}\left\{(\Delta F)\frac{\delta L_0}{\delta\varphi}\right\}+\mathrm{d}\,B_1 \\
&= \frac{\partial}{\partial s}\left\{(\Delta_{\mathbf{g}}F)(\boldsymbol{\epsilon}P)_{\mathbf{g}+s\mathbf{h}}\varphi\right\}\Big|_{s=0}+\mathrm{d}\,B_2. \qquad (191)
\end{aligned}
$$

where B_1, B_2 are local, $(D-1)$ form functional of φ and the metric, and where P is the Klein-Gordon operator. Since P is hermitian, the right side can be rewritten further as

$$
\frac{1}{2}(\Delta F)\frac{\delta(\boldsymbol{\epsilon}h_{ab}T^{ab})}{\delta\varphi} = \frac{\partial}{\partial s}\left\{(\boldsymbol{\epsilon}P)_{\mathbf{g}+s\mathbf{h}}(\Delta_{\mathbf{g}}F)\varphi+\mathrm{d}\,C\right\}\Big|_{s=0}+\mathrm{d}\,B_2 = \delta(\boldsymbol{\epsilon}P)(\Delta F)\varphi+\mathrm{d}\,B_3 \qquad (192)
$$

[26]We use the convention that whenever the expression ΔF appears in an expression to which $\delta/\delta g_{ab}$ is applied, we will view ΔF as independent of $\mathbf{g}$, i.e., $\delta/\delta g_{ab}$ does not act on ΔF in such an expression.

remembering that $\delta(\boldsymbol{\epsilon}P)$ is metric variation of the densitized Klein-Gordon operator. Thus, by the Leibniz rule, T10, we get

$$-\frac{\mathrm{i}}{2}\left[\mathscr{R}\left(\prod f_i\Phi_i;\boldsymbol{\epsilon}h_{ab}T^{ab}\right),\varphi(F)\right]=\mathscr{R}\left(\prod f_i\Phi_i;(\delta(\boldsymbol{\epsilon}P)\Delta F)\varphi\right)$$
$$+\frac{1}{2}\sum_{i=1}^{n}\mathscr{R}\left(f_1\Phi_1\cdots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\cdots f_n\Phi_n;\boldsymbol{\epsilon}h_{ab}T^{ab}\right). \quad (193)$$

We apply T11a to the first term on the right side of this equation. This gives

$$-\mathrm{i}\left[\mathscr{R}\left(\prod f_i\Phi_i;\boldsymbol{\epsilon}h_{ab}T^{ab}\right),\varphi(F)\right]=\mathrm{i}\sum_{i=1}^{n}\mathscr{T}\left(f_1\Phi_1\cdots(\Delta^{\mathrm{ret}}\delta(\boldsymbol{\epsilon}P)\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\cdots f_n\Phi_n\right)$$
$$+\sum_{i=1}^{n}\mathscr{R}\left(f_1\Phi_1\cdots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\cdots f_n\Phi_n;\boldsymbol{\epsilon}h_{ab}T^{ab}\right). \quad (194)$$

We finally take the commutator of the third term in D_n with $\varphi(F)$, and use the commutator property to simplify. This gives

$$-\left[\sum_i\mathscr{T}\left(f_1\Phi_1\cdots h_{ab}\frac{\delta(f_i\Phi_i)}{\delta g_{ab}}\cdots f_n\Phi_n\right),\varphi(F)\right]$$
$$=-\mathrm{i}\sum_{i=1}^{n}\mathscr{T}\left(f_1\Phi_1\ldots(\Delta F)\frac{\delta}{\delta\varphi}\left\{h_{ab}\frac{\delta}{\delta g_{ab}}(f_i\Phi_i)\right\}\ldots f_n\Phi_n\right)$$
$$-\mathrm{i}\sum_{i=1}^{n}\sum_{k\neq i}\mathscr{T}\left(f_1\Phi_1\ldots h_{ab}\frac{\delta(f_k\Phi_k)}{\delta g_{ab}}\ldots(\Delta F)\frac{\delta(f_i\Phi_i)}{\delta\varphi}\ldots f_n\Phi_n\right). \quad (195)$$

We have now calculated the commutator of all three terms in D_n with $\varphi(F)$, given by eqs. (189), (194) and (195) respectively. If we add these contributions up, then we see that the commutator $[D_n,\varphi(F)]$ will vanish if we can show that

$$\mathrm{i}\Delta^{\mathrm{ret}}\delta(\boldsymbol{\epsilon}P)\Delta F+\mathrm{i}\Delta\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{adv}}F=-\mathrm{i}\frac{\partial}{\partial s}\Delta_{\mathbf{g}^{(s)}}F\bigg|_{s=0} \quad (196)$$

for all compactly supported densities F. However, this identity follows immediately from $\Delta=\Delta^{\mathrm{adv}}-\Delta^{\mathrm{ret}}$ together with the identity

$$\frac{\partial}{\partial s}\Delta^{\mathrm{ret}}_{\mathbf{g}^{(s)}}F\bigg|_{s=0}=-\Delta^{\mathrm{ret}}\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{ret}}F\quad\text{and “adv”}\leftrightarrow\text{“ret”}, \quad (197)$$

for all compactly supported densities F, which in turn is seen to be true owing to the relation $(\partial/\partial s)(\boldsymbol{\epsilon}P\Delta^{\mathrm{ret}})_{\mathbf{g}^{(s)}}=0$ (and the analogous relation for the advanced propagator).

6.2.3 Proof that D_n is local and covariant and scales almost homogeneously

It is 'obvious' that D_n is a c-number functional that is constructed entirely from the metric, because all the terms in the defining equation for D_n have this property. D_n depends moreover locally and covariantly on the metric in the sense that if $\chi : N \to M$ is any causality and orientation preserving isometric embedding, then

$$D_n^{ab}[M, \mathbf{g}](\chi_* h_{ab}, \chi_* f_1, \dots \chi_* f_n) = D_n^{ab}[N, \chi^* \mathbf{g}](h_{ab}, f_1, \dots, f_n) \tag{198}$$

for all test (tensor-)fields with compact support on N. This property follows because the second and third term in the definition of D_n are local and covariant quantities by T1, and because the map $\tau^{\rm ret}$ appearing in the first term also has this property by construction.

Moreover, the functionals D_n also have an almost homogeneous scaling behavior under rescalings of the metric in the sense that

$$\frac{\partial^N}{\partial^N \ln \lambda}(\lambda^d \cdot D_n[M, \lambda^2 \mathbf{g}]) = 0 \tag{199}$$

for some natural number N, where d is the sum of the engineering dimension of the fields appearing in D_n. Again, for the second and third term in the definition of D_n, this property follows since we are assuming that our time ordered products (and hence retarded products) have an almost homogeneous scaling behavior in the sense of T2. For the first term in the definition of D_n, this follows from the fact that if $(M, \mathbf{g})$ and $(M, \mathbf{g}')$ are spacetimes whose metrics differ only within some compact set K, and if $\tau^{\rm adv/ret}$ are the corresponding algebra isomorphisms from $\mathcal{W}(M, \mathbf{g})$ to $\mathcal{W}(M, \mathbf{g}')$, then

$$\sigma'_\lambda \circ \tau^{\rm adv/ret} = \tau^{\rm adv/ret} \circ \sigma_\lambda, \tag{200}$$

where σ_λ is the natural isomorphism from $\mathcal{W}(M, \mathbf{g})$ to $\mathcal{W}(M, \lambda^2 \mathbf{g})$ introduced above in T2, and where σ'_λ is the corresponding isomorphism for $\mathbf{g}'$.

6.2.4 Proof that $D_n = 0$ when one of the Φ_i is equal to φ

Let us now assume that one of the fields Φ_i is equal to φ, say $\Phi_n = \varphi$, and as before, that the total number N_φ of free field factors in $\Phi_1, \dots, \Phi_{n-1}, \Phi_n = \varphi$ is equal to k. We will show that D_n is automatically zero in this case under our inductive assumption that $D_n = 0$ when $N_\varphi < k$.

We first look at the second term in D_n in eq. (179), setting $A_i = f_i \Phi_i$ for $i < n$ and $f_n = F$ to facilitate the notation. After some algebra, repeatedly using T10, T11a and eq. (89), we get

$$\begin{aligned}
-\frac{\mathrm{i}}{2}\mathscr{R}\left(F\varphi\prod^{n-1}A_i;\boldsymbol{\epsilon}h_{ab}T^{ab}\right) &= \frac{1}{2}\sum_j \mathscr{R}\left(A_1\dots(\Delta^{\mathrm{ret}}F)\frac{\delta A_j}{\delta\varphi}\dots A_{n-1};\boldsymbol{\epsilon}h_{ab}T^{ab}\right) \\
&- \frac{\mathrm{i}}{2}\varphi(F)\,\mathscr{R}\left(\prod^{n-1}A_i;\boldsymbol{\epsilon}h_{ab}T^{ab}\right) \\
&- \varphi(\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{adv}}F)\,\mathscr{T}\left(\prod^{n-1}A_i\right) \\
&+ \mathrm{i}\sum_j \mathscr{T}\left(A_1\dots(\Delta^{\mathrm{ret}}\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{ret}}F)\frac{\delta A_j}{\delta\varphi}\dots A_{n-1}\right)
\end{aligned} \tag{201}$$

Here $\delta(\boldsymbol{\epsilon}P)$ is the first order variation of the Klein-Gordon operator with respect to our family of metrics, see eq. (187). For the third term in D_n, we get, using T10, T11a,

$$\begin{aligned}
&-\sum_j \mathscr{T}\left(F\varphi A_1\dots h_{ab}\frac{\delta A_j}{\delta g_{ab}}\dots A_{n-1}\right) \\
= &-\mathrm{i}\sum_{j\neq k}\mathscr{T}\left(A_1\dots h_{ab}\frac{\delta A_j}{\delta g_{ab}}\dots(\Delta^{\mathrm{ret}}F)\frac{\delta A_k}{\delta\varphi}\dots A_{n-1}\right) \\
- &\ \mathrm{i}\sum_j \mathscr{T}\left(A_1\dots(\Delta^{\mathrm{ret}}F)\frac{\delta}{\delta\varphi}\left\{h_{ab}\frac{\delta}{\delta g_{ab}}A_j\right\}\dots A_{n-1}\right) \\
- &\ \varphi(F)\sum_j \mathscr{T}\left(A_1\dots h_{ab}\frac{\delta A_j}{\delta g_{ab}}\dots A_{n-1}\right).
\end{aligned} \tag{202}$$

For the first term in D_n we get, using eqs. (186) and the definition (187) of $\delta(\boldsymbol{\epsilon}P)$,

$$\begin{aligned}
\delta^{\mathrm{ret}}\left[\mathscr{T}\left(F\varphi\prod^{n-1}A_i\right)\right] &= \varphi(\delta(\boldsymbol{\epsilon}P)\Delta^{\mathrm{adv}}F)\,\mathscr{T}\left(\prod^{n-1}A_i\right) \\
&+ \mathrm{i}\sum_j \delta^{\mathrm{ret}}\left[\mathscr{T}\left(A_1\dots(\Delta^{\mathrm{ret}}F)\frac{\delta A_j}{\delta\varphi}\dots A_{n-1}\right)\right] \\
&+ \varphi(F)\,\delta^{\mathrm{ret}}\left[\mathscr{T}\left(\prod^{n-1}A_i\right)\right].
\end{aligned} \tag{203}$$

We can simplify the terms on the right side using the inductive assumption. Adding up the contributions eqs. (201), (202) and (203) to D_n, and using eq. (197), we find that all terms cancel. Thus we have shown that $D_n = 0$ when $N_\varphi = k$ and when one of the factors Φ_i is φ.

6.2.5 Proof that D_n satisfies a wave front set condition and depends smoothly and analytically on the metric

We now show that D_n is a distribution on M^{n+1}—i.e., D_n is a multilinear functional that is *continuous* in the appropriate sense—and that it satisfies the wave front set condition

$$\mathrm{WF}(D_n) \restriction_{\Delta_{n+1}} \perp T(\Delta_{n+1}). \tag{204}$$

Moreover, we will show that if $\mathbf{g}^{(s)}$ is a smooth (resp. analytic) family of metrics depending smoothly (resp. analytically) upon a set of parameters s in a parameter space $\mathcal{P}$, and if $D_n^{(s)}$ are the corresponding distributions (viewed now as a single distribution on $\mathcal{P} \times M^{n+1}$), then

$$\mathrm{WF}(D_n^{(s)}) \restriction_{\mathcal{P}\times\Delta_{n+1}} \perp T(\mathcal{P} \times \Delta_{n+1}), \tag{205}$$

(with the smooth wave front set WF replaced by the analytic wave front set WF_A in the analytic case).

Since D_n is a c-number, it is equal to the expectation value of eq. (179) in a any state ω on $\mathcal{W}(M, \mathbf{g})$. To simplify things we take ω to be a quasifree Hadamard state, and write D_n as

$$\begin{aligned} D_n^{ab}(h_{ab}; f_1, \dots, f_n) &= r_n^{ab}(h_{ab}; f_1, \dots, f_n) \\ &- \frac{\mathrm{i}}{2}\omega\left(\mathscr{R}\left(\prod_{i=1}^{n} f_i\Phi_i; \boldsymbol{\epsilon} h_{ab}T^{ab}\right)\right) \\ &- \sum_i \omega\left(\mathscr{T}\left(f_1\Phi_1 \cdots h_{ab}\frac{\delta(f_i\Phi_i)}{\delta g_{ab}} \cdots f_n\Phi_n\right)\right), \end{aligned} \tag{206}$$

where we have set

$$r_n^{ab}(h_{ab}; f_1, \dots, f_n) = \omega\left[\delta^{\mathrm{ret}}\left\{\mathscr{T}\left(\prod_{i=1}^{n} f_i\Phi_i\right)\right\}\right]. \tag{207}$$

To prove the desired properties, eqs. (204) and (205), of D_n, we show that each term on the right side of eq. (206) satisfies these properties separately. This is relatively straightforward for the second and third terms. It follows from our microlocal spectrum condition, T3, that the second and third terms in D_n each satisfy

$$\begin{aligned} \mathrm{WF}(\text{2nd and 3rd terms in eq. (206)}) \subset \{(y, p; x_1, k_1; \dots; x_n, x_n) \mid \\ \exists \text{ Feynman graph } G(q) \text{ with vertices } y, x_1, \dots, x_n \\ \text{and edges } e \text{ such that if } y = s/t(e) \text{ then } t/s(e) \in J^+(y) \\ k_i = \sum_{e:s(e)=x_i} q_e - \sum_{e:t(e)=x_i} q_e, \quad p = \sum_{e:s(e)=y} q_e - \sum_{e:t(e)=y} q_e\} \equiv \mathcal{C}_{\mathscr{R}}(M, \mathbf{g}). \end{aligned} \tag{208}$$

Since

$$\mathcal{C}_{\mathscr{R}}(M, \mathbf{g}) \restriction_{\Delta_{n+1}} \perp T(\Delta_{n+1}), \tag{209}$$

on the total diagonal, it immediately follows that the second and third terms in D_n satisfy the analog of eq. (204). Moreover, if we consider a smooth family of metrics $\mathbf{g}^{(s)}$ and a corresponding family of quasifree Hadmard states $\omega^{(s)}$ depending smoothly upon s in the sense of eq. (35), then it similarly follows from T4 that the second and third terms in $D_n^{(s)}$ (with ω in those expressions replaced by $\omega^{(s)}$) have a smooth dependence upon s. It then follows immediately that the second and third terms in $D_n^{(s)}$ satisfy the smoothness condition (205). The corresponding statement in the analytic case similarly follows from condition T5.

Having dealt with the second and third terms on the right side of eq. (206), our claims will be established by proving the following proposition:

Proposition 6.1. The first term on the right side of eq. (206) satisfies

$$\mathrm{WF}(r_n) \restriction_{\Delta_{n+1}} \perp T(\Delta_{n+1}), \tag{210}$$

as well as

$$\mathrm{WF}(r_n^{(s)}) \restriction_{\mathcal{P} \times \Delta_{n+1}} \perp T(\mathcal{P} \times \Delta_{n+1}), \tag{211}$$

where $r_n^{(s)}$ is defined by the same formula as r_n except that ω is replaced by the smooth family $\omega^{(s)}$ in that formula, and the metric $\mathbf{g}$ is replaced everywhere by $\mathbf{g}^{(s)}$. The analogous statement also holds true with regard to the analytic wave front set.

Proof. We know that r_n is a multilinear functional which is also a distribution in $f_1 \otimes \cdots \otimes f_n$ for any fixed $\mathbf{h}$ of compact support. Also, since D_n is already known to vanish for test functions $\mathbf{h} \otimes f_1 \otimes \cdots \otimes f_n$ whose support has no intersection with the total diagonal Δ_{n+1} in M^{n+1}, it follows that $r_n(\mathbf{h}, f_1, \dots, f_n)$ is equal to minus the second and third term in eq. (206). Therefore, since these terms are individually known to be distributions, we know that r_n is in fact a distribution off the total diagonal. However, our constructions so far do not tell us that r_n is also a distribution on the total diagonal, let alone whether it satisfies the wave front set conditions eqs. (210) and (211) there. Thus, in order to prove the above proposition, we must look at the detailed structure of r_n near the total diagonal.

For this, we first use our local Wick expansion (63) to write the time ordered products in the following form when $f_1 \otimes \cdots \otimes f_n$ is supported in a sufficiently small neighborhood

U_n total diagonal in M^n (which we assume from now on):

$$\begin{aligned}\mathscr{T}\left(\prod_{i=1}^n f_i \Phi_i\right) = \sum_{\alpha_1,\alpha_2,\dots} \frac{1}{\alpha_1!\dots\alpha_n!} \int \prod_j \boldsymbol{\epsilon}(y_j) \\ t\left[\delta^{\alpha_1}\Phi_1 \otimes \dots \otimes \delta^{\alpha_n}\Phi_n\right](y_1,\dots,y_n) \\ f_1(y_1)\dots f_n(y_n) : \prod_{i=1}^n \prod_j [(\nabla)^j \varphi(y_i)]^{\alpha_{ij}} :_H \\ = \sum_r \int w(y_1,\dots,y_n;x_1,\dots,x_r) \prod_{i=1}^n f_i(y_i) \ : \prod_{j=1}^r \varphi(x_j) :_H . \end{aligned} \tag{212}$$

Here, the distributions $w \in \mathcal{D}'(U_n \times M^r)$ are defined by the last equation in terms of sums of products of $t[\dots]$ and suitable delta functions and their derivatives. Since these distributions are in turn locally and covariantly constructed from the metric, it follows that also the distributions w have this property, and we will write $w = w_{\mathbf{g}}$ when we want to emphasize this fact. From the δ-functions implicit in the definition of w, one easily finds the support property

$$\begin{aligned}\operatorname{supp} w \subset \{(y_1,\dots,y_n;x_1,\dots,x_r) \mid \\ \exists \text{ partition } \{1,\dots,r\} = I_1 \cup \dots \cup I_n \text{ such that } x_i = y_l \ \forall i \in I_l\},\end{aligned} \tag{213}$$

and from the wave front set property of the t, one finds furthermore the wave front set property

$$\begin{aligned}\mathrm{WF}(w) \subset \{(y_1,k_1;\dots;y_n,k_n;x_1,p_1;\dots;x_r,p_r) \mid \\ \exists \text{ partition } \{1,\dots,r\} = I_1 \cup \dots \cup I_n \text{ such that } x_i = y_l \ \forall i \in I_l \\ \text{if } q_l \equiv k_l + \sum_{i \in I_l} p_i, \text{ then } (y_1,q_1;\dots;y_n,q_n) \in \mathcal{C}_{\mathscr{T}}(M,\mathbf{g})\} =: \mathcal{I}_{\mathscr{T}}(M,\mathbf{g})\end{aligned} \tag{214}$$

for the w. We also note that the w scale almost homogeneously under a rescaling of the metric, and vary smoothly under smooth variations of the metric in the sense that if $\mathbf{g}^{(s)}$ is a family of metrics depending smoothly on s in some parameter space $\mathcal{P}$, then the distributions $w^{(s)} = w_{\mathbf{g}^{(s)}}$ (viewed as distributions on $\mathcal{P} \times U_n \times M^r$) have wave front set

$$\begin{aligned}\mathrm{WF}(w^{(s)}) \subset \{(s,\rho;y_1,k_1;\dots;y_n,k_n;x_1,p_1;\dots;x_r,p_r) \mid \\ (y_1,k_1;\dots;y_n,k_n;x_1,p_1;\dots;x_r,p_r) \in \mathcal{I}_{\mathscr{T}}(M,\mathbf{g}^{(s)})\}.\end{aligned} \tag{215}$$

These properties follow immediately from the corresponding properties satisfied by the t (as a consequence of T3 and T4) as well as the delta functions.

We now insert eq. (212) into the definition of r_n. This gives

$$r_n(\mathbf{h}; f_1, \dots, f_n) =$$
$$\sum_r \int w^{(0)}(y_1, \dots, y_n; x_1, \dots, x_r) \prod_i f_i(y_i)\, \omega \left[\frac{\partial}{\partial s} \tau^{\text{ret}}_{\mathbf{g}^{(s)}} \left(: \prod_j \varphi(x_j) :_{H^{(s)}} \right) \Big|_{s=0} \right]$$
$$+ \sum_r \int \frac{\partial}{\partial s} w^{(s)}(y_1, \dots, y_n; x_1, \dots, x_r) \Big|_{s=0} \prod_i f_i(y_i)\, \omega \left(: \prod_j \varphi(x_j) :_{H^{(0)}} \right)$$
$$\equiv I_1 + I_2 \quad (216)$$

where $\frac{\partial}{\partial s}\mathbf{g}^{(s)} = \mathbf{h}$. Furthermore, when $\mathbf{g}$ is replaced everywhere in the above formula by a family $\mathbf{g}^{(s)}$ depending on a parameter $s \in \mathcal{P}$, we obtain a corresponding expression for $r_n^{(s)}$. The proof of the proposition will be complete if we can show that the first term, I_1, and second term, I_2, on the right side separately satisfy the wave front set condition eq. (210), and the smoothness condition eq. (211), i.e., if we can prove the following lemma:

Lemma 6.1. I_1 and I_2 are distributions satisfying

$$\text{WF}(I_j) \restriction_{\Delta_{n+1}} \perp T(\Delta_{n+1}), \tag{217}$$

as well as

$$\text{WF}(I_j^{(s)}) \restriction_{\mathcal{P} \times \Delta_{n+1}} \perp T(\mathcal{P} \times \Delta_{n+1})\,. \tag{218}$$

The remainder of this subsection consists of the proof of this lemma.

Proof of lemma 6.1 for I_1: We begin by showing eq. (217) for I_1. For this, consider the smooth 1-parameter family of metrics $\mathbf{g}^{(s)}$ with $\frac{\partial}{\partial s}\mathbf{g}^{(s)} = \mathbf{h}$, and let $\omega^{(s)}$ be the unique quasifree Hadamard state on $\mathcal{W}(M, \mathbf{g}^{(s)})$ with the property that $\omega^{(s)}$ coincides with ω on $M \setminus J^+(K)$, where K is the compact region where $\mathbf{h}$ is supported. Furthermore, let $H^{(s)}$ be the local Hadamard parametrix associated with this 1-parameter family of metrics, and, in a sufficiently small neighborhood U_2 of the diagonal, define

$$d^{(s)}(x_1, x_2) = \omega_2^{(s)}(x_1, x_2) - H^{(s)}(x_1, x_2). \tag{219}$$

Then one finds from the definition of τ^{ret} that

$$\omega \left[\tau^{\text{ret}}_{\mathbf{g}^{(s)}} \left(: \prod_j \varphi(x_j) :_{H^{(s)}} \right) \right] = \sum_{\text{pairs } ij} d^{(s)}(x_i, x_j), \tag{220}$$

and hence that

$$I_1(\mathbf{h}; f_1, \dots, f_n) = \sum_r \int w^{(0)}(y_1, \dots, y_n; x_1, \dots, x_r) \prod_i f_i(y_i) \frac{\partial}{\partial s} \sum_{\text{pairs } ij} d^{(s)}(x_i, x_j) \Big|_{s=0}. \tag{221}$$

We estimate the wave front set of I_1 by analyzing the wave front set of the individual terms in eq. (221). The wave front set of w is already known, whereas the wave front set associated with the distributions $d^{(s)}$ is given by the following lemma.

Lemma 6.2. $d^{(s)}$ is jointly smooth in s and its spacetime arguments within a sufficiently small neighborhood U_2 of the diagonal in $M \times M$. Furthermore, in such a neighborhood, if

$$(\delta d)(\mathbf{h}, f_1, f_2) = \frac{\partial}{\partial s} d^{(s)}(f_1, f_2)\Big|_{s=0}, \tag{222}$$

then

$$\begin{aligned} \mathrm{WF}(\delta d) \quad \subset \quad & \{(y, p; x_1, k_1; x_2, k_2) \mid \text{either of the following holds:} \\ & ((y,p) \sim (x_1, -k_1),\ k_2 = 0) \text{ or } ((y,p) \sim (x_2, -k_2),\ k_1 = 0) \\ & \text{or } (x_1 = x_2 = y \text{ and } p = -k_1 - k_2)\}. \end{aligned} \tag{223}$$

Proof. The bidistribution $d^{(s)}$ is symmetric, and is a bisolution of the Klein-Gordon equation modulo a smooth function, because $H^{(s)}$ is a bisolution modulo a smooth function. In fact,

$$\begin{aligned} (P^{(s)} \otimes 1) d^{(s)}(x_1, x_2) &= G^{(s)}(x_1, x_2) \\ (1 \otimes P^{(s)}) d^{(s)}(x_1, x_2) &= G^{(s)}(x_2, x_1), \end{aligned} \tag{224}$$

where $G^{(s)}$ is equal to the action of the Klein-Gordon operator on the first variable in $H^{(s)}$ (and can thereby be calculated by Hadamard's recursion procedure, at least in analytic spacetimes), and where $P^{(s)}$ is the Klein-Gordon operator associated with $\mathbf{g}^{(s)}$. It follows that $G^{(s)}$ is jointly smooth (resp. analytic, in analytic spacetimes) in s and its spacetime arguments. Furthermore, since $\omega^{(s)}$ is independent of s everywhere in $M \setminus J^+(K)$, and since $H^{(s)}$ is independent of s on any convex normal neighborhood which does not intersect K, it follows that $d^{(s)}$ is independent of s on any convex normal neighborhood which has no intersection with $J^+(K)$. Using these facts, we will now show that $d^{(s)}(x_1, x_2)$ is jointly smooth in s, x_1, x_2.

For this, we consider a globally hyperbolic subset N of M with compact closure, which contains K, and which has Cauchy surfaces S_- resp. S_+ not intersecting $J^+(K)$ resp. $J^-(K)$ (for all metrics $\mathbf{g}^{(s)}$ with s sufficiently small). Without loss of generality, we may assume that K is so small that N can be chosen to be convex and normal (again for all metrics $\mathbf{g}^{(s)}$ with s sufficiently small). By what we have said above, $d^{(s)}$ does not depend upon s in a neighborhood of S_-. Within N, we define the bi-distribution

$$\alpha^{(s)}_{ab}(x_1, x_2) = (\Delta^{\mathrm{adv}\,(s)} f_1)(x_1)(\Delta^{\mathrm{adv}\,(s)} f_2)(x_2)\ \overleftrightarrow{\nabla}_a \overleftrightarrow{\nabla}_b\ d^{(s)}(x_1, x_2), \tag{225}$$

where ∇_a acts on x_1 and ∇_b acts on x_2. We now take the divergence of $\alpha^{(s)}_{ab}(x_1, x_2)$ both in x_1 and x_2 and integrate the resulting expression over $U \times U$, where $U \subset N$ is the region enclosed by S_- and S_+. By Stokes' theorem and the support property of $\Delta^{\rm adv}$, we have

$$\int_{U\times U} \nabla^a\nabla^b\alpha_{ab}(x_1,x_2)\,\boldsymbol{\epsilon}(x_1)\boldsymbol{\epsilon}(x_2) = \int_{S_-\times S_-} \alpha_{ab}(x_1,x_2)\,\mathrm{d}\sigma^a(x_1)\mathrm{d}\sigma^b(x_2), \tag{226}$$

for any test (densities) f_1, f_2 supported in U. (Here, $\mathrm{d}\,\sigma^a$ is the usual integration element induced by $\boldsymbol{\epsilon}$, and we are suppressing the dependence upon s to lighten the notation.) Now perform the differentiation on the left side, using $(\nabla^a\nabla_a - \xi R - m^2)\Delta^{\rm adv} = \delta$, using the fact that the advanced propagator on the right side can be replaced by the causal propagator, and using the symmetry properties of G implied by eq. (224). We obtain

$$\begin{aligned} d(f_1,f_2) = &\int_{S_-\times S_-} (\Delta f_1)(x_1)(\Delta f_2)(x_2)\ \overleftrightarrow{\nabla}_a\overleftrightarrow{\nabla}_b\ d(x_1,x_2)\,\mathrm{d}\sigma^a(x_1)\mathrm{d}\sigma^b(x_2) \\ &- G(\Delta^{\rm adv}f_1,f_2) - G(\Delta^{\rm adv}f_2,f_1) - \frac{1}{2}G(Pf_1,f_2) - \frac{1}{2}G(Pf_2,f_1), \end{aligned} \tag{227}$$

where it should be remembered that all quantities depend upon s. This equation expresses $d^{(s)}(f_1,f_2)$ in terms of the advanced and retarded propagators for the metric $\mathbf{g}^{(s)}$, $G^{(s)}$, and initial data of $d^{(s)}$ on S_-. Now the retarded and advanced propagators have a smooth dependence upon s in the sense that

$$\mathrm{WF}(\Delta^{(s)\,\mathrm{ret/adv}}) \subset \{(s,\rho;x_1,k_1;x_2,k_2) \mid (x_1,k_1;x_2,k_2) \in \mathcal{C}_{\mathscr{R}/\mathscr{A}}(M,\mathbf{g}^{(s)})\}, \tag{228}$$

and $G^{(s)}$ is explicitly seen to be jointly smooth in s and its spacetime arguments. Moreover, near S_-, $d^{(s)}$ is a smooth function independent of s, since $\omega^{(s)}$ is equal to the Hadamard state ω there. It follows from these facts, together with the expression eq. (227) for $d^{(s)}$ and the wave front set calculus, that $d^{(s)}$ is jointly smooth in s and its spacetime arguments within N.

We next analyze the s-derivative of $d^{(s)}$. We denote the variation of any functional, F, of the metric by

$$\delta F_{\mathbf{g}}(\mathbf{h};f_1,\dots,f_m) = \frac{\partial}{\partial s}F_{\mathbf{g}^{(s)}}(f_1,\dots,f_m)\Big|_{s=0}, \quad \frac{\partial}{\partial s}\mathbf{g}^{(s)}\Big|_{s=0} = \mathbf{h}. \tag{229}$$

Now take the s derivative of both sides of eq. (227) at $s=0$. It follows that δd can be written as a sum of terms involving $\delta\Delta^{\rm adv}$ and $\delta\Delta^{\rm ret}$, δG and δP (the variation of the KG-operator) linearly. The wave front set of δG can be computed explicitly and is given by

$$\begin{aligned} \mathrm{WF}(\delta G) \quad \subset \quad &\{(y,p;x_1,k_1;x_2,k_2) \mid \text{either of the following holds:} \\ &(y = x_1 \text{ and } p=-k_1,\ k_2 = 0) \text{ or } (y=x_2 \text{ and } p=-k_2,\ k_1=0) \\ &\text{or } (x_1=x_2=y \text{ and } p = -k_1-k_2)\}, \end{aligned} \tag{230}$$

In order to calculate the wave front set of $\delta\Delta^{\rm ret}$ (and likewise $\delta\Delta^{\rm adv}$), we use formula (197) (and an analogous formula for the advanced propagator), as well as the wave front set of the advanced resp. retarded propagator, bounded by $\mathcal{C}_{\mathscr{A}/\mathscr{R}}(M, \mathbf{g})$. The calculus for the wave front set yields

$$\begin{aligned}\mathrm{WF}(\delta\Delta^{\rm adv/ret}) = \{(y,p;x_1,k_1;x_2,k_2) \mid y \in J^{-/+}(x_1), x_2 \in J^{-/+}(y);\\ \exists(y,q_1),(y,q_2) \text{ such that } (y,q_i) \sim (x_i,-k_i),\ p = q_1+q_2\}\end{aligned} \tag{231}$$

We now compute the wave front set of δd by expressing it in terms of δG and $\delta\Delta^{\rm adv/ret}$ via the s-derivative of eq (227), and using the wave front set calculus. This gives the bound on the wave front set of δd, thus completing the proof of lemma 6.2.

To complete the proof of eq. (217) for I_1, we estimate its wave front set using the calculus for the wave front set together with the estimates eq. (214) for the wave front set of w, and the estimates on the wave front set of δd provided in lemma 6.2. This gives

$$\begin{aligned}\mathrm{WF}(I_1) \subset \{(y,p;x_1,k_1;\dots;x_n,k_n) \mid \\ \exists(x_1,k_1;\dots;x_n,k_n;z_1,0;\dots;z_i,q_i;\dots;z_j,q_j;\dots z_r,0) \in \mathrm{WF}(w) \quad \text{such that}\\ (y,p;z_i,q_i;z_j,q_j) \in \mathrm{WF}(\delta d) \quad \text{for some } i,j\}\\ \subset \{(y,p;x_1,k_1;\dots;x_n,k_n) \mid \exists(x_i,q_i) \quad \text{such that}\\ (x_i,q_i) \sim (y,-p) \text{ and } (x_1,k_1;\dots;x_i,k_i+q_i;\dots;x_n,k_n) \in \mathcal{C}_{\mathscr{T}}(M,\mathbf{g})\\ \text{or } x_i = x_j = y \text{ and there exist } q_i,q_j \in T^*_yM \text{ such that}\\ p = -q_1-q_2 \text{ and } (x_1,k_1;\dots;y,k_i+q_i;\dots;y,k_j+q_j;\dots;x_n,k_n) \in \mathcal{C}_{\mathscr{T}}(M,\mathbf{g})\}\end{aligned} \tag{232}$$

One verifies thereby that I_1 satisfies the wave front set condition eq. (217). The smooth resp. analytic dependence of I_1 upon the metric, eq. (218), can be proved in the same way by considering metrics that have in addition a smooth (analytic) dependence upon a further parameter.

Proof of lemma 6.1 for I_2: We next show that I_2 satisfies the wave front set condition eq. (217). It was shown in our previous paper [14] that any distribution that is locally and covariantly constructed from the metric with a smooth dependence upon the metric and an almost homogeneous scaling behavior has a so called "scaling expansion". This scaling expansion for w takes the form

$$w_{\mathbf{g}}(x_1,\dots,x_{n+r}) = \sum_j (C^{a_1\dots a_j}_{\mathbf{g}} \alpha^*_{\mathbf{g}} u_{a_1\dots a_j})(x_1,\dots,x_{n+r}) + \rho_{\mathbf{g}}(x_1,\dots,x_{n+r}), \tag{233}$$

where u are tensor valued, Lorentz invariant distributions on $(\mathbb{R}^D)^{n+r-1}$ (we think of $\mathbb{R}^D$ as being identified with the tangent space on M at x_1), where C are local curvature terms (evaluated at x_1) that are polynomials in the Riemann tensor and its derivatives, and where $\alpha_{\mathbf{g}}$ is the map

$$\alpha : U_{n+1} \ni (x_1, x_2, \ldots, x_{r+n}) \to (e^\mu(x_1, x_2), \ldots, e^\mu(x_1, x_{r+n})) \in (\mathbb{R}^D)^{n+r-1}, \tag{234}$$

where $e^\mu(x, y)$ denotes the Riemannian normal coordinates y^μ of a point y relative to a point x. The "remainder" $\rho_{\mathbf{g}}$ is a local, covariant distribution that depends smoothly upon the metric and satisfies the additional properties stated in thm. 4.1 of [14]. We refer the reader to thm. 4.1 of [14] for the construction and further properties of the scaling expansion. To proceed, we split $I_2 = I_3 + I_4$ further into a contribution I_3 arising from the sum in our scaling expansion and a contribution I_4 arising from the remainder in that expansion. We analyze these separately and show that each of them satisfies the wave front set condition eq. (217).

We first analyze I_3, given by

$$I_3(\mathbf{h}, f_1, \ldots, f_n) = \sum_j \int \delta(C^{a_1 \ldots a_j} \alpha^* u_{a_1 \ldots a_j})(z, y_1, \ldots, y_n, x_1, \ldots, x_r) \\ \mathbf{h}(z) \prod_i f_i(y_i)\, \omega \left(: \prod_{j=1}^r \varphi(x_j) :_H \right). \tag{235}$$

Since the distributions u in the scaling expansion are actually independent of $\mathbf{g}$ (so that $\delta u = 0$), we have, dropping the tensor indices,

$$\mathrm{WF}[\delta(C\alpha^* u)] \subset \mathrm{WF}[(\delta C)\alpha^* u] \cup \mathrm{WF}[C(\delta\alpha)^* u]. \tag{236}$$

Thus, in order to analyze the wave front set of $\delta(C\alpha^* u)$, we only need to analyze the variations δC and $\delta\alpha$. But C is just a polynomial in the Riemann tensor and its derivatives, from which one finds

$$\mathrm{WF}(\delta C) \subset \{(y, p; x, k) \mid x = y, \quad k = -p\}. \tag{237}$$

The wave front set of $\delta\alpha$ in turn follows from the wave front set of δe^μ (recall that e^μ is essentially the inverse of the exponential map), which in turn can be calculated to be

$$\begin{aligned} \mathrm{WF}(\delta e^\mu) \quad \subset \quad & \{(y, p; x_1, k_1; x_2, k_2) \mid \text{either of the following holds:} \\ & (y = x_1 \text{ and } p = -k_1,\, k_2 = 0) \text{ or } (y = x_2 \text{ and } p = -k_2,\, k_1 = 0) \\ & \text{or } (x_1 = x_2 = y \text{ and } p = -k_1 - k_2)\}. \end{aligned} \tag{238}$$

Using the calculus for the wave front set, we find that

$$\mathrm{WF}[\delta(C\alpha^* u)] \restriction_{\Delta_{n+r+1}} \perp T(\Delta_{n+r+1}). \tag{239}$$

Since ω is a Hadamard state, the distribution $\omega\,(:\prod\varphi(x_j):_H)$ is actually a smooth function. Therefore, using again the calculus for the front set, and using the fact that $C\alpha^* u$ has the same support as t [see eq. (213)], we conclude that I_3 is a distribution jointly in $\mathbf{h}, f_1, \dots, f_n$, satisfying the wave front set condition eq. (217). The smooth resp. analytic dependence of I_3 upon the metric, eq. (218), can be proved in a similar way by considering appropriate families of metrics, instead of the fixed metric, $\mathbf{g}$.

We finally turn our attention to the functional I_4, given by

$$I_4(\mathbf{h}, f_1, \dots, f_n) = \int \delta\rho(z, y_1, \dots, y_n, x_1, \dots, x_r)\mathbf{h}(z) \prod_i f_i(y_i)\ \omega\left(:\prod_j \varphi(x_j):_H\right). \tag{240}$$

We need to show that I_4, in fact, defines a distribution on U_{n+1}, with the wave front property (217). Since $\omega\,(:\prod\varphi(x_j):_H)$ is a smooth function, the non-trivial contributions to the wave front set of I_4 arise entirely from $\delta\rho$. The wave front set of $\delta\rho$ is analyzed as follows. By construction, $\delta\rho$ is already known to be a distribution on U_{n+r+1} away from Δ_{n+r+1}. Let us denote this distribution $\delta\rho^0$. It follows from the properties of the scaling expansion (cf. thm. 4.1 of [14]) that $\delta\rho^0$ has arbitrary low scaling degree at Δ_{n+r+1} (if the scaling expansion is carried out to sufficiently large order). By the arguments given in [14], this entails that $\delta\rho$ arises from $\delta\rho^0$ by continuing the latter in a unique way to a distribution defined on all of U_{n+r+1}, in the sense that

$$\delta\rho = \lim_{\lambda\to 0+} \theta_\lambda \delta\rho^0. \tag{241}$$

Here, $\theta_\lambda(y, x_1, \dots, x_n) = \theta(\lambda^{-1} S(y; x_1, \dots, x_n))$, where S is any smooth function measuring the distance from the total diagonal, and θ is a any smooth, real valued function which vanishes in a neighborhood of the origin in $\mathbb{R}$ and which is equal to 1 outside a compact set. The key point is that we now can derive the wave front set properties of $\delta\rho$ from the fact that it is the unique continuation of $\delta\rho^0$ together with the known properties of $\delta\rho^0$. The relevant properties of $\delta\rho^0$ are that[27]

$$\left\{\text{closure of wave front set of } \delta\rho^0_{\mathbf{g}^{(s)}} \text{ in } T^*(\mathcal{P}\times M^{n+r+1})\right\}\Big|_{\mathcal{P}\times\Delta_{n+r+1}} \perp T(\mathcal{P}\times\Delta_{n+r+1}) \tag{242}$$

where $\mathbf{g}^{(s)}$ is any family of metrics depending smoothly upon a parameter $s \in \mathcal{P}$, and that $\delta\rho^0$ has a certain integral representation (see eqs. (55)–(57) of [14]) which can be derived from the fact that it is the remainder in a scaling expansion. It follows from these properties (by an argument completely analogous to the one given in the proof of [14, prop. 4.1, pp. 336]) that

$$\mathrm{WF}(\delta\rho)\restriction_{\Delta_{n+r+1}} \perp T(\Delta_{n+r+1}). \tag{243}$$

[27]Note that it is essential that we know this property for an arbitrary smooth family $\mathbf{g}^{(s)}$ and not just a fixed metric.

This estimate can be used to establish equation (217) for I_4 by applying the wave front set calculus to the defining relation (240) for I_4. The smooth resp. analytic dependence of I_4 upon the metric, eq. (218), can be shown by similar methods. This shows that I_2 satisfies relations eq. (204) and (218), and thereby concludes the proof of lemma 6.1.

6.2.6 Proof that D_n is symmetric when $\Phi_1 = T_{ab}$

We now examine the symmetry properties of D_n. It is a straightforward consequence of the definition of D_n together with the symmetry of the time-ordered products, T6, that $D_n(\mathbf{h}; f_1, \dots, f_n)$ is symmetric in $f_1, \dots, f_n$ when the fields $\Phi_1, \dots, \Phi_n$ are also exchanged accordingly. However, the symmetry properties of D_n with regard to exchanges of $\mathbf{h}$ with the f_i are not at all manifest from the definition of D_n, as $\mathbf{h}$ appears on a completly different footing than the f_i. We here examine the symmetry properties of D_n under such exchanges, which of course are relevant only when one of the fields $f_i\Phi_i$ is equal to the (densitized) stress energy tensor, say $f_1\Phi_1 = \boldsymbol{\epsilon} h_1^{ab} T_{ab}$.

We claim that the prescription for defining time ordered products can be modified (within the allowed freedom) so that the corresponding new D_n' is symmetric in the sense that

$$D_n'(\mathbf{h}_2; \mathbf{h}_1, f_2, \dots, f_n) - D_n'(\mathbf{h}_1; \mathbf{h}_2, f_2, \dots, f_n) = 0. \tag{244}$$

We note that it is an immediate consequence of this equation, the definition of D_n and the symmetry of the time ordered products, T6, that

$$D_n'(\mathbf{h}_1; \dots, \mathbf{h}_i, \dots, \mathbf{h}_j, \dots) = \text{symmetric in } \mathbf{h}_1, \dots, \mathbf{h}_i, \dots, \mathbf{h}_j, \dots, \tag{245}$$

if $f_i\Phi_i = \boldsymbol{\epsilon} h_i^{ab} T_{ab}, \dots, f_j\Phi_j = \boldsymbol{\epsilon} h_j^{ab} T_{ab}$, i.e., if any number of the fields are given by stress energy tensors.

To prove eq. (244), let us first consider the simplest case, $n = 1$, for which the anti-symmetric part of D_1 is given by[28]

$$\begin{aligned} E(\mathbf{h}_1, \mathbf{h}_2) &\equiv D_1(\mathbf{h}_1, \mathbf{h}_2) - D_1(\mathbf{h}_2, \mathbf{h}_1) \\ &= \delta_1^{\mathrm{ret}} T_{ab}(\boldsymbol{\epsilon} h_2^{ab}) - \delta_2^{\mathrm{ret}} T_{cd}(\boldsymbol{\epsilon} h_1^{cd}) + \frac{\mathrm{i}}{2}[T_{ab}(\boldsymbol{\epsilon} h_1^{ab}), T_{cd}(\boldsymbol{\epsilon} h_2^{cd})]. \end{aligned} \tag{246}$$

We already know, inductively, that D_1, and hence E, is a c-number distribution that is supported on the total diagonal in $M \times M$. Moreover, E is also locally and covariantly constructed out of the metric and scales almost homogeneously (with degree = dimension of spacetime) under a rescaling of the metric by a constant conformal factor, because D_1

[28] In this formula, and in other similar formulas below, we are assuming for simplicity that the metric variations $\mathbf{h}_1$ and $\mathbf{h}_2$ commute, i.e., that $\mathbf{h}_{[1,2]} = \delta_1 \mathbf{h}_2 - \delta_2 \mathbf{h}_1 = 0$. For non-commuting variations, there would appear the additional term $T_{ab}(\boldsymbol{\epsilon} h_{[1,2]}^{ab})$ in the formula (246) for E (and corresponding other terms in similar other formulas below). An example of non-commuting variations is $\mathbf{h}_1 = \mathbf{h}$ and $\mathbf{h}_2 = \pounds_\xi \mathbf{g}$; in that case $\mathbf{h}_{[1,2]} = -\pounds_\xi \mathbf{h}$.

has already been shown to have these properties. Finally, since D_1 satisfies the wave front set properties eqs. (204) and (205), it follows by the same arguments as in [14] that D_1 (and hence E) must, in fact, be given by a delta function times suitable curvature terms of the correct dimension,

$$E(\mathbf{h}_1, \mathbf{h}_2) = \sum_r \int \boldsymbol{\epsilon}[h_1^{ab}(\nabla_{(f_1} \cdots \nabla_{f_r)} h_2^{cd}) C_{abcd}{}^{f_1 \dots f_r} - (1 \leftrightarrow 2)], \tag{247}$$

where $C_{abcd}{}^{f_1 \dots f_r}$ are local curvature terms of dimension $D - r$.

We now claim that $E = 0$ for any prescription such that the quantum stress tensor is conserved, $\nabla^a T_{ab} = 0$. To see this, consider the variations h_{ab} and $\pounds_\xi g_{ab}$, where ξ^a is an arbitrary smooth, compactly supported vector field and h_{ab} an arbitrary smooth compactly supported symmetric tensor field, i.e., choose one of the variations to be of pure gauge. Using stress energy conservation, and the remark in footnote 28, one deduces $E(\mathbf{h}, \pounds_\xi \mathbf{g}) = 0$ for any such pair of variations. Substituting this into the above expression for E, one can show this implies that $E = 0$ by an argument similar to that given in the proof of thm. 5.1. But it follows from the analysis of section 3.2 above that when $D > 2$ we can always adjust our prescription for Wick powers and time ordered products so as to satisfy $\nabla^a T_{ab} = 0$ in addition to T1–T11a. Thus, if we take the "prime" prescription to satisfy conservation of the stress tensor, then eq. (244) follows when $n = 1$.

In order to prove eq. (244) for $n > 1$, we use the identity

$$\begin{aligned} D_n(\mathbf{h}_1; \mathbf{h}_2, \dots, f_n) - D_n(\mathbf{h}_2; \mathbf{h}_1, \dots, f_n) &= \frac{2}{\mathrm{i}}(\delta_1^{\mathrm{ret}} \delta_2^{\mathrm{ret}} - \delta_2^{\mathrm{ret}} \delta_1^{\mathrm{ret}}) \mathscr{T}\left(\prod_{i=2}^n f_i \Phi_i\right) \\ &+ E(\mathbf{h}_1, \mathbf{h}_2) \mathscr{T}\left(\prod_{i=2}^n f_i \Phi_i\right), \end{aligned} \tag{248}$$

which follows from our inductive assumptions and the definition of the retarded products by a calculation similar to those given in the previous subsections. But we have already shown that $E = 0$, and we know that $\delta_1^{\mathrm{ret}} \delta_2^{\mathrm{ret}} - \delta_2^{\mathrm{ret}} \delta_1^{\mathrm{ret}} = 0$ from the definition of the retarded variation. Hence, the right side of eq. (248) in fact vanishes, thus establishing eq. (244) for $n > 1$.

Remark concerning the cohomological nature of $E = 0$, and of T11b: There is an alternative strategy to prove the key identity $E = 0$, which shows the cohomological nature of that condition, and therefore—since it is a necessary condition for T11b to hold—that there can exist "cohomological obstructions" to imposing T11b. We define

$$\begin{aligned} \widehat{\delta} &= \delta^{\mathrm{ret}} + \frac{\mathrm{i}}{2}[T_{ab}(\boldsymbol{\epsilon} h^{ab}), \cdot\,] \\ &= \frac{1}{2}(\delta^{\mathrm{ret}} + \delta^{\mathrm{adv}}) \end{aligned} \tag{249}$$

and we view $\widehat{\delta}$ as a "gauge connection" on local covariant fields. Now apply $\widehat{\delta}_3$ to the defining relation (246) for $E(\mathbf{h}_1, \mathbf{h}_2)$, and antisymmetrize over the different metric variations $1, 2$ and 3. We obtain

$$\widehat{\delta}_{[1} E(\mathbf{h}_2, \mathbf{h}_{3]}) = \widehat{\delta}_{[1} \widehat{\delta}_2 T_{ab}(\boldsymbol{\epsilon} h^{ab}_{3]}) = 0, \tag{250}$$

where the second equality can be verified[29] by a direct calculation using the Jacobi identity (or alternatively can be viewed as the "Bianchi identity" for the "connection" $\widehat{\delta}$, because E is the "curvature" of $\widehat{\delta}$). Since E is a c-number, the antisymmetrized $\widehat{\delta}$-variation of the left side of the equation is actually equal to $\delta_{[1} E(\mathbf{h}_2, \mathbf{h}_{3]})$, where δ is the ordinary variation of a functional with respect to the metric. Hence

$$\delta_{[1} E(\mathbf{h}_2, \mathbf{h}_{3]}) = 0, \tag{251}$$

i.e., E has vanishing "curl".

In finite dimensions, every differential form with vanishing curl can be written as the curl of a form of lower degree, unless there is a topological obstruction. In the present case, the key issue is whether it is possible to write E as the curl of some F, i.e.

$$E(\mathbf{h}_1, \mathbf{h}_2) = \delta_{[1} F(\mathbf{h}_{2]}) \tag{252}$$

for some functional

$$F(\mathbf{h}) = \int C^{ab} h_{ab} \boldsymbol{\epsilon}, \tag{253}$$

where C^{ab} is a local curvature term (of the appropriate dimension). The point is that, if E could indeed be written in this way, and if we could then redefine our prescription for the stress energy tensor by $T'_{ab} = T_{ab} - C_{ab}\mathbb{1}$, then the new prescription would satisfy $E' = 0$ (as well as $\nabla^a T'_{ab} = 0$). Alternatively, if it is not always possible to write any E satisfying eq. (251) in the form (252)—i.e., if the space of functionals of the metric of this type has a non-trivial cohomology with respect to the differential δ—then if such an E arises in eq. (246) in a quantum field theory, it is clear that there would be no way consistent with axioms T1-T10 to adjust the prescription for defining time-ordered products so as to make E vanish. Consequently, by the arguments given above, it would not be possible to have a conserved stress-energy tensor in such a quantum field theory, i.e., the theory would have a "gravitational anomaly". As we have seen above, this "cohomological obstruction" does not occur for the theory of a scalar field, but it could occur for quantum field theories containing fields of higher spin.

In field theories (such as scalar field theory) that are invariant under parity, $\boldsymbol{\epsilon} \to -\boldsymbol{\epsilon}$, it follows that E must transform as[30] $E \to -E$. We are not aware of any E with this

[29] We are assuming that the variations 1, 2 and 3 commute, see footnote 28. If the variations do not commute, there would appear the additional terms $E(\mathbf{h}_1, \mathbf{h}_{[2,3]}) + E(\mathbf{h}_2, \mathbf{h}_{[3,1]}) + E(\mathbf{h}_3, \mathbf{h}_{[1,2]})$ on the left side.

[30] The minus sign arises simply because an integration is implicit in the definition of E. The integrand of such an E would be parity invariant.

transformation property which has vanishing curl but cannot be written as the curl of some F. If this could be proven, then this would provide a general proof that we can satisfy $E = 0$ in field theories preserving parity (assuming that there are no algebraic restrictions on T_{ab}). However, nontrivial cocycles E can occur when parity invariance is dropped. An example in $D = 2$ spacetime dimensions is

$$E_{D=2}(\mathbf{h}_1, \mathbf{h}_2) = \int \left[R\epsilon^{ab} h_{1\,ac} h_{2\,b}{}^{c} + 2\epsilon^{ab} \nabla_c (h_{1\,a}{}^{c} - \delta_a{}^{c} h_{1\,m}{}^{m}) \nabla_d (h_{2\,b}{}^{d} - \delta_b{}^{d} h_{2\,n}{}^{n}) \right] \boldsymbol{\epsilon} \,. \quad (254)$$

We have checked explicitly that $E_{D=2}$ has vanishing curl. However, $E_{D=2}$ is not the curl of some $F_{D=2}$, as can easily be seen from the fact that, in $D = 2$ dimensions, the only functional $F_{D=2}$ with the appropriate dimension of length is, up to a numerical factor, $F_{D=2}(\mathbf{h}) = \int R^{ab} h_{ab}\, \boldsymbol{\epsilon}$. But $F_{D=2}$ transforms as $F_{D=2} \to -F_{D=2}$ under parity, while $E_{D=2} \to +E_{D=2}$, so its antisymmetrized variation cannot be proportional to $E_{D=2}$.

This example explicitly shows that non-trivial cocycles E can be present, in principle, in parity violating theories, at least in $D = 2$ dimensions. In fact, as we have previously noted, gravitational anomalies are known to occur [1] for certain parity violating theories in $D = 4k + 2$ dimensions.

6.2.7 Proof that D_n can be absorbed in a redefinition of the time ordered products

We now complete our inductive argument by showing how to redefine our prescription for the time ordered products so that $D'_n = 0$ for the new prescription when $N_\varphi \le k$ factors of φ are present in $f_1\Phi_1, \dots, f_n\Phi_n$. To do this, we first collect the facts about D_n which we have established in the previous subsections, and we summarize the conclusions that can be can be drawn from them about the nature of the D_n

By its very definition, we know that for any choice of the fields Φ_i, $D_n(\mathbf{h}; f_1, \dots, f_n)$ is an $(n+1)$-times multilinear functional valued in $\mathcal{W}$. We showed that the values of this functional are actually proportional to the identity operator, allowing us to identify D_n with a functional taking values in the complex numbers. This functional is supported only on the total diagonal in M^{n+1}, i.e., it vanishes if the supports of $\mathbf{h}, f_1, \dots, f_n$ have no common points. We also established that the functional D_n depends locally and covariantly on the metric, and that it has an almost homogeneous scaling behavior under rescalings of the metric $\mathbf{g} \to \lambda^2 \mathbf{g}$, with λ a real constant. Furthermore, since the multilinear functional D_n has been shown to be in fact a distribution (i.e., to be *continuous* in the appropriate sense) satisfying the wave front set condition (204), it follows that

$$D(\mathbf{h}; f_1, \dots, f_n) = \sum_{\alpha_1, \dots, \alpha_n} \int_M \boldsymbol{\epsilon} h_{ab} C^{ab}{}_{\alpha_1 \dots \alpha_n} \prod_{i=1}^{n} \boldsymbol{\epsilon}^{-1} (\nabla)^{\alpha_i} f_i \cdot \mathbb{1}, \quad (255)$$

where the C are smooth tensor fields depending locally and covariantly on the metric, with a suitable almost homogeneous scaling behavior. Moreover, since we know that the dependence of D_n on the metric is actually smooth resp. analytic in the sense of eq. (210), it follows by the same arguments as in [13] that the C have to be a polynomials in the metric, its inverse, the Riemann tensor and its derivatives. The engineering dimension of the derivatives and curvature monomials in each term in eq. (255) must add up precisely to $d - nD$ where d is the sum of the engineering dimensions of the Φ_i. (Here, it should be noted that the delta function implicit in eq. (255) has engineering dimension $-nD = n \times$ engineering dimension of $\boldsymbol{\epsilon}^{-1}$ in D spacetime dimensions.) It follows from the unitarity condition on the time ordered products, T7, together with the fact that $\tau^{\rm ret}(a^*) = [\tau^{\rm ret}(a)]^*$ that the D_n are distributions satisfying the reality condition $\bar{D}_n = (-1)^{n+1} D_n$. The D_n also satisfy the symmetry condition (245) when one or more of the fields Φ_i is given by a stress energy tensor. Finally, we have shown that, when one of the fields Φ_i is equal to φ, we automatically have that $D_n = 0$.

Our proposal for redefining the prescription for time ordered products at the given induction order is now the following: If $\Phi_1, \dots, \Phi_n$ are fields in $\mathcal{V}_{\rm class}$ with a total number of $N_\varphi = k$ factors of φ, then we define

$$c\,[\varphi \nabla_a \nabla_b \varphi \otimes (\otimes_{i=1}^n \Phi_i)] = 2{\rm i} \left(D_{n\,ab} - \frac{1}{D-2} g_{ab} D_n{}^c{}_c \right). \tag{256}$$

We also define distributions $c[(\nabla)^r(\varphi \nabla_a \nabla_b \varphi) \otimes (\otimes_i \Phi_i)]$ associated with all Leibniz dependent expressions in such a way that eq. (174) is satisfied. and we define $c[\Psi \otimes (\otimes_i \Phi_i)] = 0$ for all Ψ which are "Leibniz independent" of $\varphi \nabla_a \nabla_b \varphi$ in the sense used in proposition 3.1. It is a direct consequence of these definitions that

$$c\,[T_{ab} \otimes (\otimes_{i=1}^n \Phi_i)] = 2{\rm i} D_{n\,ab}. \tag{257}$$

Because of the symmetry condition (245) satisfied by D_n, it follows that $c[T_{ab} \otimes \dots T_{cd} \otimes \dots]$ is symmetric in the respective spacetime arguments if one (or more) of the fields Φ_i is given by a stress tensor. Since the c satisfy the Leibniz rule in the first argument by construction, and since they satisfy the Leibniz rule in the remaining n arguments as a consequence of T10, an analogous statement also holds by definition for derivatives of the stress tensor. It follows that c satisfy the symmetry condition (173), and the Leibniz condition (174).

It is now clear from the properties that we have established about the D_n that the so defined coefficients c obey all further restrictions that are necessary in order that the new prescrition $\mathscr{T}'$ satisfies T1–T10 and T11a: Since D_n is of the form (255), the c are similarly local covariant delta function type distributions with coefficients that are given by local curvature terms of the appropriate dimension. The c satisfy the unitarity constraint eq. (172) because the D_n satisfy the analogous relation, and the c satisfy the constraint (178), because we showed that $D_n = 0$ when one of the Φ_i is equal to φ.

On account of the formula (6) for the free stress tensor T_{ab}, the changes in the time ordered products corresponding to the c given in eq. (256) via eqs. (170) and (171) take the following form for time ordered products with one factor of T_{ab} and n factors $\Phi_1, \dots, \Phi_n$ with $N_\varphi = k$ factors of φ:

$$\mathscr{T}'\left(\boldsymbol{\epsilon} h_{ab} T^{ab} \prod_{i=1}^{n} f_i \Phi_i\right) = \mathscr{T}\left(\boldsymbol{\epsilon} h_{ab} T^{ab} \prod_{i=1}^{n} f_i \Phi_i\right) + 2\mathrm{i} D_n^{ab}(h_{ab}; f_1, \dots, f_n) \cdot \mathbb{1} \tag{258}$$

It follows from this relation that the new prescription $\mathscr{T}'$ is designed so that $D'_n = 0$ for all $\Phi_1, \dots, \Phi_n$ such that $N_\varphi \le k$. Hence, T11b holds for the new prescription at the desired order in the induction process. This completes the proof that when $D > 2$, we can satisfy condition T11b in addition to conditions T1-T10 and T11a.

Remark: In $D = 2$ spacetime dimensions, we cannot define coefficients c by eq. (256) (because of the factor of $D-2$ in the denominator), unless D_n already happens to vanish, in which case there would of course be nothing to show in the first place. However, D_n is explicitly seen to be nonzero already for $n = 1$ and $\Phi_1 = \varphi^2$ in $D = 2$ spacetime dimensions in the local normal ordering prescription, and our previous arguments show that it cannot be made to vanish.

7 Outlook

In this paper, we have proposed two new conditions, T10 and T11, that we argued should be imposed on the definition of Wick polynomials and time-ordered products in the theory of a quantum scalar field in curved spacetime. These conditions supplement our previous conditions T1-T9, and place significant additional restrictions on the definition of Wick polynomials and time-ordered products that involve derivatives of the field. We also showed that conditions T1-T10 and T11a can always be consistently imposed, and in spacetimes of dimension $D > 2$, condition T11b also can be imposed. In addition, we proved that if these conditions are imposed on the definition of Wick polynomials and time-ordered products of the free field, then for an *arbitrary* interaction Lagrangian, L_1, the perturbatively defined stress-energy tensor of the interacting field will be conserved. We do not believe that there are any further natural conditions that should be imposed on the definition of Wick polynomials and time-ordered products for a quantum scalar field in curved spacetime. If so, axioms T1-T11 together with the existence proofs and uniqueness analyses of this paper and our previous papers essentially complete the perturbative formulation of interacting quantum field theory in curved spacetime for a scalar field with an arbitrary interaction Lagrangian.

For quantum fermion fields in curved spacetime, one can define a "canonical anti-commutation algebra" in direct analogy to the canonical commutation algebra $\mathcal{A}(M, \mathbf{g})$ defined at the beginning of subsection 2.1. The next step toward the formulation of the theory of interacting fermion fields in curved spacetime would be to define the fermionic analog of the algebra $\mathcal{W}$ and to formulate suitable fermionic analogs of our axioms T1-T11. We do not anticipate that any major difficulties would arise in carrying out these steps, although we have not yet attempted to do so ourselves. We also would expect it to be possible to prove existence and uniqueness results for the fermion case in close parallel to the scalar field case. Indeed, the only place in our entire analysis where it is clear that differences can arise is the analysis of obstructions to the implementation of condition T11b. As previously noted, the analysis of [1] establishes that the analog of condition T11b cannot hold for certain parity violating theories in spacetimes of dimension $4k + 2$.

To define the quantum theory of Yang-Mills fields in curved spacetime, one would presumably start, as in flat spacetime, by "gauge fixing" and introducing "ghost fields". However, to proceed further in the spirit of our approach, one would have to formulate the theory entirely within the algebraic framework, including procedures for extracting gauge invariant information from the field algebra. Since many subtleties already arise in the usual treatments of Yang-Mills fields in flat spacetime due to local gauge invariance, we do not anticipate that it will be straightfoward to extend our analysis to the Yang-Mills case. We expect that it would be even less straightforward to extend our analysis to a perturbative treatment of quantum gravity itself off of an arbitrary globally hyperbolic, classical solution to Einstein's equation, although we also do not see any obvious reasons why this could not be done.

Returning to the case of a scalar field, there remain some significant unresolved issues even if the renormalization theory as presently formulated turns out to be essentially complete. One such issue concerns the probability interpretation of the theory. As emphasized, e.g., in [20], there is no meaningful notion of "particle"—even asymptotically—in a general curved spacetime. Thus, the only meaningful observables are the smeared local and covariant quantum fields themselves. Let $\Phi(f) \in \mathcal{W}$ be such a field observable for the free scalar field φ, which is "self-adjoint" in the sense that $\Phi(f)^* = \Phi(f)$. For any state, ω, the very definition of ω provides one with the expectation value, $\langle \Phi(f) \rangle = \omega(\Phi(f))$, of this observable in the state ω. We also can directly obtain the moments, $\omega([\Phi(f) - \langle \Phi(f) \rangle]^n)$, of the probability distribution for measurements of $\Phi(f)$ in the state ω, since powers of $\Phi(f)$ are also in $\mathcal{W}$. However, to obtain the probability distribution itself, we need to go to a Hilbert space representation, such as the GNS representation, where ω is represented by an ordinary vector in a Hilbert space, and $\Phi(f)$ is represented by an operator $\pi[\Phi(f)]$, so that probabilities can be calculated by the usual Hilbert space methods. However, a potential difficulty arises here. Although in the GNS representation $\pi[\Phi(f)]$ is automatically a symmetric operator defined on a dense, invariant domain $\mathcal{D}$, there does not appear to be any guarantee that $\pi[\Phi(f)]$ will be essentially self-adjoint on $\mathcal{D}$. If essential self-adjointness fails, then further input would be needed to obtain a probability distribution. Specifically, if $\pi[\Phi(f)]$ has more than one self-adjoint extension, then additional rules would have to be found to determine which self-adjoint extension should be used to define the probability distribution. Worse yet, if $\pi[\Phi(f)]$ does not admit any self-adjoint extension at all, it is hard to see how any consistent probability rules can be given. As far as we are aware, this issue is unresolved for general observables in $\mathcal{W}$ even for the vacuum state in Minkowski spacetime.

Another issue of interest that has not yet been investigated in depth concerns whether a useful, non-perturbative, axiomatic characterization of interacting quantum field theory in curved spacetime can be given. The usual axiomatic formulations of quantum field theory in Minkowski spacetime, such as the Wightman axioms [19], make use of properties that are very special to Minkowski spacetime. It seems clear that a suitable replacement for the Minkowski spacetime assumption of covariance of the quantum fields under Poincare transformations is the condition that the quantum fields be local and covariant [13, 6]. It also seems clear that microlocal spectral conditions should provide a suitable replacement for the usual spectral condition assumptions in Minkowski spacetime. However, it is far less clear what should replace the Minkowski spacetime assumption of the existence of a unique, Poincare invariant vacuum state, since no analog of this property exists in curved spacetime. One possibility for such a replacement might be suitable assumptions concerning the existence and properties of an operator product expansion [11].

Undoubtedly, the foremost unresolved issue with regard to the perturbative formulation of quantum field theory in curved spacetime concerns the meaning and convergence properties of the Bogoliubov formula, eq. (91), which defines the interacting field. It is, of course, very well known that "perturbation theory in quantum field theory does not converge". However, as we pointed out in [15], the usual results and arguments against convergence concern the calculation of quantities that involve ground states or "in" and "out" states, and such states would not be expected to have the required analyticity properties. We believe that eq. (91) stands the best chance of making well defined mathematical sense if it is interpreted as determining the algebraic relations that hold in the interacting field algebra. The formula does not, of course, make sense as it stands (except as a formal power series) since we have not defined a topology on $\mathcal{W}$—so the notion of "convergence" has not even been defined—and, in any case, $\mathcal{W}$ should be "too small" to contain the elements of the interacting field algebra, since $\mathcal{W}$ consists only of *polynomial* expressions in φ smeared with appropriate distributions. However, one could imagine "enlarging" $\mathcal{W}$ by defining a suitable topological algebra $\bar{\mathcal{W}}$ into which $\mathcal{W}$ is densely embedded. We see no obvious reason why such a $\bar{\mathcal{W}}$ could not be defined so that eq. (91) would define a convergent series in $\bar{\mathcal{W}}$—but, of course, we also do not see an obvious way of carrying this out! These ideas appear to be worthy of further investigation.

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A Infinitesimal retarded variations

Let $\mathbf{g}^{(s)}$ be a smooth 1-parameter family of metrics differing from $\mathbf{g} \equiv \mathbf{g}^{(0)}$ only within a compact subset K. In this appendix, we show that the retarded variation with respect to the metric defined by

$$\delta_{\mathbf{g}}^{\mathrm{ret}} \left[\mathscr{T}_{\mathbf{g}} \left(\prod_{i=1}^{n} f_i \Phi_i \right) \right] = \frac{\partial}{\partial s} \tau_{\mathbf{g}^{(s)}}^{\mathrm{ret}} \left[\mathscr{T}_{\mathbf{g}^{(s)}} \left(\prod_{i=1}^{n} f_i \Phi_i \right) \right] \Bigg|_{s=0} \tag{259}$$

appearing in our requirement T11b is well-defined and yields an element of $\mathcal{W}(M, \mathbf{g})$. Our proof can easily be generalized to also prove the corresponding statement for an infinitesimal retarded variation of the potential, T11c, but we shall not treat this case explicitly.

Let $A^{\mathrm{ret}\,(s)}$ be the map as defined by eq. (99) above, let ω_2 be the two-point function of a Hadamard state on $(M, \mathbf{g})$ and let $\omega_2^{(s)}$ be the Hadamard 2-point functions for $(M, \mathbf{g}^{(s)})$, uniquely specified by the requirement that $\omega_2^{(s)}$ coincides with ω_2 when both arguments are taken within $M \setminus J^+(K)$. Then it can be verified that $A^{\mathrm{ret}\,(s)}$ and $\omega_2^{(s)}$ have a smooth dependence upon s in the sense that, when viewed as distributions jointly in s, x_1, x_2, we have

$$\begin{aligned} \mathrm{WF}(A^{\mathrm{ret}\,(s)}) \subset \{ (s, \rho; x_1, k_1; x_2, -k_2) \mid \exists y \in M \setminus J^+(K) \text{ and } (y, p) \in T_y^* M \setminus \{0\} \\ \text{such that } (x_1, k_1) \sim (y, p) \text{ with respect to } \mathbf{g} \text{ and} \\ \text{such that } (x_2, k_2) \sim (y, p) \text{ with respect to } \mathbf{g}^{(s)} \}, \end{aligned} \tag{260}$$

as well as eq. (35). Since the definition of $\mathcal{W}$ does not depend upon the choice of quasifree Hadamard state used in the definition of the generators W_n, we can assume without loss of generality that the generators $W^{(s)}$ of the algebra $\mathcal{W}(M, \mathbf{g}^{(s)})$ are defined using the particular 1-parameter family of states $\omega^{(s)}$ that we have just described. To compute the action of τ^{ret} on the time ordered products, we recall that the time ordered products have the following "(global) Wick expansion,"

$$\begin{aligned} \mathscr{T} \left(\prod_{i=1}^{n} f_i \Phi_i \right) = \sum_{\alpha_1, \dots, \alpha_n} \frac{1}{\alpha_1! \cdots \alpha_n!} \int \omega \left[\mathscr{T} \left(\prod_{i=1}^{n} \delta^{\alpha_i} \Phi_i(y_i) \right) \right] \prod_i f_i(y_i) \cdot \\ \cdot : \prod_i \prod_j [(\nabla)^j \varphi(y_i)]^{\alpha_{ij}} :_\omega \end{aligned} \tag{261}$$

where we are using the same notation as in the local Wick expansion[31] given in (212).

[31] Note that this expansion is entirely analogous to the local Wick expansion (212). The only difference is that in the local Wick expansion, the time ordered products are expanded in terms of the *local normal*

Inserting suitable δ-distributions, we can rewrite the Wick expansion in the form

$$\begin{aligned}
\mathscr{T}\left(\prod f_i \Phi_i\right) &= \sum_n \int u_n(y_1, \dots, y_m; x_1, \dots, x_n) \; :\prod_i^n \varphi(x_i) :_\omega \prod_j f_j(y_j) \\
&= \sum_n W_n\Big(u_n(\otimes_i f_i)\Big),
\end{aligned} \tag{262}$$

where the distributions u_n are defined in terms of the $\omega[\mathscr{T}(\prod \delta^{\alpha_i}\Phi_i(y_i))]$ with $\sum |\alpha_i| = n$, together with suitable derivatives of delta functions. On account of the delta functions, the u_n have the same support as the distributions w in eq. (213), and they satisfy the same wave front set condition as in eqs. (214). Furthermore, if we repeat the above steps for our family of metrics $\mathbf{g}^{(s)}$ instead of the single metric $\mathbf{g}$ (with ω_2 replaced by $\omega_2^{(s)}$ everywhere) then we find that the corresponding distributions $u_n^{(s)}$ have a smooth dependence upon s, i.e., that they satisfy the same wave front set condition as in eq. (215). By the wave front set calculus, we conclude that, for any n, and for any fixed choice of smooth compactly supported functions f_i, the quantity $u_n^{(s)}(\otimes_i f_i; x_1, \dots, x_n)$ is indeed a distribution in the variables $x_1, \dots, x_n$ belonging to the space $\mathscr{E}'_n(M, \mathbf{g}^{(s)})$. Moreover, it follows from the smoothness property in s of the $u_n^{(s)}$ that these distributions actually have a smooth dependence upon s in the sense that, when viewed as a distribution jointly in $s, x_1, \dots, x_n$, we have

$$\begin{aligned}
\mathrm{WF}\left(u_n^{(s)}(\otimes_i f_i)\right) \subset \{&(s, \rho; x_1, k_1; \dots; x_n, k_n) \mid \\
&(x_1, k_1; \dots; x_n, k_n) \notin [(V^{(s)\,+})^n \cup (V^{(s)\,-})^n] \setminus \{0\}\},
\end{aligned} \tag{263}$$

where $V^{(s)\,+/-}$ are the future/past lightcones associated with the metrics $\mathbf{g}^{(s)}$.

Substituting eq. (262) into the the definition of $\tau^{\mathrm{ret}}_{\mathbf{g}^{(s)}}$, we find

$$\tau^{\mathrm{ret}}_{\mathbf{g}^{(s)}}\left[\mathscr{T}_{\mathbf{g}^{(s)}}\left(\prod_i f_i \Phi_i\right)\right] = \sum_n W_n\Big((A^{\mathrm{ret}\,(s)})^{\otimes n}\left[u_n^{(s)}(\otimes_i f_i)\right]\Big) = \sum_n W_n(v_n^{(s)}), \tag{264}$$

where the distributions $v_n^{(s)}$ are the elements in the space $\mathscr{E}'_n(M, \mathbf{g})$ defined by the last equation. It follows from the calculus for wave front sets together with the wave front set of $A^{\mathrm{ret}\,(s)}$ [see eq. (260)], and the wave front property of $u_n^{(s)}$ [see eq. (263)] that $v_n^{(s)}$ are distributions depending smoothly upon s in the sense that, when viewed as distributions

ordered products (59), while we are using the normal ordered products with respect to ω_2 in eq. (262). The latter are globally defined on all of M^n, whereas the former are only defined in a neighborhood U_n of the total diagonal (but, in contrast to the normal ordered products in eq. (262), the former depend locally and covariantly on the metric).

jointly in $s, x_1, \ldots, x_n$, we have

$$\mathrm{WF}(v_n^{(s)}) \subset \{(s, \rho; x_1, k_1; \ldots; x_n, k_n) \mid \\ (x_1, k_1; \ldots; x_n, k_n) \notin [(V^{(s)+})^n \cup (V^{(s)-})^n] \setminus \{0\}\}. \quad (265)$$

It then follows that the differentiated functionals $\frac{\partial}{\partial s} v_n^{(s)}|_{s=0}$ are in fact well-defined distributions in the class $\mathcal{E}'_n(M, \mathbf{g})$. Thus, expression (259) exists as the well-defined algebra element $\sum W_n(\frac{\partial}{\partial s} v_n^{(s)}|_{s=0})$. This is what we wanted to show.

B Functional derivatives

In this appendix we define the functional derivatives, $\delta A/\delta\varphi$ and $\delta A/\delta g_{ab}$, of any element A of the space $\mathcal{F}_{\rm class}$. We shall elucidate the calculus of the functional derivative operations and, in particular, we will derive eqs. (132) and (140), which were used in the proof of theorem 5.1 and in section 6.

Let $A \in \mathcal{F}_{\rm class}$. Then A is a D-form that is locally constructed out of $\mathbf{g}$, the curvature, finitely many symmetrized derivatives of the curvature, φ, finitely many symmetrized derivatives of φ, and test tensor fields f and their symmetrized derivatives. We will denote these dependences as simply $A = A[\mathbf{g}, \varphi, f]$. The functional derivative of A with respect to φ is defined by

$$\frac{\partial}{\partial s} A[\mathbf{g}, \varphi + s\psi, f]\bigg|_{s=0} = \psi \frac{\delta A}{\delta \varphi} + \mathrm{d}\, B_\varphi[\mathbf{g}, \varphi, f, \psi], \quad (266)$$

where B_φ is a $(D-1)$-form that is similarly locally constructed out of $\mathbf{g}$, φ, f, and ψ. The deomposition of the right side of eq. (266) into the two terms written there is uniquely determined by the requirements that (1) no derivatives of ψ appear in the first term and (2) the second term is exact. The manipulations leading to this decomposition are the familiar ones that would be used to derive the Euler-Lagrange equations if A were a Lagrangian; these manipulations are usually done under an integral sign, with the "boundary term", $\mathrm{d}\, B_\varphi$, discarded. An explicit formula for $\delta A/\delta\varphi$ was given in eq. (42) above. It is worth noting that if A is an exact form, i.e., $A = \mathrm{d}\, C$ for some $C = C[\mathbf{g}, \varphi, f]$, then its functional derivative vanishes, since clearly eq. (266) holds with $\delta A/\delta\varphi = 0$ and $B_\varphi = (\partial/\partial s) C[\mathbf{g}, \varphi + s\psi, f]|_{s=0}$.

Similarly, the functional derivative of A with respect to g_{ab} is defined by

$$\frac{\partial}{\partial s} A[\mathbf{g} + s\mathbf{h}, \varphi, f]\bigg|_{s=0} = h_{ab} \frac{\delta A}{\delta g_{ab}} + \mathrm{d}\, B_{\mathbf{g}}[\mathbf{g}, \varphi, f, \mathbf{h}]. \quad (267)$$

We can obtain an explicit expression for $\delta A/\delta g_{ab}$ by introducing an arbitrary fixed, background derivative operator, $\mathring{\nabla}_a$, on M, and re-writing ∇_a and the curvature in terms of

$\overset{\circ}{\nabla}_a$ and derivatives of $\mathbf{g}$ with respect to $\overset{\circ}{\nabla}_a$. The resulting explicit formula for $\delta A/\delta g_{ab}$ was given in eq. (114) above.

Our first result is that functional derivatives with respect to φ and $\mathbf{g}$ commute modulo exact forms in the sense that

$$h_{ab}\frac{\delta}{\delta g_{ab}}\left(\psi\frac{\delta A}{\delta\varphi}\right) = \psi\frac{\delta}{\delta\varphi}\left(h_{ab}\frac{\delta A}{\delta g_{ab}}\right) + \mathrm{d}\, B \tag{268}$$

for some $(D-1)$-form, B, that is locally constructed out of $\mathbf{g}$, φ, f, ψ and $\mathbf{h}$. To prove this, we note that

$$\begin{aligned}
\frac{\partial^2}{\partial s\partial t}A[\mathbf{g}+t\mathbf{h},\varphi+s\psi,f]\bigg|_{t=s=0} &= \frac{\partial}{\partial s}\left(h_{ab}\frac{\delta A}{\delta g_{ab}} + \mathrm{d}\, B_{\mathbf{g}}\right)\bigg|_{s=0} \\
&= \frac{\partial}{\partial s}\left(h_{ab}\frac{\delta A}{\delta g_{ab}}\right)\bigg|_{s=0} + \mathrm{d}\, C_{\mathbf{g}} \\
&= \psi\frac{\delta}{\delta\varphi}\left(h_{ab}\frac{\delta A}{\delta g_{ab}}\right) + \mathrm{d}\, C_{\mathbf{g}} + \mathrm{d}\, B_{\varphi}
\end{aligned} \tag{269}$$

where $C_{\mathbf{g}} = (\partial/\partial s)B_{\mathbf{g}}[\mathbf{g},\phi+s\psi,f,\mathbf{h}]|_{s=0}$. By equality of mixed partials, we may reverse the order of differentiation with respect to s and t on the left side of eq. (269). However, $\partial^2 A/\partial t\partial s$ is given by a similar expression with the order of the functional derivatives reversed. This establishes eq. (268).

Let us now prove the relation

$$(\pounds_\xi g_{ab})\frac{\delta A}{\delta g_{ab}} + (\pounds_\xi\varphi)\frac{\delta A}{\delta\varphi} + (\pounds_\xi f)\frac{\delta A}{\delta f} = \mathrm{d}\, H. \tag{270}$$

where $\delta A/\delta f$ is defined by analogy with eqs. (266) and (267) and is given by an explicit formula analogous to eq. (42). This equation is equivalent to eq. (140) when A depends linearly upon f. Let F_s be the one-parameter family of diffeomorphisms of M generated by a smooth, compactly supported vector field ξ^a. Since A is locally and covariantly constructed from $\mathbf{g},\varphi,f$, we have

$$F_s^* A[\mathbf{g},\varphi,f] = A[F_s^*\mathbf{g},F_s^*\varphi,F_s^* f], \tag{271}$$

where F_s^* denotes the pull-back of a tensor field. We differentiate this equation at $s=0$, and use the fact that the Lie-derivative of any D-form A is given by $\pounds_\xi A = \mathrm{d}(\xi\cdot A)$, where $\xi\cdot A$ is the $(D-1)$-form obtained by contracting the index of the vector field into the first index of the form. We obtain

$$\mathrm{d}(\xi\cdot A[\mathbf{g},\varphi,f]) = \frac{\partial}{\partial s}A[\mathbf{g}+s\pounds_\xi\mathbf{g},\varphi,f]\bigg|_{s=0} + \frac{\partial}{\partial s}A[\mathbf{g},\varphi+s\pounds_\xi\varphi,f]\bigg|_{s=0} + \frac{\partial}{\partial s}A[\mathbf{g},\varphi,f+s\pounds_\xi f]\bigg|_{s=0}. \tag{272}$$

By eq. (267) (with $h_{ab} = \pounds_\xi g_{ab}$ in that equation), the first term on the right side is equal to $\pounds_\xi g_{ab} \cdot \delta A/\delta g_{ab}$ up to some exact form $\mathrm{d}\, B_{\mathbf{g}}$. Similarly, the second term is equal to $\pounds_\xi \varphi \cdot \delta A/\delta\varphi$, up to some exact from $\mathrm{d}\, B_\varphi$. Finally, the last term is given by $\pounds_\xi f \cdot \delta A/\delta f$ plus some $\mathrm{d}\, B_f$. Thus, we get eq. (270), with $H = \xi \cdot A - B_{\mathbf{g}} - B_\varphi - B_f$.

Finally, we prove the relation

$$(D_\eta D_\xi - D_\xi D_\eta)A = D_{[\xi,\eta]}A + \mathrm{d}\, C, \tag{273}$$

for some locally constructed $(D-1)$ form C, where the variational operation D_ξ is defined by

$$D_\xi A = \pounds_\xi g_{ab} \cdot \delta A/\delta g_{ab}\,. \tag{274}$$

According to eq. (267), we may write

$$D_\xi A[\mathbf{g}] = \frac{\partial}{\partial s} A[\mathbf{g} + s\pounds_\xi \mathbf{g}]\bigg|_{s=0} - \mathrm{d}\, B[\mathbf{g}, \xi] \tag{275}$$

for some B, where we are now omitting reference to the dependence upon f, φ to lighten the notation. Now apply D_η to this equation.

$$D_\eta D_\xi A[\mathbf{g}] = D_\eta \frac{\partial}{\partial s} A[\mathbf{g} + s\pounds_\xi \mathbf{g}]\bigg|_{s=0} - D_\eta\, \mathrm{d}\, B[\mathbf{g}, \xi]. \tag{276}$$

The second term on the right side of this equation vanishes, since it is the functional derivative of an exact form. Applying eq. (275) to the first term on the right side of eq. (276), we get

$$D_\eta \frac{\partial}{\partial s} A[\mathbf{g} + s\pounds_\xi \mathbf{g}]\bigg|_{s=0} = \frac{\partial^2}{\partial s \partial t} A[\mathbf{g} + s\pounds_\xi(\mathbf{g} + t\pounds_\eta \mathbf{g})]\bigg|_{s=t=0} + \mathrm{d}\, E[\mathbf{g}, \xi, \eta] \tag{277}$$

for some E. Combining these equations and antisymmetrizing over ξ and η, we obtain

$$(D_\eta D_\xi - D_\xi D_\eta)A[\mathbf{g}] = \frac{\partial^2}{\partial s \partial t} A[\mathbf{g} + st(\pounds_\xi \pounds_\eta - \pounds_\eta \pounds_\xi)\mathbf{g}]\bigg|_{s=t=0} + \mathrm{d}\, K \tag{278}$$

for some locally constructed $(D-1)$-form K. Applying eq. (275) once more to the first term on the right side of eq. (278) and using $\pounds_\xi \pounds_\eta - \pounds_\eta \pounds_\xi = \pounds_{[\xi,\eta]}$, we obtain the desired relation (273).

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