An Introduction to Algebraic QFT in Curved Spacetime

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Introduction

These lecture notes are used in one of the three possible versions of a six-month course mathematical physics that the author teaches at the University of Trento for the master's degrees in physics and mathematics. The first part of the course deals with the mathematical formulation of quantum theories in Hilbert space and is based on the text [62] by the same author. The parts relating to differential geometry are covered in the lecture notes [56, 57] by the same author.

A preliminary version of this work is a paper written in collaboration with I. Khavkine and published as [52]. Some of the proofs appearing in theses notes faithfully present arguments completely produced by I. Khavkine. A footnote acknowledges it when necessary.

The main goal of these lecture notes is to introduce the students to the algebraic approach to QFT in curved spacetime, in terms of $*$-algebras of operators. We only consider a real scalar Klein-Gordon quantum field as a model. We shall deal with some initial issues about renormalization when introducing the so-called Hadamard states.

Concerning prerequisites, the reader supposed to be familiar with the theoretical formulation of Quantum Theory in Hilbert spaces and the necessary mathematical technology from linear functional analysis and spectral theory as presented in [62].

Classical and Quantum Fields

Part of the classical (i.e. non quantum) physical matter is made of so-called *fields*. A (real scalar) field is a real-valued function defined on a *spacetime* M, for now roughly viewed as the product $\mathbb{R} \times \mathbb{R}^3$, the former representing the temporal axis and the latter the rest space of a reference frame. In practice:

$$M \ni x \mapsto \phi(x) \in \mathbb{R}\,.$$

A field satisfies a suitable dynamical equation that permits some existence and uniqueness theorem when initial data – e.g., the field values (and higher temporal derivatives) at each space point of $\mathbb{R}^3$ at the inital time $0 \in \mathbb{R}$ – are provided. More generally ϕ can take values in a vector space, with a suitable interplay with the spacetime (ϕ is a section of a *vector bundle* on the spacetime as basis)

Well known examples of fields in classical physics are the electric and the magnetic field or the gravitational one which are vector valued. The gravitational potential is an example of scalar vector field. Some of classical fields just describe some approximated phenomena, valid only at certain scales, like sound waves in a gas or a liquid, or elastic deformation waves in a continuous body or in a lattice of atoms.

When moving on to the quantum regime, a natural attempt is to define a corresponding quantum operator at least for some apparently fundamental types field, as the electromagnetic one: since the field is an observable (with some restrictions due to the so called *gauge-symmetry*), there should be a selfadjoint operator at quantum level, defined on a dense domain $D \subset \mathcal{H}$ of a suitable Hilbert space,

$$\hat{\phi}(x) : D \to \mathcal{H}$$

for every event $x \in M$. It is very well known [33] that this naive formulation is mathematically inconsistent: when adding further necessary physical restrictions to the alleged operator $\hat{\phi}(x)$, one faces insurmountable mathematical pitfalls.

What is instead possible is a *distributional* interpretation, where the field operator acts as a generalized type of distribution on *test functions.* Formally:

$$\hat{\phi}(f) = \text{``} \int_M \hat{\phi}(x) f(x) d^4x\text{''} \,.$$

More rigorously, the quantum field can be safely described by an *operator-valued* linear map

$$C_c^\infty(M) \ni f \mapsto \hat{\phi}(f) \,,$$

where all field operators $\hat{\phi}(f)$ (smeared with a test function) are really defined on a dense invariant common domain $D \subset \mathcal{H}$ of a suitable Hilbert space, where they are essentially selfadjoint. Some continuity requirements can be added in the spirt of the theory of distributions, but we shall not discuss these details here.

The idea of "quantized" fields turned out very fruitful from a physical perspective, because it showed that it is possible to associate *elementary quantum particles* to quantum fields, when these fields are "free", namely they do not have (self-)interactions with other quantum fields or themselves. Mathematically speaking, they must satisfy linear equations, even in a non trivial background, like the (non-quantized) gravitational field, as it happens in quantum field theory in curved spacetime. Especially in the absence of the gravitational field, this paradigm is known as *second quantization*, even if there is no second quantization at all! It is a direct application of general quantum theory with a suitable choice of operators and Hilbert spaces (called *Fock spaces*).

At this juncture, several important physical examples proved that the theory in a unique Hilbert space cannot account for the physical realm, when dealing with infinitely spatially extended systems (like fields which are defined in the whole space). It seems that roughly speaking, for a given quantum field, there are quantum states which cannot coexist a common Hilbert space without producing contradictions. The *algebraic approach* permits to deal with these subtleties by emancipating itself from the theory carried out in a given Hilbert space and extending the definition of quantum state. In curved spacetime, this approach produced outstanding results, like the rigorous formulation of the so called *black hole radiation.*

This is not the end of the story however! When dealing with interacting quantum fields a new family of mathematical issues pop out. It happens when interactions are described as local, i.e. in terms of products of fields evaluated at a given event in the spacetime, e.g. $\phi(x)\phi(x)\phi(x)$. These objects, as already suggested above, are ill-defined. Nevertheless, at least when dealing with fundamental interactions of fields, it seems that physics is forcing us to go back to using these ill-defined and dangerous objects.

A direct attempt to perform computations considering the fields as if they were defined at single points produces divergences. The procedure to get rid of these divergences, within a well defined perturbative approach (the *Dyson series*), is known as *renormalization*. However, the divergences are only a symptom and the reason for their presence is that mathematically ill-defined operations are being performed.

Nowadays, one can proceed with renormalization (at least the so-called *ultraviolet* one) without ever encountering infinities and fixing at each step the ill-defined procedures. The old infinities are thus tamed. In any case, even if the mathematics is known, the physical nature of the problem is not at all clear. The whole procedure seems quite hand-made and shaky. Also because some values of the constants, which appear in the formulas, have to to be fixed. More precisely, they have to be measured and then manually entered into the formulas and not fixed at the beginning. In any case, even if one introduces a finite number of values not predicted by the theory, the procedure allows one to make infinite predictions. In this sense it is scientifically sound in spite of the discussed issues.

The root of the problem is in the use of *local* interactions as said above: as far as we know from physics, everything concurs for the description of the fundamental interactions to be of this type: the *interaction Lagrangian* is made of mathematically ill-defined products of ill-defined quantum fields because evaluated at the same event of the spacetime! On the other hand when renormalization works (as in the case of *quantum electrodynamics*), one obtains the most precise predictions in the history of physics. In other cases this *perturbative* and renormalized procedure, which produced fantastic results in electrodynamics (Feynman-Tomonaga-Schwinger's Nobel prize), turns out quite useless. For example, it happens when dealing with the *strong interactions* (quantum chromodynamics).

String theory is one of the few attempts to eliminate local interactions at the root by changing the very structure of spacetime with the introduction of further compactified dimension at small scales. Unfortunately, it has not produced any confirmed predictions since it was formulated (late 60s of the last century).

Chapter 1

$*$-algebras and GNS construction for algebraic QFT

This chapter is devoted to introduce the elementary notions and constructions of the algebraic approach to QFT.

1.1 Algebraic formalism

With this preliminary section we review some basic definitions and results about the general algebraic machinery: algebras, states, GNS construction and the treatement of symmetries.

Most literature devoted to the algebraic approach to QFT is written using C^*-algebras, in particular Weyl C^*-algebras, when dealing with free fields, nevertheless the "practical" literature mostly uses *unbounded* field operators which are encapsulated in the notion of $*$-algebra instead of C^*-algebra, whose additional feature is a multiplicatively compatible norm. Actually, at the level of free theories and quasifree (Gaussian) states the two approaches are technically equivalent. Since we think more plausible that the non-expert reader acquainted with QFT in Minkowski spacetime is, perhaps unconsciously, more familiar with $*$-algebras than C^*-algebras, in the rest of the chapter we adopt the $*$-algebra framework.

Definition 1.1. [Algebras] An **algebra** $\mathcal{A}$ is a complex vector space which is equipped with an associative product

$$\mathcal{A} \times \mathcal{A} \ni (a, b) \mapsto ab \in \mathcal{A}$$

which is distributive with respect to the vector sum operation and satisfies

$$\alpha(ab) = (\alpha a)b = a(\alpha b) \quad \text{if } \alpha \in \mathbb{C} \text{ and } a, b \in \mathcal{A} .$$

Furthermore

(a) The **center** of $\mathcal{A}$ is the set $\mathcal{Z}_{\mathcal{A}}$ of elements $z \in \mathcal{A}$ commuting with all elements of $\mathcal{A}$.

(b) A set $G \subset \mathcal{A}$ is said to **generate** $\mathcal{A}$, and the elements of G are said **generators** of $\mathcal{A}$, if each element of $\mathcal{A}$ is a finite complex linear combination of products (with arbitrary finite number of factors) of elements of G.

(c) $\mathcal{A}$ is a **$*$-algebra** if admits an **involution**, namely an anti-linear map, $\mathcal{A} \ni a \mapsto a^*$, which is involutive, that is $(a^*)^* = a$, and such that $(ab)^* = b^*a^*$, for any $a, b \in \mathcal{A}$.

(d) $\mathcal{A}$ is **unital** if admits a multiplicative **unit** $\mathbb{1} \in \mathcal{A}$, that is $\mathbb{1}a = a\mathbb{1} = a$ for all $a \in \mathcal{A}$.

(e) A $*$-algebra $\mathcal{A}$ is a **C^*-algebra** if it is a Banach space with respect to a norm $||\ ||$ which satisfies $||ab|| \leq ||a||\,||b||$ and $||a^*a|| = ||a||^2$ if $a, b \in \mathcal{A}$.

(f) $\mathcal{A}_1 \subset \mathcal{A}$, where $\mathcal{A}$ is an algebra, is a **subalgebra** if it is a linear subspace of $\mathcal{A}$ closed with respect to the algebra product of $\mathcal{A}$. $\mathcal{A}_1$ is also required to include the unit of $\mathcal{A}$ if the latter is unital.

(f) If $\mathcal{A}$ is a $*$-algebra, $\mathcal{A}_1 \subset \mathcal{A}$ is a **sub $*$-algebra** if it is a subalgebra which is closed with respect to the involution of $\mathcal{A}$. ■

Regarding morphisms of algebras we shall adopt the following standard definitions

Definition 1.2. [Algebra morphisms] Consider a map $\beta : \mathcal{A}_1 \to \mathcal{A}_2$, where $\mathcal{A}_i$ are algebras.

(a) β is an **algebra homomorphism** if it is a complex linear map, preserves the product and, if the algebras are unital, preserves the unit elements.

(b) β is a **$*$-algebra homomorphism** if $\mathcal{A}_i$ are $*$-algebras, β is a **algebra homomorphism** and preserves the involution.

(c) β is an **algebra isomorphism** or a **$*$-algebra isomorphism** if it is an **algebra homomorphism** or, respectively, a **$*$-algebra homomorphism** and it is bijective.

(d) β is an **algebra automorphism** or a **$*$-algebra automorphism** if it is a **algebra isomorphism** or, respectively, a **$*$-algebra isomorphism** and $\mathcal{A}_1 = \mathcal{A}_2$.

Corresponding **anti-linear morphisms** are defined analogously replacing the linearity condition with anti-linearity. ■

Remark 1.3.
(1) The unit $\mathbb{1}$, if exists, turns out to be unique. In $*$-algebras it satisfies $\mathbb{1} = \mathbb{1}^*$. The proofs are elementary.

(2) Although we shall not deal much with C^*-algebras, we recall the reader that a unital $*$-algebra admits at most one norm making it a C^*-algebra. Finally, $*$-homomorphisms between two unital C^*-algebras are automatically continuous because norm-decreasing [61, 62]

Definition 1.4. [Two-sided ideals] A **two-sided ideal** of an algebra $\mathcal{A}$ is a linear complex subspace $\mathfrak{I} \subset \mathcal{A}$ such that $ab \in \mathfrak{I}$ and $ba \in \mathfrak{I}$ if $a \in \mathcal{A}$ and $b \in \mathfrak{I}$.

In a $*$-algebra, a two-sided ideal $\mathfrak{I}$ is said to be a **two-sided $*$-ideal** if it is also closed with respect to the involution: $a^* \in \mathfrak{I}$ if $a \in \mathfrak{I}$.

An algebra $\mathcal{A}$ is **simple** if it does not admit two-sided ideals different form $\{0\}$ and $\mathcal{A}$ itself. ■

Remark 1.5. It should be evident that the intersection of a class of two-sided ideals (two-sided $*$-ideals) is a two-sided ideal (resp. two-sided $*$-ideal). ■

1.1.1 The general algebraic approach to quantum theories

In the algebraic formulation of a quantum theory [33], observables are viewed as abstract self-adjoint objects instead of operators in a given Hilbert space. These observable generate a $*$-*algebra* or a C^*-*algebra* depending on the context. The algebra also includes a formal identity $\mathbb{1}$ and *complex* linear combinations of observables which, consequently cannot be interpreted as observables. Nevertheless the use of complex algebras is mathematically convenient. The justification of a linear structure for the set of the observables is quite easy, the presence of an associative product is instead much more difficult to justify [76]. However, *a posteriori*, this approach reveals to be powerful and it is particularly convenient when the theory encompasses many unitarily inequivalent representation of the algebra of observables, as it happens in quantum field theory.

1.1.2 Defining $*$-algebras by generators and relations

In the algebraic approach, the $*$-algebra of observables cannot be defined simply as some concrete set of (possibly unbounded) operators on some Hilbert space. Instead, the $*$-algebra must be defined abstractly, using some more basic objects. Below we recall an elementary algebraic construction that will be of use in Section 1.2.1 in defining the CCR algebra of a scalar field.

We will construct a $*$-algebra from a presentation by *generators* and *relations*. As we shall see in the Section 1.2.1, the CCR algebra is *generated* by abstract objects, the *smeared fields*, $\phi(f)$ and the unit $\mathbb{1}$. In other words, the elements of the algebra are finite linear combinations of products of these objects. However there also are *relations* among these objects, e.g. $[\phi(f), \phi(g)] = iE(f, g)\mathbb{1}$. We therefore need an abstract procedure to define this sort of algebras, starting form generators and imposing relations. We make each of these concepts precise in a general context.

Let us start with the notion of algebra, $\mathcal{A}_G$, *generated* by a set of generators G. Intuitively, the algebra $\mathcal{A}_G$ is the *smallest* algebra that contains the elements of the generator set G (yet without any algebraic relations between these generators). The following is an example of a definition by a *universal property* [54, §I.11].

Definition 1.6. [Free algebra] Given a set G of elements called **generators** (not necessarily finite or even countable) the following definitions are valid.

(a) An algebra $\mathcal{A}_G$ is said to be **freely generated by** G (or **free on** G) if there is a (necessarily injective) map $\gamma\colon G \to \mathcal{A}_G$ such that, for any algebra $\mathcal{B}$ and map $\beta\colon G \to \mathcal{B}$, there exists a *unique* algebra homomorphism $b\colon \mathcal{A}_G \to \mathcal{B}$ such that $\beta = b \circ \gamma$.

(b) A (unital) $*$-algebra $\mathcal{A}_G$ is said to be **freely generated by** G (or **free on** G) if there is a (necessarily injective) map $\gamma\colon G \to \mathcal{A}_G$ such that, for any (unital) $*$-algebra $\mathcal{B}$ and map $\beta\colon G \to \mathcal{B}$, there exists a *unique* $*$-algebra homomorphism $b\colon \mathcal{A}_G \to \mathcal{B}$ such that $\beta = b\circ\gamma$. ■

Remark 1.7.

(1) The elements of $\gamma(G) \subset \mathcal{A}_G$ are necessarily *generators* of $\mathcal{A}_G$ according to Definition 1.1.

(2) Any two algebras freely generated by G, given by say $\gamma\colon G \to \mathcal{A}_G$ and $\gamma'\colon G \to \mathcal{A}'_G$, are *naturally isomorphic*. In this sense $\mathcal{A}_G$ is uniquely determined by G. By definition, there exist unique homomorphisms $a\colon \mathcal{A}'_G \to \mathcal{A}_G$ and $a'\colon \mathcal{A}_G \to \mathcal{A}'_G$ such that $\gamma = a \circ \gamma'$ and $\gamma' = a' \circ \gamma$. Their compositions satisfy the same kind of identity as b in the above definition, namely $\gamma = \mathrm{id} \circ \gamma = (a \circ a') \circ \gamma$ and $\gamma' = \mathrm{id} \circ \gamma' = (a' \circ a) \circ \gamma'$, where we use id to denote the identity homomorphism on any algebra. Invoking once again uniqueness shows that $a \circ a' = \mathrm{id} = a' \circ a$ and hence that $\mathcal{A}_G$ and $\mathcal{A}'_G$ are naturally isomorphic. So, any representative of this isomorphism class could be called *the* algebra freely generated by G.

(3) To make the above definition useful we must prove that a pair $(\mathcal{A}_G, \gamma)$ exists for every set G. Consider the complex vector space spanned by the basis $\{e_S\}$, where S runs through all finite ordered sequences of the elements of G, say $S = (g_1, \dots g_k)$, with $k > 0$. Define multiplication on basis elements by concatenation, $e_S e_T = e_{ST}$, where $(g_1, \dots, g_k)(g'_1, \dots, g'_l) = (g_1, \dots, g_k, g'_1, \dots, g'_l)$ and extend it to the whole vector space by linearity. It is straight forward to see that we have defined an algebra that satisfies the property of being freely generated by G.

(4) In the case of unital $*$-algebras (assuming that the unit does not belong to G), we use the same construction, except that the basis of e_S is augmented by the element $\mathbb{1}$, with the extra multiplication rule $\mathbb{1} e_S = e_S \mathbb{1} = e_S$, and S now runs through finite ordered sequences of the elements of $G \sqcup G^*$, where G^* is in bijection with G, denoted by $*\colon G \to G^*$ and its inverse also by also $*\colon G^* \to G$. The $*$-involution is defined on the basis as $\mathbb{1}^* = \mathbb{1}$ and $e_S^* = e_{S^*}$, where $S^* = (*g_k, \dots, *g_1)$ for $S = (g_1, \dots, g_k)$, and extended to the whole linear space by complex anti-linearity. ■

Let us pass to the discussion of how to impose some algebraic relations on the (unital $*$-) algebra $\mathcal{A}_G$ freely generated by G. To be concrete, think of an algebra $\mathcal{A}_G$ freely generated by G and assume that we want to impose the relation l stating that $ba - ab = 0$ for a certain couple of elements $a, b \in \mathcal{A}_G$. We can define $\mathcal{A}_{G,l} \cong \mathcal{A}_G/\mathcal{I}_l$, where $\mathcal{I}_l \subset \mathcal{A}_G$ is the two-sided ideal (resp. $*$-ideal, in the case of $*$-algebras) generated by l, the set of finite linear combinations of products of $(ba - ab)$ and any other elements of $\mathcal{A}_G$. In case a set R of relations is imposed, one similarly takes the quotient with respect to the intersection $\mathcal{I}_R$ of the ideals ($*$-ideals if working with $*$-algebras) generated by each relation separately, $\mathcal{A}_{G,R} \cong \mathcal{A}_G/\mathcal{I}_R$.

The projection homomorphism $r : \mathcal{A}_G \to \mathcal{A}_G/\mathfrak{I}_R$ maps the generators of $\mathcal{A}_G$, the elements of G, to generators of $\mathcal{A}_{G,R} \cong \mathcal{A}_G/\mathfrak{I}_R$.

The construction of a unital algebra out of a freely generated algebra can be obtained as discussed, using the family R of relations $\mathbb{1}a - a\mathbb{1} = 0$ and $\mathbb{1}a = a$ for every $a \in \mathcal{A}_G$, where $\mathbb{1}$ is a preferred element of $\mathcal{A}_G$.

At this juncture we can state the crucial definition in terms of an universal property.

Definition 1.8. [Presentation by generators and relations] Let $\mathcal{A}_G$ be a (unital $*$-) algebra $\mathcal{A}_G$ free on G, R a set whose elements are called **relations** (again, not necessarily finite or even countable), and an injective map $\rho\colon R \to \mathcal{A}_G$.
A (unital $*$-) algebra $\mathcal{A}_{G,R}$ is said to be **presented by the generators** G **and relations** R if there exists a ($*$-) algebra homomorphism $r\colon \mathcal{A}_G \to \mathcal{A}_{G,R}$ that satisfies the following requirement. For any other ($*$-) algebra $\mathcal{B}$ and a map $\beta\colon G \to \mathcal{B}$ such that the composition of the relations with the canonical homomorphism $b\colon \mathcal{A}_G \to \mathcal{B}$ gives $b \circ \rho = 0$, there exists a *unique* ($*$-) homomorphism $b_R\colon \mathcal{A}_{G,R} \to \mathcal{B}$ such that $b = b_R \circ r$. ■

Remark 1.9.

(1) The (unital $*$-) algebra $\mathcal{A}_{G,R} = \mathcal{A}_G/\mathfrak{I}_R$ defined with respect to a ($*$-) ideal associated to relations, *satisfies* the previous abstract definition. We leave the proof to the reader.

(2) Analogously to the case of $\mathcal{A}_G$, Definition 1.8 easily implies that any two (unital $*$) algebras $\mathcal{A}_{G,R}$, $\mathcal{A}'_{G,R}$ presented by the generators G and relations R are *naturally isomorphic* as the reader can immediately prove by using the universal property of the definition. Intuitively, the algebra $\mathcal{A}_{G,R}$ is therefore *the* (unital $*$-) algebra that is generated by G satisfying *only* the relations $\rho(R) = 0$. ■

The presentation in terms of generators and relations works for a variety of algebraic structures, like groups, rings, module, algebras, etc. In fact, the universal property of objects defined in this way is most conveniently expressed using commutative diagrams in the corresponding category [54, §I.11]. The case of groups is extensively discussed in [54, §I.12]. Note that, though uniqueness of these objects is guaranteed by abstract categorical reasoning, their existence is not automatic and must be checked in each category of interest.

1.1.3 The GNS construction

When adopting the algebraic formulation, the notion of (quantum) state must be similarly generalized as follows.

Definition 1.10. [States] Given an unital $*$-algebra $\mathcal{A}$, an (algebraic) **state** ω over $\mathcal{A}$ is a $\mathbb{C}$-linear map $\omega : \mathcal{A} \to \mathbb{C}$ which is *positive* (i.e. $\omega(a^*a) \geq 0$ for all $a \in \mathcal{A}$) and *normalized* (i.e. $\omega(\mathbb{1}) = 1$). ■

The overall idea underlying this definition is that if, for a given observable $a = a^* \in \mathcal{A}$ we know all moments $\omega(a^n)$, and thus all expectation values of polynomials $\omega(p(a))$, we also know the probability distribution associated to every value of a when the state is ω. To give a precise meaning to this idea, we should represent observables a as self-adjoint operators $\hat{a}$ in some Hilbert space $\mathcal{H}$, where the values of a correspond to the point of spectrum $\sigma(\hat{a})$ and the mentioned probability distribution is that generated by a vector ψ state representing ω in $\mathcal{H}$, and the spectral measure of $\hat{a}$. We therefore expect that, in this picture, $\omega(a) = \langle\psi|\hat{a}\psi\rangle$ for some normalized vector $\psi \in \mathcal{H}$. This is, in fact, a consequence of the content of the celebrated GNS re-construction procedure for unital C^*-algebras [33, 75, 61]. We will discuss shortly the unital $*$-algebra version of that theorem. Note that the general problem of reconstructing even a unique classical state (a probability distribution on phase space) from the knowledge of all of its polynomial moments is much more difficult and is sometimes impossible (due to non-uniqueness). This kind of reconstruction goes under the name of the Hamburger moment problem [71, §X.6 Ex.4]. In this case, the successful reconstruction of a representation from a state succeeds because of the special hypotheses that go into the GNS theorem, where we know not only the expectation values of a (and the polynomial $*$-algebra generated by it) but also those of all elements of the algebra of observables. Nevertheless several open problems remain (see [19] for a general discussion on these still partially open issues.)

Notation 1.11. In the rest of the chapter $\mathscr{L}(V)$ will denote the linear space of linear operators $T : V \to V$ on the vector space V. If $\mathcal{H}$ is a complex Hilbert space, † henceforth denotes the Hermitian adjoint operation of densely defined linear operators in $\mathcal{H}$. ■

Definition 1.12. [$*$-Representations] Let $\mathcal{A}$ be a complex algebra and $\mathcal{D}$ a linear subspace of the Hilbert space $\mathcal{H}$.

(a) A map $\pi : \mathcal{A} \to \mathscr{L}(\mathcal{D})$ such that it is linear and product preserving is called **representation** of $\mathcal{A}$ on $\mathcal{H}$ with **domain** $\mathcal{D}$. If $\mathcal{A}$ is furthermore unital, a representation is also required to satisfy: $\pi(\mathbb{1}) = I$.

(b) If $\mathcal{A}$ is a $*$-algebra, a **$*$-representation** of $\mathcal{A}$ on $\mathcal{H}$ with *dense*[1] **domain** $\mathcal{D}$ is a representation which satisfies

$$\pi(a^*) = \pi(a)^\dagger\restriction_{\mathcal{D}} \quad \forall a \in \mathcal{A} .$$

(c) A vector $\psi \in \mathcal{D}$ is said to be **cyclic** for a representation $\pi : \mathcal{A} \to \mathscr{L}(\mathcal{D})$ if the subspace $\pi(\mathcal{A})\psi$ is dense in $\mathcal{H}$. ■

Remark 1.13. If $\mathcal{A}$ is a unital C^* algebra, a special case of $*$-representation is a $*$-homomorphism $\pi : \mathcal{A} \to \mathfrak{B}(\mathcal{H}) \subset \mathscr{L}(\mathcal{H})$. In this case $\mathcal{D} = \mathcal{H}$ and $\pi(a^*) = \pi(a)^\dagger$. Tought purely algebraically defined, these $*$-representations turn out to be automatically continuous, **norm decreasing**, with respect to the operator norm $|| \ ||$ in $\mathfrak{B}(\mathcal{H})$. Moreover such a π is isometric if and only if it is injective [33, 10]. ■

[1]So that the adjoint operator $\pi(a)^\dagger$ exists for every $a \in \mathcal{A}$.

Proposition 1.14. [On faithful representations] *If $\mathcal{A}$ is a complex algebra is simple, then every representation is either faithful – i.e., injective – or it is the zero representation.* ■

Proof. If $\pi : \mathcal{A} \to \mathscr{L}(\mathcal{D})$ is a $*$-representation, $Ker(\pi)$ is evidently a two-sided ideal. Since $\mathcal{A}$ is simple there are only two possibilities either $Ker(\pi) = \mathcal{D}$ so that π is the zero representation, or $Ker(\pi) = \{0\}$ and thus π is injective. □

We are now in a position to state and prove the fundamental theoretical theorem of the algebraic formulation of Quantum Theory. It regards the so called *GNS constuction* and relates the algebraic machinery to the Hilbert space formulation of Quantum Theory.

Theorem 1.15. [GNS construction] *If $\mathcal{A}$ is a complex unital $*$-algebra and $\omega : \mathcal{A} \to \mathbb{C}$ is a state, the following facts hold.*
(a) *There is a quadruple $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$, where:*

- *(i) $\mathcal{H}_\omega$ is a (complex) Hilbert space,*
- *(ii) $\mathcal{D}_\omega \subset \mathcal{H}_\omega$ is a dense subspace,*
- *(iii) $\pi_\omega : \mathcal{A} \to \mathscr{L}(\mathcal{D}_\omega)$ a $*$-representation of $\mathcal{A}$ on $\mathcal{H}_\omega$ with domain $\mathcal{D}_\omega$,*
- *(iv) $\Psi_\omega \in \mathcal{H}_\omega$ satisfies $\pi_\omega(\mathcal{A})\Psi_\omega = \mathcal{D}_\omega$, in particular Ψ_ω is cyclic for $\mathcal{H}_\omega$,*
- *(v) $\omega(a) = \langle \Psi_\omega | \pi_\omega(a)\Psi_\omega \rangle$ for every $a \in \mathcal{A}$, in particular $||\Psi_\omega|| = 1$.*

(b) *If $(\mathcal{H}'_\omega, \mathcal{D}'_\omega, \pi'_\omega, \Psi'_\omega)$ satisfies (i)-(v) in (a), then there is a unique $U : \mathcal{H}_\omega \to \mathcal{H}'_\omega$ linear surjective and isometric (sometimes called* unitary*) such that:*

- *(i) $U\Psi_\omega = \Psi'_\omega$,*
- *(ii) $U\mathcal{D}_\omega = \mathcal{D}'_\omega$,*
- *(iii) $U\pi_\omega(a)U^{-1} = \pi'_\omega(a)$ if $a \in \mathcal{A}$.*

(c) *If $\mathcal{A}$ is C^*, then π_ω uniquely continuously extends to a $*$-homomorphism $\pi_\omega : \mathcal{A} \to \mathfrak{B}(\mathcal{H}_\omega)$. (In particular $||\pi_\omega(a)|| \leq ||a||$ and $\pi_\omega(a^*) = \pi_\omega(a)^\dagger$ for every $a \in \mathcal{A}$.)*
(d) *If $\mathcal{A}$ is C^* and $(\mathcal{H}'_\omega, \pi'_\omega, \Psi'_\omega)$ is such that $\mathcal{H}'_\omega$ is a Hilbert space, $\pi'_\omega : \mathcal{A} \to \mathfrak{B}(\mathcal{H}'_\omega)$ is a $*$-homomorphism, $\Psi'_\omega \in \mathcal{H}'_\omega$ satisfies (v) in (a) and $\overline{\pi'_\omega(\mathcal{A})\Psi'_\omega} = \mathcal{H}'_\omega$, then there is a unique $U : \mathcal{H}_\omega \to \mathcal{H}'_\omega$ linear surjective and isometric such that (i) and (ii) in (b) are satisfied.*

Proof. (a)
(a1) Let us first construct $\mathcal{D}_\omega$ and $\mathcal{H}_\omega$.
Consider $\mathcal{A}$ as complex vector space and define $N_\omega := \{a \in \mathcal{A} \mid \omega(a^*a) = 0\}$. N_ω is a subspace. Indeed, it is closed under multiplication with complex numbers since ω is linear. It is also closed under sum of elements as easily follows from the Cauchy-Schwartz inequality

$$|\omega(a^*b)| \leq \sqrt{\omega(a^*a)}\sqrt{\omega(b^*b)}$$

which holds because the sesquilinear form $(a, b) \mapsto \omega(a^*b)$ is non-negative by definition of ω. We therefore have, if $a, b \in N_\omega$,

$$|\omega((a+b)^*(a+b))| = |0 + 0 + \omega(a^*b) + \omega(b^*a)| \leq 2\sqrt{\omega(a^*a)}\sqrt{\omega(b^*b)} = 0 .$$

Define

$$\mathcal{D}_\omega := \mathcal{A}/N_\omega$$

as a complex vector space and equip it with the Hermitian scalar product $\langle [a]|[b]\rangle := \omega(a^*b)$. This sesquilinear form is well defined because, if $a', b' \in N_\omega$,

$$\omega((a+a')^*(b+b')) = \omega(a^*b) + \omega(a'^*b) + \omega(a'^*b') + \omega(ab'^*)$$

the last three terms vanish again from Cauchy-Schwartz inequality. Finally $\langle [a]|[a]\rangle \geq 0$ by construction and $\langle [a]|[a]\rangle = 0$ trivially implies $a \in N_\omega$, i.e., $[a] = [0]$. In summary $\langle \cdot|\cdot\rangle$ is a Hermitian scalar product on $\mathcal{D}_\omega$. $\mathcal{H}_\omega$ is, by definition, the Hilbert completion of $\mathcal{D}_\omega$ with respect to the constructed Hermitian scalar product. With this definition $\mathcal{D}_\omega$ is automatically dense in $\mathcal{H}_\omega$.

(a2) Let us move on to define the representation π_ω.
First of all, observe that N_ω is also a left-ideal: if $a \in N_\omega$ then $ba \in N_\omega$ for $b \in \mathcal{A}$. Indeed

$$\omega((ba)^*ba) = \omega((b^*(ba))^*a) = 0 \quad \text{if } a \in N_\omega ,$$

where we used Cauchy-Schwartz inequality once more. At this juncture, define

$$\pi_\omega(a)[b] := [ab] \quad a, b \in \mathcal{A} .$$

This map is well-defined: if $[b] = [c]$ then $[ab] - [ac] = [a(b-c)] = 0$ because $b - c \in N_\omega$ and thus $a(b-c) \in N_\omega$ it being a left ideal. It is clear that $\pi_\omega : \mathcal{A} \to \mathscr{L}(\mathcal{D}_\omega)$ is linear, product preserving and unit preserving, and thus it is an algebra representation. We postpone the proof of the $*$-preservation property.

(a3) Let us define Ψ_ω also establishing (v), (iv) and the $*$-preservation property.
Defining

$$\Psi_\omega := [\mathbb{1}] ,$$

we have that (v) holds. Indeed $\langle \Psi_\omega|\pi_\omega(a)\Psi_\omega\rangle = \langle [\mathbb{1}]|[a]\rangle = \omega(\mathbb{1}^*a) = \omega(\mathbb{1}a) = \omega(a)$. Furthermore also (iv) is valid, since $\pi_\omega(a)\Psi_\omega = [a]$ for every $a \in \mathcal{A}$. Let us eventually prove that π_ω is a $*$-representation. We start by observing that $\pi_\omega(a)^\dagger$ exists because the domain $\mathcal{D}_\omega$ of $\pi_\omega(a)$ is a dense subspace of a Hilbert space [61, 62]. Next we consider the following immediate identity,

$$\langle \pi_\omega(a)^\dagger \pi_\omega(c)\Psi_\omega|\pi_\omega(b)\Psi_\omega\rangle = \langle \pi_\omega(c)\Psi_\omega|\pi_\omega(a)\pi_\omega(b)\Psi_\omega\rangle = \omega(c^*(a^*)^*b) = \omega((a^*c)^*b)$$

$$= \langle \pi_\omega(a^*c)\Psi_\omega|\pi_\omega(b)\Psi_\omega\rangle = \langle \pi_\omega(a^*)\pi_\omega(c)\Psi_\omega|\pi_\omega(b)\Psi_\omega\rangle .$$

In summary,

$$\langle (\pi_\omega(a)^\dagger - \pi_\omega(a^*))\pi_\omega(c)\Psi_\omega|\pi_\omega(b)\Psi_\omega\rangle = 0 .$$

Since b is arbitrary $\pi_\omega(b)\Psi_\omega$ ranges in $\mathcal{D}_\omega$ which is dense,

$$(\pi_\omega(a)^\dagger - \pi_\omega(a^*))\pi_\omega(c)\Psi_\omega = 0 \,.$$

Again, since c is arbitrary $\pi_\omega(c)\Psi_\omega$ ranges in $\mathcal{D}_\omega$, we have found that $\pi(a)^\dagger|_{\mathcal{D}_\omega} = \pi(a^*)$ concluding the proof of (a).
(b) Let us assume that U exists, then it must satisfy

$$U(\pi_\omega(a)\Psi_\omega) = \pi'_\omega(a)\Psi'_\omega \,, \quad \forall a \in \mathcal{A} \,. \tag{1.1}$$

Actually there is a unique map defined on $\mathcal{D}_\omega$ and taking values on $\mathcal{D}'_\omega$ which satisfies the requirement (1.1) thus making true (i) automatically. This is true *if* the definition above is well posed. In other words we have to prove that $\pi_\omega(a)\Psi_\omega = \pi_\omega(a')\Psi_\omega$ if and only if $\pi'_\omega(a)\Psi'_\omega = \pi'_\omega(a')\Psi'_\omega$. In fact, condition (v) valid for both representations yields

$$||\pi_\omega(a)\Psi_\omega - \pi_\omega(a')\Psi_\omega||^2 = \omega(a^*a) + \omega(a'^*a') - \omega(a^*a') - \omega(a'^*a) = ||\pi'_\omega(a)\Psi_\omega - \pi'_\omega(a')\Psi_\omega||^2 \,.$$

We conclude that there is a unique map $U : \mathcal{D}_\omega \to \mathcal{D}'_\omega$ which satisfies (1.1). By construction U is linear and the above reasoning, taking $a' = 0$, also proves that U, is isometric and thus injective. Its unique continuous (and linear) extension from the whole $\mathcal{H}_\omega$ to $\mathcal{H}'_\omega$, which exists because $\mathcal{D}_\omega$ is a dense subspace e of $\mathcal{D}_\omega$, is isometric as well [61, 62]. We indicate this continuous extension with the same symbol $U : \mathcal{H}_\omega \to \mathcal{H}'_\omega$. Surjectivity of the extension also holds since an analogous procedure permits to write down the inverse operator of the extended U. It is nothing but the unique continuous extension of the unique linear operator $U' : \mathcal{D}'_\omega \to \mathcal{D}_\omega$ such that

$$U'\pi'_\omega(a)\Psi'_\omega := \pi_\omega(a)\Psi_\omega \,, \quad \forall a \in \mathcal{A} \,.$$

By definition $U'U = I_{\mathcal{D}_\omega}$ and $UU' = I_{\mathcal{D}'_\omega}$ so that these compositions extend to the identities on $\mathcal{H}_\omega$ and $\mathcal{H}'_\omega$, respectively, when considering the unique continuous extensions of U and U'. Observe that $U'U = I_{\mathcal{D}_\omega}$ and $UU' = I_{\mathcal{D}'_\omega}$ imply (ii) trivially. Property (iii) can be established as follows. (1.1) and and standard algebra-representation properties entail

$$U\pi_\omega(a)\pi_\omega(b)\Psi_\omega = U\pi_\omega(ab)\Psi_\omega = \pi'_\omega(ab)\Psi'_\omega = \pi'_\omega(a)\pi'(b)\Psi'_\omega = \pi'_\omega(a)U\pi(b)\Psi_\omega \,.$$

Since $\pi(b)\Psi_\omega$ ranges on the whole $\mathcal{D}_\omega$, taking (ii) into account, we conclude that

$$U\pi_\omega(a) = \pi'_\omega(a)U$$

which is (iii).
(c) and (d). In this case $||\pi_\omega(a)|| \leq ||a||$ as proved in the proof of Theorem 8.7 n [62]. Therefore $\pi_\omega(a) : \mathcal{D}_\omega \to \mathcal{H}_\omega$ uniquely continuously extends to the whole $\mathcal{H}$, since $\mathcal{D}_\omega$ is dense. The extension, indicated with the same symbol, is the $*$-homomorphism of the thesis. The last statement in (c) is obvious from $\pi_\omega(a)^\dagger|_{\mathcal{D}_\omega} = \pi_\omega(a^*)$ since $\pi_\omega(a) \in \mathfrak{B}(\mathcal{H})$. The proof of (d) is the one of (b) with trivial re-adaptations. $\square$

The left ideal $N_\omega := \{a \in \mathcal{A} \,|\, \omega(a^*a) = 0\}$ used in the proof is called **Gelfand ideal** of ω. It plays several roles in algebraic quantum (field) theory and pure mathematics.

Corollary 1.16. *Referring to Theorem 1.15 π_ω is faithful if the Gelfand ideal of ω is trivial.*

Proof. $ker(\pi_\omega) = \{a \in \mathcal{A} \mid [ab] = 0\,, \quad \forall b \in \mathcal{A}\}$. Therefore, taking b as the unit of the algebra we have $ker(\pi_\omega) \subset N_\omega$. The thesis follows. $\square$

Remark 1.17.

(1) The quadruple $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ is often called **GNS triple** (!) the name is due to the fact that for C^*-algebras the representation is defined on the whole $\mathcal{H}_\omega$ as stated in (c) [33, 10, 61].

(2) There are unitarily non-equivalent GNS representations of the same unital $*$-algebra $\mathcal{A}$ associated with states ω, ω'. In other words there is no surjective isometric operator $U : \mathcal{H}_\omega \to \mathcal{H}_{\omega'}$ such that $U\pi_\omega(a) = \pi_{\omega'}(a)U$ for all $a \in \mathcal{A}$. (Notice that, in the notion of *unitary equivalence* it is not required that $U\Psi_\omega = \Psi_{\omega'}$). Appearance of unitarily inequivalent representations is natural when $\mathcal{A}$ has a non-trivial *center*, $\mathcal{Z}_\mathcal{A}$, i.e., it contains something more than the elements $c\mathbb{1}$ for $c \in \mathbb{C}$. Pure states ω, ω' such that $\omega(z) \neq \omega'(z)$ for some $z \in \mathcal{Z}_\mathcal{A}$ give rise to unitarily inequivalent GNS representations. This easily follows from the fact that $\pi_\omega(z)$ and $\pi_{\omega'}(z)$, by irreducibility of the representations, must be operators of the form $c_z I$ and $c'_z I$ for complex numbers c_z, c'_z in the respective Hilbert spaces $\mathcal{H}_\omega$ and $\mathcal{H}_{\omega'}$. It should be noted that such representations remain inequivalent even if the unitarity of U is relaxed. However, it can happen that some representations are unitarily inequivalent even when the algebra has a trivial center. See Section 1.5.5 for a relevant example

(3) Since $\mathcal{D}_\omega$ is dense, $\pi_\omega(a)^\dagger$ is always well defined and, in turn, densely defined for (iii) in (a). Hence, $\pi_\omega(a)$ is always closable. Therefore, if $a = a^*$, $\pi(a)$ is at least symmetric. Under suitable conditions on $\mathcal{A}$, it is also self-adjoint [75]. When $\pi_\omega(a)$ is selfadjoint, the probability distribution of the observable a in the state ω mentioned in the comment after Def. 1.10 is $\mathcal{B}(\mathbb{R}) \ni E \mapsto \langle \Psi_\omega | P^{(\pi_\omega(a))}_E \Psi_\omega \rangle$, where $\mathcal{B}(\mathbb{R})$ is the class of Borel sets on $\mathbb{R}$ and $P^{(\pi_\omega(a))}$ the projection-valued measure of $\pi_\omega(a)$. Actually the known conditions are very strong and the study of essential selfadjointness of $\pi_\omega(a)$ for $a = a^*$ is quite difficult and the issue is essentially open [19].

(4) The positivity requirement on states is physically meaningful when every self-adjoint element of the $*$-algebra is a physical observable. It is also a crucial ingredient in the GNS reconstruction theorem. However, in the treatment of gauge theories in the Gupta-Bleuler or BRST formalisms, in order to keep spacetime covariance, one must enlarge the $*$-algebra to include unobservable or *ghost* fields. Physically meaningful states are then allowed to fail the positivity requirement on $*$-algebra elements generated by ghost fields. The GNS reconstruction theorem is then not applicable and, in any case, the $*$-algebra is expected to be represented on an indefinite scalar product space (a *Krein space*) rather than a Hilbert space. Fortunately, several extensions of the GNS construction have been made, with the positivity requirement replaced by a different one that, instead, guarantees the reconstructed $*$-representation to be on an indefinite scalar product space. Such generalizations and their technical details are discussed in [38]. ■

1.1.4 More on states of $*$-algebras and their GNS representations

When $\mathcal{A}$ is a unital C^*-algebra, so that every GNS representation is made of bounded operators in $\mathcal{H}_\omega$ according to (c) Theorem 1.15, the set of (algebraic) states on $\mathcal{A}$ is hugely larger that the (Hilbert space) states of the form

$$\mathcal{A} \ni a \mapsto \omega_\rho(a) := tr(\rho \pi_\omega(a)) \tag{1.2}$$

for a fixed (algebraic) state ω and where $\rho \in \mathfrak{B}(\mathcal{H}_\omega)$ is a positive trace class operator with unit trace [62]. These special states of the form (1.2) associated with an algebraic state ω form the **folium** of ω and are called **normal states** of ω or **normal states** in $\mathcal{H}_\omega$. We stress again that these states are very few in comparison to the full set of algebraic states: the normal states of $\omega' \neq \omega$, in general are *not* normal states of ω
If $\mathcal{A}$ is not C^* but is a simple $*$-algebra, so that the operators $\pi_\omega(a)$ are not bounded nor everywhere defined in general, the trace $tr(\rho\pi_\omega(a))$ is not defined in general, because $\pi_\omega(a)$ is not bounded and $\rho\pi_\omega(a)$ may not be well defined nor trace class in general. Nevertheless, even if $\mathcal{A}$ is just a unital $*$-algebra, a unit vector $\Phi \in \mathcal{D}_\omega$ defines however a state by means of

$$\mathcal{A} \ni a \mapsto \omega_\Phi(a) := \langle \Phi | \pi_\omega(a) \Phi \rangle \ ,$$

recovering the standard formulation of elementary quantum mechanics.

In the formulation of Quantum Theory [62] on a fixed Hilbert space $\mathcal{H}$, there exists a distinction between *pure* and *mixed* states. In the absence of superselection rules and gauge group, so that the (von Neumann) algebra of observables is the whole $\mathfrak{B}(\mathcal{H})$, the pure states are represented by equivalence classes of vectors: unit vectors up to phases $[\psi]$, and mixed states are represented by positive, trace-class, unit-trace operators ρ. Notice that the latter family includes the former. In fact, an equivalence class $[\psi]$ of unit vectors carries the same information as the orthogonal projector $\langle \psi | \cdot \rangle \psi$. This is in fact a positive, trace-class, unit-trace operator.

According to the GNS construction, it seems that all types of states are instead representable as unit vectors, so that they are all pure states! This assertion is false and relies upon a prejudice. Pure states are unit vectors, in the Hilbert space formulation, *when the algebra of observables is the full* $\mathfrak{B}(\mathcal{H})$. The true definition, even in Hilbert space [62], is different. The set of positive, trace-class, unit-trace operators on $\mathcal{H}$ is a convex body and the pure states are the *extremal* elements of this body: the ones which cannot be decomposed into non-trivial convex combinations. If the algebra of observables is $\mathfrak{B}(\mathcal{H})$, these extremal operators are in fact exactly the ones of the form $\langle \psi | \cdot \rangle \psi$. This definition of pure state is valid in general. Pure states are the extremal elements of the convex set of states. Their relevance is due to the fact that the remaining states are convex combinations of them, at most in suitable topologies. When the observables are not all (selfadjoint) elements of $\mathfrak{B}(\mathcal{H})$, it is possible that couples of different positive, trace-class, unit-trace operators cannot be distinguished by the observables: observables do not separate these operators when considering expectation values. In the presence of superselection rules, which decrease the number of observables, states represented by unit vectors up to phases are indistinguishable from states represented by proper trace class-operators [62]: they are actually the same states! Nevertheless, taking the quotient with respect to this redundancy, the set of states remains a convex body and the definition of pure states in terms of extremal elements works well.

This perspective applies to the case of algebraic states on a unital $*$-algebra (also C^*). The set of states over a unital *-algebra $\mathcal{A}$ is a **convex body** in the $\mathbb{C}$-vector space of functionals $\mathcal{A} \to \mathbb{C}$. In other words *convex combinations* of states are states: $\omega = p\omega_1 + (1-p)\omega_2$ with $p \in [0,1]$ is a state if ω_1, ω_2 are.

Definition 1.18. A state ω on a unital $*$-algebra is **pure** if it is extremal: if $\omega = p\omega_1 + (1-p)\omega_2$ with $p \in (0,1)$ then $\omega_1 = \omega_2 = \omega$. Non pure states are said **mixed**. ■

We move on to briefly discuss the notion of pure state for unital $*$-algebras (see [61, 62] for the case of C^*-algebras). When dealing with representations of $*$-algebras, two notions are important for characterizing pure states.

Definition 1.19. The **weak commutant** π'_w of a $*$-representation π of a unital $*$-algebra $\mathcal{A}$ on $\mathcal{H}$ with domain $\mathcal{D}$, is defined as

$$\pi'_w := \{A \in \mathfrak{B}(\mathcal{H}) \mid \langle \psi | A\pi(a)\phi \rangle = \langle \pi(a)^\dagger \restriction_{\mathcal{D}} \psi | A\phi \rangle \quad \forall a \in \mathcal{A}\,, \forall \psi, \phi \in \mathcal{D}\}\,, \tag{1.3}$$

The **strong commutant** π'_s is defined as

$$\pi'_s := \{A \in \mathfrak{B}(\mathcal{H}) \mid A\pi(a)\phi = \pi(a)A\phi \quad \forall a \in \mathcal{A}\,, \forall \phi \in \mathcal{D}\}\,, \tag{1.4}$$

where it is implicitly required that $A(\mathcal{D}) \subset \mathcal{D}$. ■

Remark 1.20. Using the definition of adjoint and $\pi(a)^\dagger \restriction_{\mathcal{D}} = \pi(a^*)$, one immediately sees that π'_w can equivalently be defined as

$$\pi'_w = \{A \in \mathfrak{B}(\mathcal{H}) \mid A\pi(a) \subset \pi(a^*)^\dagger A\,, \quad \forall a \in \mathcal{A}\}\,.$$

Similarly

$$\pi'_s := \{A \in \mathfrak{B}(\mathcal{H}) \mid A\pi(a) \subset \pi(a)A \quad \forall a \in \mathcal{A}\}\,.$$

Evidently

$$\pi'_s \subset \pi'_w\,, \tag{1.5}$$

but the converse inclusion generally fails. However, if $\mathcal{A}$ is a unital C^*-algebra and $\pi : \mathcal{A} \to \mathfrak{B}(\mathcal{H})$ is a $*$-homomorphism, then the weak commutant and the strong commutant of π evidently coincide to the standard **commutant**

$$\pi' := \{A \in \mathfrak{B}(\mathcal{H}) \mid A\pi(a) = \pi(a)A \quad \forall a \in \mathcal{A}\}\,,$$

and is a *von Neumann algebra*. ■

Definition 1.21. We say that a $*$-representation π of a unital $*$-algebra $\mathcal{A}$ on $\mathcal{H}$ is

(a) **weakly irreducible** if its weak commutant is trivial, that is, it coincides with the set of operators $cI : \mathcal{H} \to \mathcal{H}$ for $c \in \mathbb{C}$.

(b) **irreducible** if its strong commutant does not contain nontrivial orthogonal projectors. In other words, the only orthogonal projectors are 0 and I.

Representations which are not (weakly) irreducible are said (weakly) **reducible**. ■

Remark 1.22. Saying that the strong commutant π'_s does not contain a nontrivial orthogonal projectors, without further conditions on the representation, is not equivalent to requiring that $\pi'_s = \mathbb{C}I$, though this latter requirement implies the former evidently. If $\mathcal{A}$ is also C^* the two conditions coincide as it is easy to prove. ■

Irreducibility can be equivalently characterised in terms of invariant closed subspaces[2].

Proposition 1.23. *Let π be a $*$-representation of a unital $*$-algebra $\mathcal{A}$ on $\mathcal{H}$ with domain $\mathcal{D}$. The following holds.*
(a) *π is reducible if and only if there exist a closed subspace $\mathcal{H}_0 \subset \mathcal{H}$ which is non-trivial – i.e., $\mathcal{H}_0 \neq \{0\}$, $\mathcal{H}_0 \neq \mathcal{H}$ – and* **reduces** *$\pi(a)$ for all $a \in \mathcal{A}$:*

(i) $\pi(a)(\mathcal{H}_0 \cap \mathcal{D}) \subset \mathcal{H}_0$ *and* $\pi(a)(\mathcal{H}_0^\perp \cap \mathcal{D}) \subset \mathcal{H}_0^\perp$,

(ii) $\mathcal{D} = (\mathcal{D} \cap \mathcal{H}_0) \oplus (\mathcal{D} \cap \mathcal{H}_0^\perp)$,

(b) *If $\mathcal{A}$ is C^*, a $*$-homomorphism $\pi : \mathcal{A} \to \mathfrak{B}(\mathcal{H})$ is reducible if and only if there exist a closed subspace $\mathcal{H}_0 \subset \mathcal{H}$ which is non-trivial and is invariant under π, i.e., $\pi(\mathcal{H}_0) \subset \mathcal{H}_0$.*

Proof. (a) First of all observe that, in (i), $\mathcal{H}_0$ can equivalently be replaced for $\mathcal{H}_0 \cap \mathcal{D}$ and $\mathcal{H}_0^\perp$ for $\mathcal{H}_0^\perp \cap \mathcal{D}$ since $Ran\pi(a) = \mathcal{D}$. Let us assume that $\mathcal{H}_0$ exists satisfying (i)-(ii) and we prove that π is reducible. Let P be the orthogonal projector onto $\mathcal{H}_0$ and $P^\perp$ be the one onto $\mathcal{H}_0^\perp$. In view of the uniqueness of the direct orthogonal decomposition with respect to $\mathcal{H}_0$ and $\mathcal{H}_0^\perp$, (ii) yields $P(\mathcal{D}) \subset \mathcal{H}_0 \cap \mathcal{D}$ and $P^\perp(\mathcal{D}) \subset \mathcal{H}_0^\perp \cap \mathcal{D}$. If $\psi \in \mathcal{D}$, using (i) we therefore have $P\pi(a)P\psi = \pi(a)P\psi$. On the other hand, $\psi = P\psi + P^\perp\psi$ and $P\pi(a)P^\perp\psi = 0$ since $\pi(a)P^\perp\psi \in \mathcal{H}_0^\perp$. In summary $P\pi(a)\psi = \pi(a)\psi$. Hence $P \in \pi'_s$ proving that π is reducible. To conclude, we assume that π is reducible and we prove that (i) and (ii) are satisfied for a non trivial $\mathcal{H}_0$. According to the hypothesis $\mathcal{H}_0$ denotes the non trivial subspace projection of $P \in \pi'_s$ different from 0 and I. Since $\pi(a)P\psi = P\psi(a)\psi$ for every $\psi \in \mathcal{D}$ and $a \in \mathcal{A}$, using also the fact that $\pi(\mathcal{D}) = \mathcal{D}$, we immediately have that the first inclusion in (i) is true. Concerning the second one observe that $P^\perp = I - P$ so that it also belongs to π'_s and the same argument

[2]In [75] this characterization is adopted as the definition.

can be used. Regarding (ii), the requirement $P\pi(a)\psi = \pi(a)P\psi$ valid for every $\psi \in \mathcal{D}$ includes the condition that $P(\mathcal{D}) \subset \mathcal{D}$ since the latter is the domain of $\pi(a)$. The same procedure also yields $P^{\perp}(\mathcal{D}) \subset \mathcal{D}$. At this point (ii) is obvious.
(b) The proof is trivial using the fact that we can replace $\mathcal{D}$ for $\mathcal{H}$ in all the discussion above. □

We come to the fundamental result.

Proposition 1.24. [Pure states and irreducible representations] *Suppose that $\mathcal{A}$ is a unital $*$-algebra and ω a state on it. ω is pure if and only if π_ω is weakly irreducible. In this case π_ω is also irreducible due to (1.5).* ■

Proof. See Corollary 5.4 in [75] □

If $\mathcal{A}$ is a unital C^*-algebra the same statement holds but "weakly" is omitted together with the last corollary. A direct proof of the statement below can be found in [61, 62].

Corollary 1.25. *Suppose that $\mathcal{A}$ is a unital C^*-algebra. A state ω on it is pure if and only if $\pi_\omega : \mathcal{A} \to \mathfrak{B}(\mathcal{H}_\omega)$ is irreducible.*

Proof. In case of unital C^*-algebras weak and strong commutant of π_ω coincide, this immediately implies the thesis. □

To conclude we come back to the initial issue. Even if, according to the GNS construction, ω is represented by a unit vector Ψ_ω in $\mathcal{H}_\omega$, it does not mean that ω is pure! In standard quantum mechanics it happens because $\mathcal{A}$ is implicitly assumed to coincide to the whole C^*-algebra $\mathfrak{B}(\mathcal{H})$ of everywhere-defined bounded operators over $\mathcal{H}$ and π_ω is the identity map $\pi_\omega : \mathfrak{B}(\mathcal{H}) \ni A \to A \in \mathfrak{B}(\mathcal{H})$ when ω corresponds to a unit vector (up to phases) of $\mathcal{H}$. We have a final corollary.

Corollary 1.26. *Suppose that $\mathcal{A}$ is a unital C^*-algebra and ω a pure state on it. Consider a unit vector $\psi \in \mathcal{H}$, and define the algebraic state $\omega_\psi(a) := \langle \psi | \pi_\omega(a)\psi \rangle$ for every $a \in \mathcal{A}$. The following holds.*

(a) A GNS triple of ω_ψ is $(\mathcal{H}_\psi, \pi_\psi, \Psi_\psi) := (\mathcal{H}_\omega, \pi_\omega, \psi)$.

(b) ω_ψ is pure as well. ■

Proof. Define $\mathcal{H}_0 := \overline{\pi_\omega(\mathcal{A})\psi}$. It is obvious that this closed vector space must coincide with the whole space $\mathcal{H}$. Otherwise π_ω would be reducible, since $\mathcal{H}_0$ is invariant under π_ω that, in the considered case, is continuous and defined on the whole $\mathcal{H}$. Finally $(\mathcal{H}_\omega, \pi_\omega, \psi)$ respects the definition of GNS triple. The state ω_ψ is pure just because $\pi_\psi = \pi_\omega$ is irreducible and Corollary 1.25 holds. □

1.1.5 Symmetries from the algebraic perspective

Another relevant result arising from the GNS theorem concerns *symmetries*. In the algebraic approach quantum symmetries are represented by $*$-algebra automorphisms or anti-linear automorphisms. When transformations of this tipe exist which furthermore leaves invariant some preferred state, then a noticeable result arises.

Proposition 1.27. [Automorphisms induced by invariant states] *Let $\mathcal{A}$ be an unital $*$-algebra, ω a state on it and consider its GNS representation. The following facts hold.*
(a) *If $\beta : \mathcal{A} \to \mathcal{A}$ is a unital $*$-algebra automorphism (resp. anti-linear automorphism) which leaves fixed ω, i.e., $\omega \circ \beta = \omega$, then there exist a unique surjective isometric linear (resp. anti-linear) operator $U^{(\beta)} : \mathcal{H}_\omega \to \mathcal{H}_\omega$ such that:*

(i) $U^{(\beta)}\Psi_\omega = \Psi_\omega$ *and* $U^{(\beta)}(\mathcal{D}_\omega) = \mathcal{D}_\omega$,

(ii) $U^{(\beta)}\pi_\omega(a)U^{(\beta)-1} = \pi_\omega(\beta(a))$ *if* $a \in \mathcal{A}$.

(b) *If, varying $t \in \mathbb{R}$, $\beta_t : \mathcal{A} \to \mathcal{A}$ defines a one-parameter group of unital $*$-algebra automorphisms*[3] *which leaves fixed ω, the corresponding unitary operators $U_t^{(\beta)}$ as in (a) define a one-parameter group of unitary operators in $\mathcal{H}_\omega$.*
(c) $\{U_t^{(\beta)}\}_{t\in\mathbb{R}}$ *as in (b) is strongly continuous (thus it admits a self-adjoint generator by Stone's theorem [61, 62]) if and only if*

$$\lim_{t\to 0} \omega(a^*\beta_t(a)) = \omega(a^*a) \quad \textit{for every } a \in \mathcal{A}.$$

Proof. (a) Let us start by supposing that β is a $*$-automorphism. If an operator satisfying (i) and (ii) exists it also satisfies $U^{(\beta)}\pi_\omega(a)\Psi_\omega = \pi_\omega(\beta(a))\Psi_\omega$. Since $\pi_\omega(\mathcal{A})\Psi_\omega = \mathcal{D}_\omega$ is this identity determines $U^{(\beta)}$ on $\mathcal{D}_\omega$. Therefore we are lead to try to define

$$U^{(\beta)}(\pi_\omega(a)\Psi_\omega) := \pi_\omega(\beta(a))\Psi_\omega \,.$$

Let us prove that this definition is well-posed: if $\pi_\omega(b)\Psi_\omega = \pi_\omega(b')\Psi_\omega$ then $\pi_\omega(\beta(b))\Psi_\omega = \pi_\omega(\beta(b'))\Psi_\omega$. From (v) in (a) of Theorem 1.15, β invariance of ω and the fact that β is a $*$-automorphism, it immediately arises that

$$||\pi_\omega(\beta(a))\Psi_\omega||^2 = \langle\Psi_\omega|\pi_\omega(\beta(a))^\dagger\pi_\omega(\beta(a))\Psi_\omega\rangle = \langle\Psi_\omega|\pi_\omega(\beta(a^*a))\Psi_\omega\rangle$$

$$= \omega(\beta(a^*a)) = \omega(a^*a) = ||\pi_\omega(a)\Psi_\omega||^2 \,.$$

In summary

$$||\pi_\omega(a)\Psi_\omega||^2 = ||\pi_\omega(\beta(a))\Psi_\omega||^2 \,. \tag{1.6}$$

[3] There do not exist one-parameter group of unital $*$-algebra *anti-linear* automorphisms, this is because $\beta_t = \beta_{t/2} \circ \beta_{t/2}$ is linear both for $\beta_{t/2}$ linear or anti-linear.

Exactly as in the proof of (b) of the GNS theorem (1.15), when using $a = b - b'$, we have

$$||\pi_\omega(b)\Psi_\omega - \pi_\omega(b')\Psi_\omega||^2 = ||\pi_\omega(\beta(b))\Psi_\omega - \pi_\omega(\beta(b'))\Psi_\omega||^2$$

and this proves that $U^{(\beta)}$ is well defined because if $\pi_\omega(b)\Psi_\omega = \pi_\omega(b')\Psi_\omega$ then $U^{(\beta)}(\pi_\omega(b)\Psi_\omega) = U^{(\beta)}(\pi_\omega(b')\Psi_\omega)$. On the other hand (1.6) proves that $U^{(\beta)}$ is isometric on $\mathcal{D}_\omega$. By construction, the so far defined map $U : \mathcal{D}_\omega \to \mathcal{D}_\omega$ is also linear as the reader immediately proves. If we analogously define the other isometric operator $V^{(\beta)}\pi_\omega(a)\Psi_\omega := \pi_\omega\left(\beta^{-1}(a)\right)\Psi_\omega$ on $\mathcal{D}_\omega$, we see that $U^{(\beta)}Vx = VU^{(\beta)}x = x$ for every $x \in \mathcal{D}_\omega$. Since $\mathcal{D}_\omega$ is dense in $\mathcal{H}_\omega$, these identities extend to analogous identities for the unique bounded extensions of $U^{(\beta)}$ and V valid over the whole Hilbert space. In particular the former operator extends into an isometric surjective operator (thus unitary) $U^{(\beta)}$ which, by construction, satisfies (i) and (ii). Notice that V, defined on $\mathcal{D}_\omega$, is the inverse of $U^{(\beta)}$ so that, in particular $U^{(\beta)}(\mathcal{D}_\omega) = U^{(\beta)}(\mathcal{D}_\omega) = \mathcal{D}_\omega$. The followed procedure also proves that $U^{(\beta)}$ is uniquely determined by (i) and (ii). The anti-linear case is proved analogously. Anti-linearity of β implies that, in $U^{(\beta)}\pi_\omega(a)\Psi_\omega := \pi_\omega\left(\beta(a)\right)\Psi_\omega$, $U^{(\beta)}$ must be anti-linear.

(b) Let β_t, $t \in \mathbb{R}$, denote the generic element of the one-parameter group of $*$-automorphisms β. With the given defintion of $U^{(\beta_t)}$:

$$U^{(\beta_s)}U^{(\beta_t)}\pi_\omega(a)\Psi_\omega = U^{(\beta_s)}\pi_\omega\left(\beta_t(a)\right)\Psi_\omega = \pi_\omega\left(\beta_s(\beta_t(a))\right)\Psi_\omega = \pi_\omega\left(\beta_{s+t}(a)\right)\Psi_\omega = U^{(\beta_{s+t})}\pi_\omega(a)\Psi_\omega .$$

Since $\pi_\omega(\mathcal{A})\Psi_\omega$ is dense, we have found that $U^{(\beta_s)}U^{(\beta_t)} = U^{(\beta_{s+t})}$. The same argument proves that $U^{(\beta_0)} = I$. $U_t^{(\beta)} := U^{(\beta_t)}$ for $t \in \mathbb{R}$ is the wanted one-parameter group of unitary operators.

(c) We observe that, if $x = \pi_\omega(a)\Psi_\omega$ one has for $t \to 0$ by the GNS theorem,

$$\langle x|U_t^{(\beta)}x\rangle = \omega(a^*\beta_t(a)) \quad \text{in particular} \quad \omega(a^*a) = \langle x|x\rangle \,.$$

This proves that $\omega(a^*\beta_t(a)) \to \omega(a^*a)$ for every $a \in \mathcal{A}$ is true if strong cotinuity holds for $U^{(\beta)}$, since $\langle x|U_t^{(\beta)}x\rangle \to \langle x|x\rangle$ for $t \to 0$.
Let us prove the converse implication: $\omega(a^*\beta_t(a)) \to \omega(a^*a)$ for every $a \in \mathcal{A}$ implies that the one-parameter group of unitary operators $\{U_t^{(\beta)}\}_{t\in\mathbb{R}}$ is strongly continuous. First of all, it is clear that $\{U_t^{(\beta)}\}_{t\in\mathbb{R}}$ is strongly continuous (at every t) if it is strongly continuous for $t = 0$ since

$$||U_{t+h}^{(\beta)}x - U_t^{(\beta)}x|| = ||U_t^{(\beta)}(U_h^{(\beta)}x - x)|| = ||U_h^{(\beta)}x - x|| \to 0 \,.$$

We now observe tha continuity at $t = 0$ can be imposed with an apparently even weaker condition: if $\langle x|U_t^{(\beta)}x\rangle \to \langle x|x\rangle$ for $t \to 0$, we also have

$$||U_t^{(\beta)}x - x||^2 = ||U_t^{(\beta)}x||^2 + ||x||^2 - 2Re\langle x|U_t^{(\beta)}x\rangle = 2||x||^2 - 2Re\langle x|U_t^{(\beta)}x\rangle \to 0 \,.$$

In summary, if $\omega(a^*\beta_t(a)) \to \omega(a^*a)$ for every $a \in \mathcal{A}$ this condition, and thus $U_t^{(\beta)}x \to x$, is true for the special case $x = \pi_\omega(a)\Psi_\omega$. However, since the span of thes vectors $x = \pi_\omega(a)\Psi_\omega$ is dense in $\mathcal{H}_\omega$, the argument extends to every $\phi \in \mathcal{H}_\omega$ as follows.

$$\left|\left|U_t^{(\beta)}\phi - \phi\right|\right| \leq \left|\left|U_t^{(\beta)}\phi - U_t^{(\beta)}x\right|\right| + \left|\left|U_t^{(\beta)}x - x\right|\right| + ||x - \phi|| = \left|\left|U_t^{(\beta)}x - x\right|\right| + 2\,||x - \phi||\ .$$

Using the density of $\mathcal{D}_\omega$, we can fix $x \in \mathcal{D}_\omega$ such that $||x - \phi|| < \epsilon/2$. Now

$$\left|\left|U_t^{(\beta)}x - x\right|\right| \leq \sqrt{2||x||^2 - 2Re\langle x|U_t x\rangle} \leq \epsilon/2$$

for $|t| < \delta$ and $\delta > 0$ small enough. Hence $||U_t^{(\beta)}\phi - \phi|| < \epsilon$ if $|t| < \delta$, proving the claim. □

Remark 1.28.

(1) Evidently, the statements (b) and (c) can immediately be generalized to the case of a representation of a generic *group* or, respectively, *connected topological group*, G. Assume that G is represented in terms of automorphisms of unital $*$-algebras $\beta_g : \mathcal{A} \to \mathcal{A}$ for $g \in G$. With the same proof of (c), it turns out that, if ω is invariant under this representation of G, the associated representation in the GNS Hilbert space of ω, $\{U_g^{(\beta)}\}_{g\in G}$ is strongly continuous if and only if

$$\lim_{g\to e} \omega(a^*\beta_g(a)) = \omega(a^*a) \quad \text{for every } a \in \mathcal{A},$$

where $e \in G$ is the unit element.

(2) The algebraic approach permits us to deal with a physically important situation where a symmetry exists only at the level of the algebra of observables, but it 'breaks down' at the level of states. This situation is usually called *spontaneous breaking of symmetry*. There are several interpretations of this idea (see [53] for a broad, up-to-date review on the subject and [33, 76] for more specific results in relativistic local QFT). Generally speaking, the **spontaneous breaking of symmetry** occurs when the $*$-algebra of observables $\mathcal{A}$ admits a symmetry α described by an (anti-)automorphism, but there is no state invariant under α in a class of states of physical relevance (depending on the physical context one is interested in), for instance in the class of *pure states*, in the class of *extremal ground states*, or also in the class of *extremal KMS states*. In general,

Definition 1.29. The symmetry $\alpha : \mathcal{A} \to \mathcal{A}$ is said to be **spontaneously broken** by a given algebraic state $\omega : \mathcal{A} \to \mathbb{C}$ if ω is *not* invariant under α. ■

In this case α could still be implemented in the GNS representation of ω: (ii) Proposition1.27 might hold for some (anti-)unitary operator U on $\mathcal{H}_\omega$, although U does not satisfy (i). This situation calls for a stronger version of symmetry breakdown.

Definition 1.30. The symmetry $\alpha : \mathcal{A} \to \mathcal{A}$ is **spontaneously broken** by an algebraic state $\omega : \mathcal{A} \to \mathbb{C}$ in **strong sense**, if α cannot be implemented in the GNS representation of ω: no (anti-)unitary operator U on $\mathcal{H}_\omega$ satisfies (ii) Proposition 1.27 (hence in particular ω cannot be invariant under α, by Proposition 1.27). ■

1.2 The $*$-algebra of a Klein-Gordon quantum field

This section deals with the case of a real scalar field, we will denote by ϕ, on a given (time oriented by definition) *globally hyperbolic spacetime* $\boldsymbol{M} = (M, g, \mathfrak{o})$ of dimension $n \geq 2$, where g is the metric with signature $(p, n-p)$, $\mathfrak{o}$ the *time orientation.* The special case of Minkowski spacetime will be denoted by $\mathbb{M}$ and its metric by η. Regarding geometrical notions, we adopt throughout the definitions of the appendix (Chapter 3) which includes a recap of the most relevant notions of differential geometry and theory of spacetimes we shall use henceforth.

In the rest of this paper $C_c^\infty(M)$ denotes the real vector space of compactly-supported and *real*-valued smooth functions on the manifold M and, if $\boldsymbol{M} := (M, g)$ is Lorentzian manifold.

$$\Box_{\boldsymbol{M}} \psi := \mathrm{div}_{\boldsymbol{M}} d\psi^\sharp = g^{ab} \nabla_a \nabla_b \psi \tag{1.7}$$

is the **d'Alembert operator** on $\boldsymbol{M}$. We address the reader to Sections 3.3.4 and 3.3.6 for the basic theory of the Klein-Gordon equation in curved spacetime.

Remark 1.31. Contrarily to Chapter 3, in the following we adopt *Einstein's convention of sum over repeated indices.* ■

1.2.1 The algebra of observables of a real scalar Klein-Gordon field

In order to deal with QFT in curved spacetime, a convenient framework is the algebraic one. This is due to various reasons. Especially because, in the absence of Poincaré symmetry, there is no preferred Hilbert space representation of the field operators, but several unitarily inequivalent representations naturally show up. Furthermore, the standard definition of the field operators based on the decomposition of field solutions in positive and negative frequency part is not allowed here, because there is no preferred notion of (Killing) time.

As is well known a quantum field is a *locally covariant notion*, functorially defined in *all* globally hyperbolic spacetimes simultaneously [14]. Nevertheless, since this chapter is devoted to discussing algebraic *states* of a QFT in a given manifold we can deal with a fixed spacetime. All our discussion will be confined to a real scalar (Bosonic) field. The results we shall present can be extended to charged and higher spin fields.

Moreover we shall not construct the $*$-algebras as *Borchers-Uhlmann-like* [34, 5] algebras nor use the *deformation approach* [20] (see also [34]) to define the algebra structure, in order to simplify the technical structure and focus on the properties of the states.

The elementary algebraic object, i.e., a **scalar quantum field** ϕ over the globally hyperbolic spacetime $\boldsymbol{M} := (M, g, \mathfrak{o})$ is captured by a unital $*$-algebra $\mathcal{A}(\boldsymbol{M})$ called the CCR algebra of the quantum field ϕ. According to the discussion in Section 1.1.2, the following abstract definition is sufficient to uniquely define $\mathcal{A}(\boldsymbol{M})$ up to isomorphism. An alternative construction using tensor products of spaces $C_c^\infty(M)$ is presented in, e.g. [34]. That construction yields a concrete representative of the isomorphism class of $\mathcal{A}(\boldsymbol{M})$.

Definition 1.32. [CCR algebra] The **CCR algebra** $\mathcal{A}(\boldsymbol{M})$ of a scalar bosonic quantum field ϕ over a globally hyperbolic spacetime $\boldsymbol{M} := (M, g, \mathfrak{o})$ is the complex $*$-algebra with unit $\mathbb{1}$ – where we explicitly assume that the algebra is not trivial: $\mathbb{1} \neq 0$ – presented by the following generators and relations (cf. Section 1.1.2).

(a) The generators, indicated by $\phi(f)$, $f \in C_c^\infty(M)$, are called (**abstract**) **field operators**. They are **smeared** with – i.e. labeled by – functions $f \in C_c^\infty(M)$.

(b) The generators satisfy the following relations, where $V \in C^\infty(M)$ is a given real function:

$\mathbb{R}$-Linearity: $\phi(af + bg) - a\phi(f) - b\phi(g) = 0 \quad \text{if } f, g \in C_c^\infty(M) \text{ and } a, b \in \mathbb{R}$.

Hermiticity: $\phi(f)^* - \phi(f) = 0 \quad \text{for } f \in C_c^\infty(M)$.

Klein-Gordon equation: $\phi\left((\Box_{\boldsymbol{M}} + V)g\right) = 0 \quad \text{for } g \in C_c^\infty(M)$.

Commutation relations: $[\phi(f), \phi(g)] - iE(f, g)\mathbb{1} = 0 \quad \text{for } f \in C_c^\infty(M)$ with E defined in (1.15).

The Hermitian elements of $\mathcal{A}(\boldsymbol{M})$ are called **observables** of the Klein-Gordon field ϕ. Furthermore,

(i) an element of $a \in \mathcal{A}(\boldsymbol{M})$, thus made of a finite linear combination of $\mathbb{1}$ and finite products of smeared fields $\phi(f)$, is said to be **localized** in an open set $O \subset M$, if $supp(f) \subset O$ for all supports of the smearing functions f concurring to define a.

(ii) $\mathbb{1}$ is *per definition* localized in every open set $O \subset M$.

(ii) $\mathcal{A}(O)$ denotes the sub $*$-algebra of $\mathcal{A}(\boldsymbol{M})$ of the elements localized in O. ■

We note that necessarily $\phi(f) \neq \mathbb{1}$ for every $f \in C_c^\infty(M)$, otherwise *Commutation relations* would imply $\mathbb{1} = 0$ as $E(f, g) \neq 0$ for some choices of g. Furthermore it is not necessary to include $\mathbb{1}$ in the set of generators (though it is permitted), since $\mathbb{1} = -iE(f, g)^{-1}[\phi(f), \phi(g)]$.

The formal meaning of $\phi(f)$ is

$$\phi(f) \text{“} = \int_M \phi(x) f(x) \mathrm{dvol}_{\boldsymbol{M}} \text{''} , \tag{1.8}$$

even if the object $\phi(x)$ does not exist. Assuming that it exists leads to mathematical contradictions. This formal identity should be taken into account in interpreting the formalism. For instance the linearity requirement in the definition above. The idea at the basis of this formal identity is that the object $\phi(x)$ is too singular to be defined rigorously and it needs a sort of average (perhaps the measurement instrument which occupies a certain location in spacetime) represented by the smooth function f.

Several technical comments about mathematical properties of Klein-Gordon equation theory used in Definition 1.32 and the internal consistence of the given axioms are necessary.

(AKG1) If $\boldsymbol{M} := (M, g, \mathfrak{o})$ is a spacetime and $V \in C^\infty(M)$ is a given real function, the **Klein-Gordon operator** is

$$P := \Box_{\boldsymbol{M}} + V : C^\infty(M) \to C^\infty(M) . \tag{1.9}$$

In concrete cases relevant in physics

$$V := m^2 + \xi R , \tag{1.10}$$

where R is the *scalar curvature* of the metric g of $\boldsymbol{M}$, $\xi \in \mathbb{R}$ a constant, and $m \geq 0$ is the mass of the particles associated to the field. The restriction $m^2 \geq 0$ is of purely physical nature and using $m^2 < 0$, or m^2 depending on the event in spacetime, has no mathematical consequences even regarding causality.

(AKG2) The associated **Klein-Gordon equation** reads

$$P\psi = 0 , \quad \psi \in C^\infty(M) . \tag{1.11}$$

The condition indicated in Definition 1.32 as *Klein-Gordon equation* is the requirement that ϕ *distributionally* satisfies the equation of Klein-Gordon. This interpretation makes sense since P is *formally selfadjoint* as established in Proposition 3.3.6. In terms of the formal manipulations at the basis of (1.8), the afore-mentioned requirement is "explained" as follows, in the spirit of the *theory of distributions*:

$$0 = \int_M \phi(x)(Pf)(x)\mathrm{dvol}_{\boldsymbol{M}} = \int_M (P\phi)(x)f(x)\mathrm{dvol}_{\boldsymbol{M}} .$$

Arbitrariness of f, if $\phi(x)$ existed, would imply $(P\phi)(x) = 0$.

(AKG3) According to Theorem 3.59, if the spacetime is globally hyperbolic and smooth compactly supported Cauchy data are given on a Cauchy surface, the solutions of the Klein-Gordon equation are uniquely determined. Furthermore their support is compact for *every* Cauchy surface of $\boldsymbol{M}$ as asserted in Corollary 3.61. Hence the following definition is well posed for a Klein-Gordon operator P in a *globally hyperbolic* spacetime $\boldsymbol{M}$:

$$\textsf{Sol} := \{\psi \in C^\infty(M) \mid P\psi = 0, \quad \psi \text{ has compact Cauchy data on every Cauchy surface}\} . \tag{1.12}$$

We stress that $\textsf{Sol}$ is a *real vector space*.

(AKG4) For a Klein-Gordon operator P in a *globally hyperbolic* spacetime $\boldsymbol{M}$, the linear map

$$E := A - R : C_c^\infty(M) \to \textsf{Sol} \tag{1.13}$$

appearing in Definition 1.32 is the **advanced-minus-retarded fundamental solution** of the KG operator also known as the **causal propagator**. The *advanced* and *retarded* propagators (also called *advanced* and *retarded fundamental solutions*), A and R respectively, are defined in Proposition 3.62. There the elementary theory of Klein-Gordon equation in globally-hyperbolic spacetime is presented. The map (1.13) associates compactly supported smooth functions to solutions of the KG equation, sometimes (improperly) called *wavefunctions*

$$C_c^\infty(M) \ni f \mapsto \psi_f := Ef \in \mathsf{Sol}\,. \tag{1.14}$$

In fact,

(a) if $f \in C_c^\infty(M)$ then $P\psi_f = PEf = PAf - PRf = f - f = 0$ due to (3.55);

(b) *supp*$(Af) \subset J^-($*supp*$(f))$ and *supp*$(Rf) \subset J^+($*supp*$(f))$ according to Proposition 3.62, so that *supp*$(Ef) \subset J^+($*supp*$(f)) \cup J^-($*supp*$(f))$. The intersection of the latter set with a Cauchy surface is compact as established in Proposition 3.57 since *supp*(f) is compact. Hence $Ef \in \mathsf{Sol}$.

(AKG5) In Definition 1.32 we used also the definition

$$E(f,g) := \int_M f(Eg)\,\mathrm{dvol}_{\boldsymbol{M}} \quad \text{if} \quad f,g \in C_c^\infty(M)\,. \tag{1.15}$$

thus viewing E as a bilinear map : $C_c^\infty(M) \times C_c^\infty(M) \to \mathbb{R}$.
At this juncture is worth observing that the *Commutation relations* requirement implies $iE(f,h)\mathbb{1} = [\phi(f), \phi(h)] = -[\phi(h), \phi(f)] = -iE(g,f)\mathbb{1}$ so that the identity

$$E(f,h) = -E(h,f) \quad \text{if } f,h \in C_c^\infty(M) \tag{1.16}$$

must be true to make consistent the list of axioms that define $\mathcal{A}(\boldsymbol{M})$. In fact, (1.16) is satisfied in view of the properties of A, R presented in Proposition 3.62:

$$E(f,h) = \int_M (fAh - fRh)\mathrm{dvol}_{\boldsymbol{M}} = \int_M ((Rf)h - (Af)h)\mathrm{dvol}_{\boldsymbol{M}} = -E(h,f)\,.$$

(AKG5) Once a state ω is given, we can implement the GNS machinery obtaining a $*$-representation $\pi_\omega : \mathcal{A}(\boldsymbol{M}) \to \mathscr{L}(\mathcal{D}_\omega)$ over the Hilbert space $\mathcal{H}_\omega$ including the dense invariant linear subspace $\mathcal{D}_\omega$. The **smeared field operators** in proper sense appear here as the densely defined symmetric operators:

$$\hat{\phi}_\omega(f) := \pi_\omega(\phi(f)) : \mathcal{D}_\omega \to \mathcal{H}_\omega\,, \quad f \in C_c^\infty(M)\,.$$

We stress that in general $\hat{\phi}_\omega(f)$ is not self-adjoint nor essentially self-adjoint on $\mathcal{D}_\omega$ (even if we are considering real smearing functions). A state ω on $\mathcal{A}(\boldsymbol{M})$ and its GNS representation are said to be **regular** if $\hat{\phi}_\omega(f)$ is essentially self-adjoint on $\mathcal{D}_\omega$ for every $f \in C_c^\infty(M)$.

From a physical perspective, it should be evident that $\mathcal{A}(\boldsymbol{M})$ is by no means sufficient to faithfully describe physics involved with the quantum field ϕ. For instance $\mathcal{A}(\boldsymbol{M})$ does not include any element which can be identified with the *stress energy tensor* of ϕ. Also the local interactions like ϕ^4 cannot be described as elements of this algebra either. We shall tackle this problem later.

1.2.2 Implementation of local causality in the algebraic formulation

An important consequence of Definition 1.32 is stated in Proposition 1.35 below which deserves a theoretical introduction.

In local quantum field theory [33], the physical hypothesis that physical information cannot travel between causally separated regions is interpreted by stating that *observables* localized in causally separated regions must be *compatible* in a quantum sense. The direct, perhaps technically naive, interpretation of compatibility is that these observables must *commute* as we are about discussing. In this form, the requirement can be promoted to the algebraic-formulation level.

Remark 1.33. Physically speaking, the commutativity requirement, due to causal separation, distinguishes observable fields, like Bosons, from unobservable ones, like Fermions, since the asserted commutativity, that is necessary for physical reasons, does not hold for Fermions. ■

We present here a precise justification of this relation between local causality and commutativity, using the Hilbert space formulation before to promote it to the algebraic level and to prove that this requirement is automatically valid for our Klein-Gordon field.

Suppose that the observables of QFT are organized in a net of local families of operators as in Definition 1.32, even if the theory is explicitly developed in a given Hilbert space. For each open region O of spacetime $\boldsymbol{M}$ there is a family $\mathfrak{A}(O)$ of operators in the Hilbert space $\mathcal{H}$ of the theory. The observables of $\mathfrak{A}(O)$ are measured by instruments localized in O. The nature of $\mathfrak{A}(O)$ is typically a *von Neumann algebra* [33], but we do not need a that sophisticated structure in this discussion. To have a concrete case to focus on we can assume that $\mathfrak{A}(O)$ contains in particular the elements of the projection valued measures of the selfadjoint operators $\overline{\hat{\phi}_\omega(f)}$, assuming that the state ω is regular.

Consider a couple of regions $O, O' \subset M$ which are *causally separated* and pick out a pair of corresponding observables $T \in \mathfrak{A}(O)$, $T' \in \mathfrak{A}(O')$, namely two selfadjoint operators densely defined in $\mathcal{H}$. Consider the spectral measures of T and T' respectively denoted by $P_E^{(T)}$ and $P_{E'}^{(T')}$, where E and E' range in family of Borel sets in the spectra of the associated selfadjoint operators.

Suppose that the measurement in O is not *selective* and that the measurement procedure is described by the *Lüders-von Neumann projection postulate* [62]. We therefore test $P_E^{(T)}$ and $\neg P_E^{(T)} := I - P_E^{(T)}$ and then we collect together all possible out coming states. If the generically mixed initial state is ρ, the *post-measurement state* is

$$\rho' := P_E^{(T)} \rho P_E^{(T)} + (I - P_E^{(T)})\rho(I - P_E^{(T)}) .$$

The probability to next measure E' in O' is therefore

$$\operatorname{tr}\left(P_{E'}^{(T')} \rho'\right) .$$

Since this measurement is located in a causally separated region from O, the same probability should arise when we do *not* perform a measurement on the initial state ρ: That is because physical communications between O and O' are impossible and no causal relation can be defined. Finally there is an observer who describes the measurement in T' *before* the one in T. Hence, it seems physically plausible to assume that the statistics of outcomes in O' does not depend on possible measurements performed or *not* performed in O[4]. In formulae:

$$\mathrm{tr}\left(P^{(T')}_{E'}\rho\right) = \mathrm{tr}\left(P^{(T')}_{E'}\rho'\right).$$

An easy computation based on linearity and the cyclic property of the trace yields

$$\mathrm{tr}\left(\rho\left(P^{(T')}_{E'} - P^{(T)}_{E}P^{(T')}_{E'}P^{(T)}_{E} - (I - P^{(T)}_{E})P^{(T')}_{E'}(I - P^{(T)}_{E})\right)\right) = 0\,.$$

Arbitrariness of ρ entails

$$P^{(T')}_{E'} = P^{(T)}_{E}P^{(T')}_{E'}P^{(T)}_{E} + (I - P^{(T)}_{E})P^{(T')}_{E'}(I - P^{(T)}_{E})\,.$$

Applying $P^{(T)}_{E}$ separately on both sides produces:

$$P^{(T)}_{E}P^{(T')}_{E'} = P^{(T)}_{E}P^{(T)}_{E}P^{(T')}_{E'}P^{(T)}_{E} + 0 = P^{(T)}_{E}P^{(T')}_{E'}P^{(T)}_{E}$$

and

$$P^{(T')}_{E'}P^{(T)}_{E} = P^{(T)}_{E}P^{(T')}_{E'}P^{(T)}_{E}P^{(T)}_{E} + 0 = P^{(T)}_{E}P^{(T')}_{E'}P^{(T)}_{E}\,.$$

So that we conclude that

$$P^{(T')}_{E'}P^{(T)}_{E} = P^{(T)}_{E}P^{(T')}_{E'}\,. \tag{1.17}$$

As is well known [61, 62], this requirement is equivalent to commutativity of unitary one-parameters groups generated by T and T':

$$e^{itT}e^{isT'} = e^{isT'}e^{itT}\,, \quad \forall s,t \in \mathbb{R}\,.$$

Now suppose that there is a common dense invariant subspace $\mathcal{D} \subset \mathcal{H}$ for T and T', and $\psi, \psi' \in \mathcal{D}$. From

$$\langle e^{-itT}\psi|e^{isT'}\psi'\rangle = \langle e^{-isT'}\psi|e^{itT}\psi'\rangle\,, \quad \forall s,t \in \mathbb{R}\,,$$

taking the derivatives for $t = s = 0$, we have

$$\langle T\psi|T'\psi'\rangle = \langle T'\psi|T\psi'\rangle\,.$$

Hence

$$\langle\psi|[T,T']\psi'\rangle = 0\,.$$

[4]We stress that *quantum entanglemen* and the EPR correlations respect this requirement [62] even if non local correlations between single couples of outcomes in O and O' are predicted and are experimentally observed. In single couples of measurements for an entangled state correlations may exist, but there is no way to transmit information through these correlations because the correlated outcomes in O and O' are separately stochastic.

Density of $\mathcal{D}$ finally yields

$$[T, T'] \restriction_{\mathcal{D}} = 0\,. \tag{1.18}$$

Under suitable mathematical assumptions (e.g. $T^2 + T'^2$ is essentially selfadjoint on $\mathcal{D}$, see [62]), this condition implies (1.17) and, in those cases, is equivalent to it.

Remark 1.34. The weakness of this justification of the equivalence of local causality and commutativity, for theories formulated in a Hilbert space, is due to the fundamental use of Lüders-von Neumann projection postulate for the post-measurement state. It is well known that it describes just a very ideal type of measurement and other descriptions, physically more meaningful, are possible in the modern theory of quantum measurements. A better perspective is perhaps directly assuming commutativity as *the* axiomatic description of local causality from scratch. ■

Requirement (1.18) can be promoted to the level of algebraic theory formulated in terms of $*$ algebras. With our formulation of the basic axioms for the Klein-Gordon field, the requirement corresponding to (1.18) is automatically satisfied for all elements of $\mathcal{A}(\boldsymbol{M})$.

Proposition 1.35. [Local Causality] *Referring to $\mathcal{A}(\boldsymbol{M})$, let $O, O' \subset M$ be a pair of open sets. Then*

$$[a, a'] = 0 \quad \textit{if } a \in \mathcal{A}(O) \textit{ and } a' \in \mathcal{A}(O') \textit{ with } O \textit{ and } O' \textit{ causally separated.}$$

Proof. Let us first consider the case $a := \phi(f)$ and $a' := \phi(g)$ where the supports of f and g are causally separated. It holds

$$[\phi(f), \phi(g)] = iE(f, g)\mathbb{1} = i\int_M f(Eg)\,\mathrm{dvol}_{\boldsymbol{M}}\mathbb{1} = i\int_M f(Ag)\,\mathrm{dvol}_{\boldsymbol{M}}\mathbb{1} - i\int_M f(Rg)\,\mathrm{dvol}_{\boldsymbol{M}}\mathbb{1}\,.$$

From Proposition 3.62 we know that $supp(Ag) \subset J^-(supp(g))$ and $supp(Rg) \subset J^+(supp(g))$. If the supports of f and g are causally separated, then $supp(f) \cap J^{\pm}(supp(g)) = \varnothing$ and thus the integrals vanish and the commutator does. The general case easily follows by induction from the elementary case $a = \phi(f)$ and $a' = \phi(g)$, taking advantage of bi-linearity of the commutator and using the properties $[a_1 a_2, b] = a_1[a_2, b] + [a_1, b]a_2$, $[a, b_1 b_2] = b_1[a, b_2] + [a, b_1]b_2$. □

1.2.3 Further properties of the causal propagator E

We move on to illustrate some further features of the smeared field operators and the CCR algebra. An important technical result [3, 79] is necessary.

Theorem 1.36. *In a globally hyperbolic spacetime $\boldsymbol{M}$ equipped with a Klein-Gordon operator P (1.9), the associated causal propagator $E : C_c^\infty(M) \to$ **Sol** defined in (1.13) satisfies the following properties.*

(a) *It is surjective.*

(b) *Its kernel is*

$$Ker(E) = \{Ph \mid h \in C_c^\infty(M)\} . \tag{1.19}$$

(c) *If $\Sigma \subset M$ is any smooth space-like Cauchy surface $f, h \in C_c^\infty(M)$ and $\psi_f := Ef$ and $\psi_h := Eh$ are the associated elements of* **Sol** *according to (1.14), it holds*

$$E(f,h) = \int_M f\psi_h \mathrm{dvol}_{\boldsymbol{M}} = \int_\Sigma \left(\psi_f \nabla_{\boldsymbol{n}_\Sigma}\psi_h - \psi_h \nabla_{\boldsymbol{n}_\Sigma}\psi_f\right) d\Sigma\,, \tag{1.20}$$

where $d\Sigma := \mathrm{dvol}_\Sigma$ is the standard measure associated to metric g_Σ induced by g on Σ and $\boldsymbol{n}_\Sigma$ the future-directed normal unit vector field to Σ.

Proof. This proof is an extended version of the proof of an analogous result in [79]. (a) Let Σ be a smooth space-like Cauchy surface of the globally hyperbolic spacetime $\boldsymbol{M}$. Referring to (a),(b),(c) Theorem 3.55, represent the spacetime as $\mathbb{R} \times \Sigma$. Take the open spacetime region O_ϵ between two slices $\{-\epsilon\} \times \Sigma$ and $\{\epsilon\} \times \Sigma$ for $\epsilon > 0$, if $\Sigma \equiv \{0\} \times \Sigma$ according to the said theorem. Let us define $\chi \in C^\infty(\mathbb{R})$ such that $\chi = 0$ in $(-\infty, -\epsilon]$ and $\chi = 1$ in $[\epsilon, +\infty)$. For any given $\psi \in$ **Sol**, we want to pick out $f \in C_c^\infty(M)$ such that $Pf = \psi$. To this end, define $f := -P\chi\psi$. With the help of Proposition 3.57, it is easy to see that $f \in C_c^\infty(M)$ by construction: this support included in $J^+(K_-) \cap J^-(K_+)$, where $K_\pm \subset \{\pm\epsilon\} \times \Sigma$ are compact sets which include the Cauchy data of ψ on the respective Cauchy surface. We know that $J^+(K_-) \cap J^-(K_+)$ is compact due to Proposition 3.57. In particular $\mathrm{supp}\,(f)$ stays in the slab between $\{-\epsilon\} \times \Sigma$ and $\{\epsilon\} \times \Sigma$. Furthermore the following identities are valid

$$Af = (1-\chi)\psi \quad \text{and} \quad Rf = -\chi\psi\,.$$

In fact, concerning the former, the right hand side satisfies $P(1-\chi)\psi = -P\chi\psi = f$ and $(1-\chi)\psi$ vanishes on $\{2\epsilon\} \times \Sigma$ and therefore agrees with the definition of $A(1-\chi)\psi$ for Proposition 3.62. Tha analogous corresponding fact is true for the latter identity. The two identities yield $Ef = Af - Rf = \psi$.
(b) If $f = Ph$ with $h \in C_c^\infty(M)$, then $Ef = APh - RPh = h - h = 0$ according to (b) Proposition 3.68. Conversely, if $Ef = 0$, it must hold $Af = Rf$ so that both $Af, Rf \in C_c^\infty(M)$ because their supports are included in $J^+(supp(f)) \cap J^-(supp(f))$ that is compact in view of Proposition 3.57. Furthermore by applying P to both sides of $Af = Rf$ we get, $f = PAf$ and thus $f = Ph$ where $h = Af \in C_c^\infty(M)$.
(c) Take $\psi \in$ **Sol** and $f \in C_c^\infty(M)$. Fix $\epsilon > 0$ as above in order that $f(p) = 0$ if $t(p) \notin [-\epsilon, \epsilon]$. We have

$$\int_M f\psi \ \mathrm{dvol}_{\boldsymbol{M}} = \int_M \psi f \ \mathrm{dvol}_{\boldsymbol{M}} = \int_M \psi P(Af)\mathrm{dvol}_{\boldsymbol{M}} = \int_{t\in[-2\epsilon,2\epsilon]} \psi P(Af)\mathrm{dvol}_{\boldsymbol{M}}\,.$$

Now we can take advantage of the Green identity (3.65) for $\Box_{\boldsymbol{M}}$, on a smoothed cylinder with sufficiently large bases parallel to Σ such that the lateral surface does not meet the supports of Af, Rf and ψ. Use the fact that $P\psi = 0$, and that the terms containing V cancel each other

$$\int_{t\in[-2\epsilon,2\epsilon]} \psi P(Af)\mathrm{dvol}_{\boldsymbol{M}} = \int_{t\in[-2\epsilon,2\epsilon]} \left(\psi P(Af) - (P\psi)Af\right)\mathrm{dvol}_{\boldsymbol{M}}$$

$$= \int_{t\in[-2\epsilon,2\epsilon]} (\psi\Box_{\boldsymbol{M}}(Af) - (\Box_{\boldsymbol{M}}\psi)Af)\,\mathrm{dvol}_{\boldsymbol{M}}$$

$$= \int_{\Sigma_{-2\epsilon}} (\psi\nabla_{-\boldsymbol{n}}(Af) - (Af)\nabla_{-\boldsymbol{n}}\psi)\ d\Sigma_{-2\epsilon} + \int_{\Sigma_{2\epsilon}} (\psi\nabla_{\boldsymbol{n}}(Af) - (Af)\nabla_{-\boldsymbol{n}}\psi)\ d\Sigma_{2\epsilon}\ .$$

Above $\boldsymbol{n}$ is the future-oriented normal unit vector to the relevant Cauchy surfaces (we write $\boldsymbol{n}$ in place of, e.g., $\boldsymbol{n}_{\Sigma_{2\epsilon}}$ for shortness). We can omit the contribution on $\Sigma_{2\epsilon} \equiv \{2\epsilon\} \times \Sigma$ since Af vanishes thereon. Since $-Rf = 0$ on $\Sigma_{-2\epsilon} \equiv \{-2\epsilon\} \times \Sigma$, we can safely replace Af for $Af - Rf = Ef$ in the former integral above, obtaining

$$\int_M f\psi \mathrm{dvol}_{\boldsymbol{M}} = -\int_{\Sigma_{-2\epsilon}} (\psi\nabla_{\boldsymbol{n}}(Ef) - (Ef)\nabla_{\boldsymbol{n}}\psi)\ d\Sigma_{-2\epsilon}\ .$$

Since $\psi = \psi_h = Eh$ for some $h \in C_c^\infty(M)$, we established that, if $S := \Sigma_{-2\epsilon}$ and restoring the notation $\boldsymbol{n}_S$ for its future oriented-unit normal vector

$$E(f,h) = \int_M f(Eh)\,\mathrm{dvol}_{\boldsymbol{M}} = \int_S (\psi_f\nabla_{\boldsymbol{n}_S}\psi_h - \psi_h\nabla_{\boldsymbol{n}_S}\psi_f)\ dS\ .$$

In other words,

$$E(f,g) = \int_S f\psi_h \mathrm{dvol}_{\boldsymbol{M}} = \int_S (\psi_f\nabla_{\boldsymbol{n}_S}\psi_h - \psi_h\nabla_{\boldsymbol{n}_S}\psi_f)\ dS$$

as wanted. The proof is concluded for the given S. However, if Σ is another generic spacelike Cauchy surface (not necessarily the initial one), the identity holds, working with a sufficiently large solid with bases contained in the two Cauchy surfaces S and Σ and such that it includes the supports of ψ_f and ψ_h in the considered region:

$$\int_\Sigma (\psi_f\nabla_{\boldsymbol{n}_\Sigma}\psi_h - \psi_h\nabla_{\boldsymbol{n}_\Sigma}\psi_f)\ d\Sigma = \int_S (\psi_f\nabla_{\boldsymbol{n}_S}\psi_h - \psi_h\nabla_{\boldsymbol{n}_S}\psi_f)\ dS$$

as a consequence of the divergence-theorem identity applied to the vector field

$$X = \psi_f d\psi_h^\sharp - \psi_h d\psi_f^\sharp$$

since $div_{\mathbb{M}}X = 0$ in view of $P\psi_f = P\psi_h = 0$ as the reader immediately proves in local coordinates. $\Box$

For future convenience we extract part (a) of the proof of the theorem in form of a lemma.

Lemma 1.37. *Let Σ be a smooth space-like Cauchy surface of the globally hyperbolic spacetime $\boldsymbol{M}$. Referring to (a),(b),(c) Theorem 3.55, take the open spacetime region O_ϵ between two slices $\{-\epsilon\} \times \Sigma$ and $\{\epsilon\} \times \Sigma$ for $\epsilon > 0$, if $\Sigma \equiv \{0\} \times \Sigma$ according to the said theorem.*
For every $\psi \in \mathsf{Sol}$, there is $f_\psi \in C_c^\infty(M)$ whose support is contained in O_ϵ, such that $\psi = Ef_\psi$.

Proof. It has been already established in the proof of (a) Theorem 1.36. $\square$

Linearity and *Commutation relations* conditions in Definition 1.32 together with (1.19) imply the next elementary but important result.

Proposition 1.38. *Referring to the smeared fields $\phi(f) \in \mathcal{A}(\boldsymbol{M})$ in Definition 1.32, the following facts are equivalent for $f, g \in C_c^\infty(M)$.*

(a) $\phi(f) = \phi(g)$;

(b) $f = g + Ph$ *for some* $h \in C_c^\infty(M)$;

(c) $\psi_g = \psi_f$ *where* $\psi_f := Ef$ *and* $\psi_g := Eg$.

Proof. Assume (a): $\phi(f) = \phi(g)$. Linearity implies $\phi(f-g) = 0$ and thus $iE(h,(f-g)) = [\phi(h), \phi(f-g)] = 0$ for all $h \in C_c^\infty(M)$. From (1.15) and Lemma 3.66, $E(f-g) = 0$ holds, that is $f - g \in Ker(E)$. Finally (1.19) implies (b): $f = g + Ph$ for some $h \in C_c^\infty(M)$. We established that $(a) \Rightarrow (b)$. Assume (b). Applying E to both sides we have $\psi_f = Ef = Eg = \psi_g$ for (1.19) and (c) arises. We established that $(b) \Rightarrow (c)$. To conclude, observe that, if (c) holds, $E(f-g) = 0$ so that $f - g = Ph$ for some $h \in C_c^\infty(M)$ and $\phi(f) - \phi(g) = \phi(Ph) = 0$ in view of the *Klein-Gordon equation* requirement in Definition 1.32, hence (a) holds closing the loop. $\square$

Remark 1.39.

(1) The above proposition shows that the generators $\phi(f)$ of $\mathcal{A}(\boldsymbol{M})$ are not faithfully labeled by the functions $f \in C_c^\infty(M)$. To remove this this redundancy one should re-label them in terms of wavefunctions $\psi = Ef \in \textsf{\textbf{Sol}}$ in view of the equivalence (a) and (b), or using classes $[f] \in C_c^\infty(M)/Ker(E) = C_c^\infty(M)/P(C_c^\infty(M))$ due to the equivalence of (a) and (b). In both cases, the requirement $\phi(Pf) = 0$ imposed on the generators of $\mathcal{A}(\boldsymbol{M})$ ceases to be necessary, since it is the reason of the redundancy: $\phi(f) = \phi(f')$ if and only if $f - f' = Ph$ with $h \in C_c^\infty(M)$ in view of the very Proposition 1.38.

As a matter of fact we shall follow this route, equivalently redefining $\mathcal{A}(\boldsymbol{M})$, in Proposition 1.49.

(2) The causal propagator (1.13) $\mathbb{C}$-linearly extends to a continuous map

$$E : \mathcal{D}(M) \to \mathcal{E}(M) \subset \mathcal{D}'(M) .$$

Here, as usual we use the notation $\mathcal{D}(M) := C_c^\infty(M) \oplus iC_c^\infty(M)$ for the space of *complex* test functions, $\mathcal{D}'(M)$ is the dual space of distributions, and $\mathcal{E}(M) := C^\infty(M) \oplus iC^\infty(M)$. Remark 3.69 immediately implies that $E : \mathcal{D}(M) \to \mathcal{D}'(M)$ is continuous. As a consequence of the *Schwartz kernel theorem* [44], it defines a distribution, indicated with the same symbol $E \in \mathcal{D}'(M \times M)$, uniquely determined by

$$E(f_1, f_2) = E(f_1 \otimes f_2) , \quad f_1, f_2 \in \mathcal{D}(M) .$$

All that leads to an equivalent interpretation of the left-hand side of (1.15), which is actually a bit more useful, because it permits to consider the action of E on non-factorized test functions $h \in \mathcal{D}(M \times M)$. $\blacksquare$

1.2.4 Time slice axiom

The smeared field $\phi(f)$ can be thought of as localized within the support of its argument f, this idea is consistent with local causality as seen above.

On the other hand, $\phi(f)$ really depends on f only up to addition of terms from $Ker(E)$, as established in the previous section. We can use this freedom to move and shrink the support of f to be arbitrarily close to any Cauchy surface [79], which is a technically useful possibility. On the other hand, this possibility gives rise to a direct proof of the so called *Time-slice axiom* for the CCR algebra (which therefore turns out to be a theorem in this elementary case).

The physical idea underpinning this principle is to promote Cauchy surfaces to a quantum level. Not only they define solutions of hyperbolic equations when initial data are given on them, but they also determine the whole algebra of observables on $\boldsymbol{M}$ when focusing on the algebra in an arbitrary small neighborhood of the surface. This determination is independent from a notion of time evolution.

Proposition 1.40. ["Time-slice axiom" validity] *Referring to the globally hyperbolic spacetime $\boldsymbol{M}$ and the algebra $\mathcal{A}(\boldsymbol{M})$, let O be a neighborhood of a smooth spacelike Cauchy surface Σ such that, with obvious notation, $(O, g\restriction_O, \mathfrak{o}\restriction_O)$ is a globally hyperbolic spacetime in its own right. Then*

$$\mathcal{A}(\boldsymbol{M}) = \mathcal{A}(O)\,. \tag{1.21}$$

Remark 1.41. A neighborhood O as in the hypothesis does exist as an immediate consequence of Theorem 3.55, simply taking the open spacetime region between two slices $\{-\epsilon\} \times \Sigma$ and $\{\epsilon\} \times \Sigma$ for $\epsilon > 0$, if $\Sigma \equiv \{0\} \times \Sigma$ according to the said theorem. ■

Sketch of proof of Theorem 1.40. Let $S \subset O$ be a smooth spacelike Cauchy surface of the globally hyperbolic spacetime $(O, g\restriction_O, \mathfrak{o}\restriction_O)$. It is not difficult to prove that S is also a Cauchy surface for $\boldsymbol{M}$ (every inextendible future-directed timelike smooth curve of $\boldsymbol{M}$ must enter O because $\Sigma \subset O$ and Σ is Cauchy for $\boldsymbol{M}$; there the curve must also meet S once because S is a Cauchy surface of O). Remaining in the globally spacetime $(O, g\restriction_O, \mathfrak{o}\restriction_O)$ and applying Theorem 3.55, consider the family of Cauchy surfaces $S_t := \{t\} \times S$ of O and $\boldsymbol{M}$. Construct the open slab O_ϵ in O between $S_{-\epsilon}$ and $S_{+\epsilon}$. According to Lemma 1.37 and Proposition 1.38, if $f \in C_0^\infty(M)$, there exists $f_O \in C_c^\infty(M)$ such that $supp(f_O) \subset O_\epsilon$ and $\phi(f) = \phi(f_O)$. Therefore, all elements of $\mathcal{A}(\boldsymbol{M})$ can be written as finite linear combinations of $\mathbb{1}$ and finite products of fields smeared with functions supported in O, proving the thesis. □

1.3 Symplectic reformulations

We move on to present an alternative but equivalent formulation of the theory known as the *symplectic formulation.* This formulation permits us to construct $\mathcal{A}(\boldsymbol{M})$ in another equivalent way which is more useful when dealing with some types of states. Furthermore this formulation allows one to give a rigorous meaning to the so called *equal time CCR* used by physicists.

1.3.1 Symplectic and Poisson structures

We start by recalling for the reader the following elementary definitions.

Definition 1.42. [Symplectic form and vector space] Let V be a (**real**) a real vector space.

(a) A **symplectic form** is a *bilinear*, *antisymmetric* map $\tau : V \times V \to \mathbb{R}$.

(b) (V, τ) is a **symplectic space** if the symplectic form τ is **weakly non-degenerate**: if $\tau(x, y) = 0$ for all $x \in V$ implies $y = 0$. ■

Next, we would like to define a *Poisson vector space*. In the finite dimensional case, it is simply a pair (V, Π), where V is a real vector space and $\Pi \in \Lambda^2 V$, which is the same as being a bilinear, antisymmetric form on the (algebraic) linear dual V^*. However, in our cases of interest, V is infinite dimensional and Π belongs to a larger space than $\Lambda^2 V$, that could be defined using linear duality. Constructions involving linear duality necessarily bring into play the topological structure on V (or lack thereof). We will not enter topological questions in detail, so we content ourselves with a formal notion of duality, which will be sufficient for our purposes.

Definition 1.43. [Poisson vector space] Let V and W be two real vector space.

(a) V and W, together with a bilinear pairing $\langle \cdot, \cdot \rangle \colon W \times V \to \mathbb{R}$, are in **formal duality** when the bilinear pairing is **non-degenerate** in either argument: $\langle x, y \rangle = 0$ implies $x = 0$ if it holds for all $y \in V$, or it implies $y = 0$ if it holds for all $x \in W$.

(b) Given V and W in formal duality, we call $(V, \Pi, W, \langle \cdot, \cdot \rangle)$ a (**real**) **Poisson vector space** if $\Pi \colon W \times W \to \mathbb{R}$ is a bilinear, antisymmetric map, called the **Poisson bivector**. Π is said to be **weakly non-degenerate** if $\Pi(x, y) = 0$ for all $x \in W$ implies $y = 0$. ■

The Poisson vector $\Pi : W \times W \to \mathbb{R}$ can be considered a symplectic form and we adopt this perspective in the rest of the section. However this viewpoint is a bit misleading since these two structures actually live on vector spaces in duality. At this level, there are only subtle differences between symplectic and Poisson vector spaces. In fact, the two structures have often been confounded in the literature on QFT on curved spacetime [2, 22, 23, 18, 36, 30]. The differences become more pronounced when we consider symplectic differential forms and Poisson bivector fields on manifolds locally modeled on the vector space V. A form is a section of an antisymmetric power of the cotangent bundle, while a bivector field is a section of an antisymmetric power of the tangent bundle. In infinite dimensional settings, one has to choose a precise notion of tangent and cotangent bundle, among several inequivalent possibilities. This ambiguity is reflected in our need to introduce formal duality for the definition of a Poisson vector space.

The above abstract definitions are concretely realized for a Klein-Gordon operator $P = \Box_{\boldsymbol{M}} + V$ in a globally hyperbolic spacetime $\boldsymbol{M} = (M, g, \mathfrak{o})$ as in the Proposition that we present below. Let us use the formula on the right-hand side of (1.20) to define a bilinear, antisymmetric map $\sigma\colon \mathsf{Sol} \times \mathsf{Sol} \to \mathbb{R}$ by

$$\sigma(\psi, \psi') := \int_\Sigma (\psi \nabla_{\boldsymbol{n}_\Sigma} \psi' - \psi' \nabla_{\boldsymbol{n}_\Sigma} \psi)\, d\Sigma, \tag{1.22}$$

where Σ is a spacelike smooth Cauchy surface of $\boldsymbol{M}$, $\boldsymbol{n}$ is the future-directed unit normal vector to Σ. As we already know, the value of the integral does not depend on the choice of Σ as established in Theorem 1.36.
As a further step, taking advantage of the causal propagator $E : C_0^\infty(M) \to \mathsf{Sol}$ (1.13), we define the real vector space of equivalence classes

$$\mathcal{E} := C_0^\infty(M)/P(C_c^\infty(M)) = C_c^\infty(M)/Ker(E) \tag{1.23}$$

where we used $Ker(E) = PC_c^\infty(M)$ from (b) Theorem 1.36, so that a corresponding well-defined bijective linear map exists $E : \mathcal{E} \to \mathsf{Sol}$

$$E[f] := Ef\ . \tag{1.24}$$

From (1.15), the advanced-minus-retarded fundamental solution E also defines a bilinear, antisymmetric map $E\colon \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ by

$$E([f], [g]) := E(f, g)\ , \quad \forall f, g \in C_c^\infty(M)\ . \tag{1.25}$$

This bilinear form is again well defined because $Ker(E) = P(C_c^\infty(M))$ from (b) Theorem 1.36 and (1.16). Finally, there is a bilinear pairing $\langle \cdot, \cdot \rangle\colon \mathcal{E} \times \mathsf{Sol} \to \mathbb{R}$ given by

$$\langle [f], \psi \rangle := \int_M f\psi \,\mathrm{dvol}_{\boldsymbol{M}}\ . \tag{1.26}$$

Also this bilinear pairing is well defined due to the formal selfadjointness of P as stated in Proposition 3.67 and exploiting $Ker(E) = P(C_c^\infty(M))$ once more.

Given the above definitions for the Klein-Gordon real scalar field, we have the following proposition which collects the various relations in the perspective of symplectic and Poisson structures.

Proposition 1.44. *Referring to the theory of Klein-Gordon operator P (1.9) in a globally hyperbolic spacetime $\boldsymbol{M}$, the following facts are true.*

- **(a)** *The pairs (Sol, σ) and $(\mathcal{E}, E)$ are symplectic vector spaces: σ and E are weakly non-degenerate.*
- **(b)** *(Sol, σ) and $(\mathcal{E}, E)$ are isomorphic through the linear bijective map $E : \mathcal{E} \to \mathsf{Sol}$ (1.24) since*

$$\sigma(E[f], E[g]) = E([f], [g]) \quad \forall [f], [g] \in \mathcal{E}\ .$$

(c) *The spaces* Sol *and* $\mathcal{E}$ *are in formal duality, with respect to the pairing* $\langle\cdot,\cdot\rangle$ *(1.26) and* $(\mathsf{Sol}, E, \mathcal{E}, \langle\cdot,\cdot\rangle)$ *is a Poisson vector space. In particular,* $\langle\cdot,\cdot\rangle$ *is weakly non-degenerate.*

(d) $E : \mathcal{E} \to \mathsf{Sol}$*, its inverse* $\sigma\colon \mathsf{Sol} \to \mathcal{E}$ *and the pairing* $\langle\cdot,\cdot\rangle\colon \mathcal{E} \times \mathsf{Sol} \to \mathbb{R}$ *satisfy*

$$\sigma(\psi,\xi) = \langle\sigma\psi,\xi\rangle\,, \quad E([f],[g]) = \langle[f],E[g]\rangle\,.$$

Proof. (a) and (b). The proof of the identity in (b) immediately arises from the given definitions and Theorem 1.36. Let us prove (a). We prove that σ is weakly non degenerate. To this end choose a spacelike smooth Cauchy surface Σ and assume that $\sigma(\psi,\phi) = 0$ for all $\psi \in \mathsf{Sol}$. In other words

$$\sigma(\psi,\phi) = \int_\Sigma (\psi\nabla_{\boldsymbol{n}_\Sigma}\phi - \phi\nabla_{\boldsymbol{n}_\Sigma}\psi)d\Sigma = 0$$

for every choice of the smooth compactly supported functions $\psi\restriction_\Sigma$ and $\nabla_{\boldsymbol{n}_\Sigma}\psi$ on Σ. We stress that these two functions can be chosen freely because, for every choice of them in $C^\infty_c(\Sigma)$, there is an element ψ of Sol which restricts to them on Σ in view of the existence part in Theorem 3.59. Arbitrariness of $\psi\restriction_\Sigma$ and $\nabla_{\boldsymbol{n}_\Sigma}\psi$, taking advantage of Lemma 3.66, implies that $\phi\restriction_\Sigma = 0$ and $\nabla_{\boldsymbol{n}_\Sigma}\phi = 0$. Again, the uniqueness part in Theorem 3.59 shows that $\phi = 0$ is the unique element of Sol compatible with these initial data on Σ. We proved that σ is weakly non degenerate. At this juncture, the fact that E in (1.24) is a vector space isomorphism and preserves the symplectic forms as proved in (b) implies that the symplectic form $E : \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ is weakly non degenerate as well. Indeed, if $E([f],[g]) = 0$ for all $[f]$, we also have $\sigma(E[f],E[g]) = 0$. Since $E[f]$ everywhere ranges in Sol – E is surjective – non degenerateness of σ implies $E[g] = 0$, namely, $[g] = 0$ since E is linear and injective.
(c) and (d). Let us start from (d). The two written identities are immediate consequences of the given definitions and of Theorem 1.36. We finally prove (c). Weak non-degenerateness of $\langle\cdot,\cdot\rangle$ immediately arises from (d) and the fact that $E : \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ is weakly non degenerate and $E : \mathcal{E} \to \mathsf{Sol}$ in (1.24) is linear and bijective. □

Given the isomorphism between $\mathcal{E}$ and Sol and the close relationship between E and σ, it is not surprising these two spaces and bilinear forms have often been used interchangeably in the context of the QFT of the Klein-Gordon real scalar field. However, this interchangeability may fail for more complicated field theories, as we remark next. This is another reason why it is important to keep track of the difference between the respective symplectic and Poisson vector spaces, (Sol,σ) and $(\mathsf{Sol}, E, \mathcal{E}, \langle\cdot,\cdot\rangle)$.

Remark 1.45. References [49, Sec.5] and [50, Sec.3] also address in detail the question of whether similar statements hold for *gauge theories* (electrodynamics, linearized gravity, etc.) or for theories with constraints (massive vector field, etc.). Related questions were also studied in [36]. The answer turns out to be rather subtle. The bilinear forms σ and E can essentially always be defined. A reasonable choice of the spaces $\mathcal{E}$ and Sol also make sure that the linear maps $\sigma\colon \mathsf{Sol} \to \mathcal{E}$ and $E\colon \mathcal{E} \to \mathsf{Sol}$ are also well-defined and are mutually inverse. However, the pairing $\langle\cdot,\cdot\rangle$ appearing in the formulas $\sigma(\psi,\xi) = \langle\sigma\psi,\xi\rangle$ and $E([f],[g]) = \langle[f],E[g]\rangle$, need no longer be non-degenerate. Hence, the bilinear forms σ and E may be degenerate themselves. The conditions under which these degeneracies do or do not occur subtly depend on the geometry of the gauge transformations and the constraints of the theory. ■

We now turn to applying the above symplectic and Poisson structures to the study of the properties of the CCR algebra $\mathcal{A}(\boldsymbol{M})$ of a Klein-Gordon field.

Definition 1.46. [CCR algebra of a vector space with symplectic form] Let (V, τ) be a real vector space with a symplectic form (also weak degenerate). The **CCR algebra** $\mathcal{A}(V, \tau)$ is defined as the $*$-algebra with unit $\mathbb{1}$ – where we explicitly assume that the algebra is not trivial: $\mathbb{1} \neq 0$ – presented by the generators $\Phi(x)$, $x \in V$, subject to the relations

(i) $\Phi(ax + by) - a\Phi(x) - b\Phi(y) = 0$,

(ii) $\Phi(x)^* - \Phi(x) = 0$,

(iii) $[\Phi(x), \Phi(y)] - i\tau(x, y)\mathbb{1} = 0$,

for any $a, b \in \mathbb{R}$ and $x, y \in V$. ■

Remark 1.47.

(1) If τ is weakly non-degenerate, then $\Phi(x) \neq \mathbb{1}$ and $\Phi(x) = 0$ only if $x = 0$. Both statements immediately follow from (iii).

(2) A similar CCR algebra $\mathcal{A}(V, \Pi, W, \langle\cdot,\cdot\rangle)$ can be defined for a Poisson structure $(V, \Pi, W, \langle\cdot,\cdot\rangle)$. Here the relevant couple corresponding to (V, σ) in Definition 1.46 is (W, Π). The generators are labeled by elements of W and the symplectic form to be used in (iii) (without the restriction of non-degenerateness) is Π. ■

1.3.2 Induced automorphisms and the interplay of $\mathcal{A}(\mathsf{Sol}, \sigma)$, $\mathcal{A}(\mathcal{E}, E)$ and $\mathcal{A}(\boldsymbol{M})$

We start with a technical result of great relevance for its applications. Next we apply the result to prove in particular that the various representations of the CCRs so far accumulated are equivalent.

Proposition 1.48. [Induced homomorphism][5] *Let $\mathcal{A}(V, \tau)$ and $\mathcal{A}(V', \tau')$ be two CCR algebras as in Definition 1.46 and let $\gamma\colon V \to V'$ be a linear map such that*

$$\tau'(\gamma x, \gamma y) = \tau(x, y) \quad (\textit{resp. } \tau'(\gamma x, \gamma y) = -\tau(x, y)), \quad \forall x, y \in V. \tag{1.27}$$

Then, there exists a homomorphism (resp. anti-linear homomorphism) of unital $*$-algebras, $\alpha^{(\gamma)}\colon \mathcal{A}(V, \tau) \to \mathcal{A}(V', \tau')$ uniquely defined by its values on the generators of $\mathcal{A}(V, \tau)$ as

$$\alpha^{(\gamma)}(\Phi(x)) := \Phi'(\gamma x), \quad \forall x \in V \tag{1.28}$$

If γ is bijective, then $\alpha^{(\gamma)}$ is an isomorphism of unital $*$-algebras.

[5] This proof is due to I. Khavkine

Proof. First of all observe that the uniqueness property is obvious by definition of generators provided the considered homomorphism exists. Recall the definition of an algebra presented by generators and relations by its universal property, as discussed in Section 1.1.2, as well as such a presentation of the algebra $\mathcal{A}(V,\tau)$ given in Definition 1.46.

Let us denote by $\mathcal{A}(V)$ and $\mathcal{A}(V')$ the algebras freely generated by the elements of the vector space V and V' respectively. Following our notation, the map embedding the generators in these algebras can be denoted as $A\colon V \to \mathcal{A}(V)$ and $A'\colon V' \to \mathcal{A}(V')$ respectively. The composition $A' \circ \gamma$ is another such map. Therefore, by the universal property, there exists a unique homomorphism $\beta\colon \mathcal{A}(V) \to \mathcal{A}(V')$ such that $\beta(A(x)) = A'(\gamma x)$, for all $x \in V$, and $\beta(\mathbb{1}) = \mathbb{1}'$.

We now need to check whether β transforms the kernel of the projection $\mathcal{A}(V) \to \mathcal{A}(V,\tau)$ into the kernel of the projection $\mathcal{A}(V') \to \mathcal{A}(V',\tau')$. This kernel is the two-sided ideal generated by the relations $A(ax+by) - aA(x) - bA(y) = 0$, $A(x)^* - A(x) = 0$ and $[A(x), A(y)] - i\tau(x,y)\mathbb{1} = 0$, for any $a, b \in \mathbb{R}$ and $x, y \in V$, so it is sufficient to check the invariance of these relations. The first two are obviously invariant. The last commutator identity is invariant upon invoking the hypothesis that γ transforms τ to τ', up to sign. We deal with the two cases separately.

In the case when γ transforms τ to τ', we have

$$\beta\left([A(x), A(y)] - i\tau(x,y)\mathbb{1}\right) = [A'(\gamma x), A'(\gamma y)] - i\tau(x,y)\mathbb{1}' = [A'(\gamma x), A'(\gamma y)] - i\tau'(\gamma x, \gamma y)\mathbb{1}'. \tag{1.29}$$

Hence, the homomorphism β induces a uniquely defined homomorphism on the quotiented algebra, which we call $\alpha^{(\gamma)}\colon \mathcal{A}(V,\tau) \to \mathcal{A}(V',\tau')$, which given by $\alpha^{(\gamma)}([a]) = [\beta a]$, and which has all the desired properties. In particular $\alpha^{(\gamma)}(\Phi(x)) = \Phi'(\gamma x)$ where, as usual, $\Phi(x) := [A(x)]$ and $\Phi'(x') := [A'(x')]$.

In the case when γ changes the sign of Π, we need to change perspective slightly. Recall that we defined $\mathcal{A}(V,\tau)$ as a complex algebra, which then automatically has the structure of a real algebra. Equivalently, we could have also defined it directly as a real algebra, by throwing in an extra generator i, satisfying the relations $i^2 = -\mathbb{1}$, $[i, \mathbb{1}] = [i, \Phi(x)] = 0$ and $i^* = -i$. We define an analogous generator i' for $\mathcal{A}(V')$. If the homomorphism β is extended to this generator as $\beta(i) = -i'$, then it preserves the new relations that need to be satisfied by i' and also the commutator identity, since

$$\beta\left([\Phi(x), \Phi(y)] - i\tau(x,y)\mathbb{1}\right) = [\Phi'(\gamma x), \Phi'(\gamma y)] - (-i)\tau(x,y)\mathbb{1}' = [\Phi'(\gamma x), \Phi'(\gamma y)] - i'\tau'(\gamma x, \gamma y)\mathbb{1}. \tag{1.30}$$

Hence, the real algebra homomorphism β induces a uniquely defined homomorphism on the quotiented algebra, which also happens to be an anti-linear homomorphism in the sense of complex algebras, which we call $\alpha^{(\gamma)}\colon \mathcal{A}(V,\tau) \to \mathcal{A}(V',\tau')$, and which has all the desired properties.

Finally, when γ is a bijection, we can define an analogous isomorphism $\alpha^{(\gamma^{-1})} : \mathcal{A}(V',\tau') \to \mathcal{A}(V,\tau)$ which uniquely extends $\alpha^{(\gamma^{-1})}(\Phi'(x')) = \Phi'(\gamma^{-1}x)$. The isomorphisms $\alpha^{(\gamma)} \circ \alpha^{(\gamma^{-1})}$ and $\alpha^{(\gamma^{-1})} \circ \alpha^{(\gamma)}$ are the identity maps on $\mathcal{A}(V',\tau')$ and $\mathcal{A}(V,\tau)$ respectively, since they are the identity maps on corresponding generators. Therefore, $\alpha^{(\gamma)}$ is an isomorphism of the algebras becuse $(\alpha^{(\gamma)})^{-1} = \alpha^{(\gamma^{-1})}$. $\square$

The interplay of $\mathcal{A}(\boldsymbol{M})$, $\mathcal{A}(\mathsf{Sol},\sigma)$, and $\mathcal{A}(\mathcal{E},E)$ is trival: they are all $*$ isomorphic. We prove this nice fact in the following proposition which is an elementary corollary of Proposition 1.48.

Proposition 1.49. *Consider a globally hyperbolic spacetime $\boldsymbol{M}$, a Klein-Gordon operator $P = \Box_{\boldsymbol{M}} + V$ on it and the associated symplectic spaces (Sol,σ) and $(\mathcal{E},E)$, with respective symplectic forms $\sigma : \mathsf{Sol}\times\mathsf{Sol}\to\mathbb{R}$ defined in (1.22) and $E:\mathcal{E}\times\mathcal{E}\to\mathbb{R}$ defined in (1.25). The following facts hold.*

(a) *The CCR algebras $\mathcal{A}(\mathsf{Sol},\sigma)$ and $\mathcal{A}(\mathcal{E},E)$ are $*$-isomorphic. The isomorphism is the unique homomorphism of unital $*$-algebras $F:\mathcal{A}(\mathcal{E},E)\to\mathcal{A}(\mathsf{Sol},\sigma)$ which extends*[6]

$$F:\mathcal{A}(\mathcal{E},E)\ni\Phi([f])\mapsto\Phi(E[f])\in\mathcal{A}(\mathsf{Sol},\sigma)\quad f\in C^\infty_c(M). \tag{1.31}$$

(b) *The unital $*$-algebras $\mathcal{A}(\boldsymbol{M})$ and the CCR algebra $\mathcal{A}(\mathcal{E},E)$ are $*$-isomorphic. The isomorphism is the unique homomorphism of unital $*$-algebras $G:\mathcal{A}(\mathcal{E},E)\to\mathcal{A}(\boldsymbol{M})$ which extends*

$$G:\mathcal{A}(\mathcal{E},E)\ni\Phi([f])\mapsto\phi(f)\in\mathcal{A}(\boldsymbol{M})\quad f\in C^\infty_c(M). \tag{1.32}$$

(c) *The unital $*$-algebras $\mathcal{A}(\boldsymbol{M})$ and the CCR algebra $\mathcal{A}(\mathsf{Sol},\sigma)$ are $*$-isomorphic. The isomorphism is the unique homomorphism of unital $*$-algebras $H:\mathcal{A}(\mathsf{Sol},\sigma)\to\mathcal{A}(\boldsymbol{M})$ which extends*

$$H:\mathcal{A}(\mathsf{Sol},\sigma)\ni\Phi(Ef)\mapsto\phi(f)\in\mathcal{A}(\boldsymbol{M})\quad f\in C^\infty_c(M), \tag{1.33}$$

where E is the causal propagator (1.13) of P.

Proof. (a) The thesis is an immediate application of Proposition 1.48, taking (b) Proposition 1.44 into account.
(b) According to Proposition 1.38, the generators $\phi(f)$ of $\mathcal{A}(\boldsymbol{M})$ satisfy $\phi(f)=\phi(f')$ if and only if $[f]=[f']$. Therefore we can faithfully re-label the generators using classes $[f]\in\mathcal{E}$ and defining $\phi'([f]):=\phi(f)$. With this procedure, the requirements stated in Definition 1.32 which define $\mathcal{A}(\boldsymbol{M})$ up to isomorphisms according to the procedure described in Section 1.1.2, exactly become the conditions (i)-(iii) which define $\mathcal{A}(\mathcal{E},E)$, when taking (1.25) into account, provided the identification $\Phi([f])\equiv\phi'([f])$ is assumed. The requirement called *Klein-Gordon equation* in Definition 1.32 is automatically true with the new choice of generators. According to (1) Remark 1.9 and Definition 1.8, there is a unique $*$-homomorphism $\mathcal{A}(\mathcal{E},E)\to\mathcal{A}(\boldsymbol{M})$ which extends the map $\Phi([f])\mapsto\phi'([f])=\phi(f)$. This homomorphism is surjective because the image includes a set of generators. It is also injective according to Proposition 1.50 below, whose proof does not depend on this proof. The found $*$-isomorphism is G.
(c) According to Proposition 1.38, the generators $\phi(f)$ of $\mathcal{A}(\boldsymbol{M})$ satisfy $\phi(f)=\phi(f')$ if and only if $Ef=Ef'$. As before we can therefore faithfully re-label the generators using the images

[6] We use the same symbol Φ to denote the generators of $\mathcal{A}(\mathsf{Sol},\sigma)$ and $\mathcal{A}(\mathcal{E},E)$, the relevant algebra is evident from the argument of Φ.

$Ef \in \mathsf{Sol}$ and defining $\phi'(Ef) := \phi(f)$. As before, the requirements stated in Definition 1.32 which define $\mathcal{A}(\boldsymbol{M})$ up to isomorphisms according to the procedure described in Section 1.1.2, exactly become the conditions (i)-(iii) which define $\mathcal{A}(\mathsf{Sol}, \sigma)$, when taking (1.20) into account, provided the identification $\Phi(\psi) \equiv \phi(\psi)$ is assumed. The requirement called *Klein-Gordon equation* in Definition 1.32 is automatically true with the new choice of generators. According to (1) Remark 1.9 and Definition 1.8, there is a unique $*$-homomorphism $\mathcal{A}(\mathsf{Sol}, \sigma) \to \mathcal{A}(\boldsymbol{M})$ which extends the map $\Phi(\psi) \mapsto \phi'(\psi) = \phi(f)$ with $\psi = Ef$. This homomorphism is surjective because the image includes a set of generators. It is also injective according to Proposition 1.50 below, whose proof does not depend on this proof. The found $*$-isomorphism is H. $\square$

Homomorphisms of CCR algebras are in particular important because the composition of a state with an homomorphism gives a way to define more states, once at least one is known. The isomorphisms $\mathcal{A}(\boldsymbol{M}) \cong \mathcal{A}(\mathsf{Sol}, \sigma)$ and $\mathcal{A}(\boldsymbol{M}) \cong \mathcal{A}(\mathcal{E}, E)$ allow us to construct lots of automorphisms of $\mathcal{A}(\boldsymbol{M})$, induced by transformations of Sol or $\mathcal{E}$ that, respectively, leave σ or E invariant.

1.3.3 The meaning of the Equal-Time CCR

In physically minded QFT textbooks, quantized fields are often described in the so called *canonical formalism*. Here the fields are smeared with smooth functions defined on an arbitrary Cauchy surface S of a globally hyperbolic spacetime $\boldsymbol{M}$. Two types of formal field operators enter the game. If, as usual, we assume that the theory is developed in a Hilbert space, these formal operators are $\hat{\varphi}(t, x)$ and its *conjugated momentum* $\hat{\pi}(t, x) := \nabla_{\mathbf{n}}\hat{\varphi}(t, x)$, where $t \in \mathbb{R}$ is a notion of global time and $x \in S$. As said. $S \subset M$ is a spacelike smooth Cauchy surface and the spacetime is decomposed as $M \equiv \mathbb{R} \times S$ according to Theorem 3.55, so that $S_t \equiv \{t\} \times S$ (in particular $S \equiv \{0\} \times S$), and finally $\mathbf{n}$ is the unit future-oriented normal vector to S_t. The **Equal-Time CCR** read

$$[\hat{\varphi}(t, x), \hat{\varphi}(t, x')] = 0\,, \quad [\hat{\pi}(t, x), \hat{\pi}(t, x')] = 0\,, \quad [\hat{\varphi}(t, x), \hat{\pi}(t, x')] = i\delta(x, y)I\,. \tag{1.34}$$

To produce some rigorous intepretation, it is usefult to pass to a smeared version of the identities:

$$[\hat{\varphi}_t(f), \hat{\varphi}_t(h)] = 0\,, \quad [\hat{\pi}_t(f), \hat{\pi}_t(h)] = 0\,, \quad [\hat{\varphi}_t(f), \hat{\pi}_t(h)] = i\int_{S_t} f(x)h(x)dS_tI\,, \tag{1.35}$$

where $f, h \in C_c^\infty(S_t)$ and dS_t is the natural volume measure induced by the Riemannian metric on S, finally, with the usual formal distributional sense

$$\hat{\varphi}_t(f) := \int_{S_t} f(x)\hat{\varphi}(t, x)dS_t\,, \quad \hat{\pi}_t(f) := \int_{S_t} f(x)\hat{\pi}(t, x)dS_t\,. \tag{1.36}$$

We move on to prove that a $*$-algebraic version of this formalism can be rigorously embodied in the very nature of $\mathcal{A}(\mathsf{Sol}, \sigma)$ as follows. Every $\psi \in \mathsf{Sol}$ is completely determined by its Cauchy data $f := \psi\restriction_{S_t}$ and $h := \nabla_{\mathbf{n}}\psi|_{S_t}$ due to the existence and uniqueness Theorem 3.59. Referring to Definition 1.46, we define the elements of $\mathcal{A}(\textsf{\textbf{Sol}}, \sigma)$

$$\varphi_t(f) := \Phi(\psi_{0,f}) \,, \quad \pi_t(h) := -\Phi(\psi_{h,0}) \,, \tag{1.37}$$

where $\psi_{f_1,f_2} \in Sol$ is the solution of the Klein-Gordon equation with Cauchy data $\psi\restriction_{S_t}= f_1$ and $\nabla_{\mathbf{n}}\psi|_{S_t} = f_2$, for $f_1, f_2 \in C^\infty_c(S_t)$. Notice that $C^\infty_0(S) \ni f \mapsto \varphi_t(f) \in \mathcal{A}(\textsf{\textbf{Sol}}, \sigma)$ and $C^\infty_0(S) \ni h \mapsto \pi_t(h) \in \mathcal{A}(\textsf{\textbf{Sol}}, \sigma)$ turn out to be linear by construction. By linearity, we also have

$$\Phi(\psi_{f,h}) = \varphi_t(f) - \pi_t(h) \,. \tag{1.38}$$

Requirement (iii) in Definition 1.46 reads now $[\Phi(\psi_{f,h}), \Phi(\psi_{f',h'})] = i\sigma(\psi_{f,h}, \psi_{f',h'})\mathbb{1}$. With the given definitions, it can be rephrased to

$$[\varphi_t(f) - \pi_t(h), \varphi_t(f') - \pi_t(h')] = i \int_{S_t} (hf' - h'f)\, dS_t \mathbb{1} \,.$$

If we consider the cases where only two functions among f, h, f', h' do not vanish, the previous identity gives rise to the following three subcases (the forth one coincides with the third just in view of antisymmetry of the commutator):

$$[\varphi_t(f), \varphi_t(h)] = 0 \,, \quad [\pi_t(f), \pi_t(h)] = 0 \,, \quad [\varphi_t(f), \pi_t(h)] = i \int_{S_t} f(x)h(x) dS_t \mathbb{1} \,. \tag{1.39}$$

We eventually found the algebraic (and rigorous) version of (1.35). In this sense the symplectic formalism embodies the equal-time canonical commutation relations. On the other hand the identities (1.39), taking (1.37) and (1.38) into account (where linearity is implicitly assumed), imply properties (i),(ii),(iii) of Definition 1.46. In summary, the equal-time CCR are nothing but an equivalent way to describe the generators of $\mathcal{A}(\textsf{\textbf{Sol}}, \sigma)$.

1.3.4 Simplicity and faithfulness of CCR

This generic definition of $\mathcal{A}(V, \tau)$ allows us to state and prove the following useful result.

Proposition 1.50. [Simplicity and faithfulness] *Given a symplectic space (V, τ) – thus τ is explicitly required to be weakly non degenerate – the corresponding CCR algebra $\mathcal{A}(V, \tau)$ is simple and thus admits only zero or faithful representations for Proposition 1.14.*

Before giving the proof, we note its main consequence. Thus, given Proposition 1.49 and Proposition 1.44, we have the immediate

Corollary 1.51. *The CCR algebra $\mathcal{A}(\boldsymbol{M})$ of a real Klein-Gordon quantum field on the globally hyperbolic spacetime $\boldsymbol{M}$ is simple. Therefore it admits only either zero or faithful representations.*

Remark 1.52.

(1) The proposition above is also valid (with the same proof just replacing τ for Π) when spaces V and W are in formal duality and the Poisson bivector Π of the Poisson vector space $(V, \Pi, W, \langle\cdot,\cdot\rangle)$ is weakly non-degenerate (as a bilinear form on W). In this case the corresponding CCR algebra $\mathcal{A}(V, \Pi, W, \langle\cdot,\cdot\rangle)$ is simple. Further, it admits only zero or faithful representations.

(2) The result established in the Corollary above is *not* valid form more complicated QFTs like *electromagnetism* [74] and *linearized gravity* [21]. The physical reason is the appearance of the *gauge invariance*. Mathematically it is related to the fact that the Poisson bivector corresponding to our E is *degenerate* on the space $\mathcal{E}$ of compactly supported observables, as discussed in [49, Sec.5] and [50, Sec.3]. ■

The proof of Proposition 1.50 makes use of the following two lemmata[7].

Lemma 1.53. *Let τ be a bilinear form (we need not even assume it to be antisymmetric) on a vector space V. Further, let $v_i \in V$, $i = 1, \dots, N$, be a set of linearly independent vectors and $c^{i_1\cdots i_k}$ a collection of scalars, not all zero, with each index running through $i_j = 1, \dots, N$. Then, if*

$$\sum_{i_1,\dots,i_k} c^{i_1\cdots i_k}\tau(v_{i_1}, u_1)\cdots\tau(v_{i_k}, u_k) = 0 \tag{1.40}$$

for each set of vectors $u_i \in V$, $i = 1, \dots, k$. Then there exists a non-zero vector $w \in V$ such that $\tau(w, u) = 0$ for any $u \in V$.

Proof. The proof is by induction on k. Let $k = 1$, then the right-hand side of the equation in the hypothesis is $\tau(w', u_1)$, where

$$w' = \sum_i c^i v_i. \tag{1.41}$$

Since not all c^i are zero and the v_i, $i = 1, \dots, N$ are linearly independent, we have $w' \neq 0$. We can then set $w = w'$ and we are done, since u_1 can be arbitrary.

Now, assume that the case $k-1$ has already been established. Note that we can write the right-hand side of the above equation as $\tau(w', u_k)$, where

$$w' = \sum_{i_1,\dots,i_k} c^{i_1\cdots i_k}\tau(v_{i_1}, u_1)\cdots\tau(v_{i_{k-1}}, u_{k-1})v_{i_k}. \tag{1.42}$$

If $w' \neq 0$ for some choice of $u_i \in V$, $i = 1, \dots, k-1$, then we can set $w = w'$ and we are done, since u_k can be arbitrary.

Consider the case when $w' = 0$ for all $u_i \in V$, $i = 1, \dots, k-1$. Then, choose j_k such that $c^{i_1\cdots i_{k-1}j_k}$ are not all zero. Since, by linear independence, the coefficients of the v_{i_k} in w' must vanish independently, we have

$$\sum_{i_1,\dots,i_{k-1}} c^{i_1\cdots i_{k-1}j_k}\tau(v_{i_1}, u_1)\cdots\tau(v_{i_{k-1}}, u_{k-1}) = 0 \tag{1.43}$$

[7] This proof is due to I. Khavkine

for all $u_i \in V$, $i = 1, \dots, k-1$. In other words, by the inductive hypothesis, the last equality implies the existence of the desired non-zero $w \in V$, which concludes the proof. □

A bilinear form τ on V naturally defines a bilinear form $\tau^{\otimes k}$ on the k-fold tensor product $V^{\otimes k}$. Let $S_k \colon V^{\otimes k} \to V^{\otimes k}$ denote the symmetrization priojector

$$S_k(u_1 \otimes \cdots \otimes u_k) := \frac{1}{k!} \sum_{\sigma \in \mathcal{P}_k} u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(k)} ,$$

($\mathcal{P}_k$ is the permutation group of k objects, i.e., the group of bijective maps $\sigma : \{1, 2, \dots, k\} \to \{1, 2, \dots, k\}$ with respect to the composition product of maps.) We denote its image, the space of fully symmetric k-tensors, by

$$S^k V := S_k(V^{\otimes k}) .$$

Of course, $\tau^{\otimes k}$ also restricts to $S^k V$. If τ is antisymmetric, then $\tau^{\otimes k}$ is symmetric when k is even and antisymmetric when k is odd.

Lemma 1.54. [8] *If the antisymmetric bilinear form τ is weakly non-degenerate on W, then the antisymmetric bilinear form $\tau^{\otimes k}$ is weakly non-degenerate on $S^k V$.*

Proof. Assume the contrary, that $\tau^{\otimes k}$ is degenerate. By its (anti-)symmetry, we need only consider the degeneracy in its first argument. That is, there exists a vector $v = \sum_{i_1, \dots i_k} d^{i_1 \cdots i_k} v_{i_1} \otimes \cdots \otimes v_{i_k}$, where $v_i \in V$, $i = 1, \dots, N$, constitute a linearly independent set and the $d^{i_1 \cdots i_k}$ coefficients are not all zero and are symmetric under index interchange, such that

$$\tau^{\otimes k}(v, S_k(u_1 \otimes \cdots \otimes u_k)) = 0. \tag{1.44}$$

for any $u_i \in V$, $i = 1, \dots, k$. But then, the above equality is precisely of the form of the hypothesis of Lemma 1.53, with

$$c^{i_1 \cdots i_k} = k!\, d^{i_1 \cdots i_k}, \tag{1.45}$$

due to the symmetry of $d^{i_1 \cdots i_k}$ under index interchanges. Therefore, by Lemma 1.53, there must exist a $w \in V$ such that $\tau(w, u) = 0$ for all $u \in V$, which contradicts the weak non-degeneracy of τ on V. Therefore, $\tau^{\otimes k}$ cannot be degenerate on $S^k V$, and hence is weakly non-degenerate. □

Proof of Proposition 1.50. [9] Suppose that $\mathcal{A}(V, \tau)$ is not simple, and so has a non-trivial two-sided ideal $\mathcal{I}$. If we can deduce that $\mathbb{1} \in \mathcal{I}$, then any non-trivial two-sided ideal must be all of $\mathcal{A}(V, \tau)$, implying that the algebra is simple.

Take any non-zero element $a \in \mathcal{I}$ and recall the idea behind Equation (1.48). That is, there exists integers $k, N \geq 0$, linearly independent elements $v_i \in V$, $i = 1, \dots, N$, and complex coefficients $c_{(l)}^{i_1 \cdots i_l}$, $i_j = 1, \dots, N$ and $l = 0, \dots, k$, such that[10]

[8] This proof is due to I. Khavkine

[9] This proof is due to I. Khavkine

[10] Actually the term $c_{(0)}\mathbb{1}$ can be omitted since it is a special case of $\sum_{i_1, i_2} c_{(2)}^{i_1 i_2} \Phi(v_{i_1}) \Phi(v_{i_2})$ in view of the commutation relations.

$$a = c_{(0)}\mathbb{1} + \sum_{i_1} c^{i_1}_{(1)}\Phi(v_{i_1}) + \sum_{i_1,i_2} c^{i_1 i_2}_{(2)}\Phi(v_{i_1})\Phi(v_{i_2}) + \cdots + \sum_{i_1,\ldots,i_k} c^{i_1\ldots i_k}_{(k)}\Phi(v_{i_1})\cdots\Phi(v_{i_k}), \quad (1.46)$$

where not all of the components of $c^{i_1\ldots i_k}_{(k)}$ are zero. If $k = 0$, the $\mathbb{1} \in \mathfrak{I}$ and we are done. If $k > 0$, note that $\mathfrak{I}$ also contains the iterated commutator $[\cdots[a, \Phi(u_1)], \ldots, \Phi(u_k)]$, for any $u_i \in V$, $i = 1, \cdots, k$. A straight forward calculation shows that, up to (non-zero) numerical factors, the iterated commutator is equal to

$$\tau^{\otimes k}\left(\sum_{i_1,\ldots,i_k} c^{i_1,\ldots,i_k}_{(k)} S_k(v_{i_1} \otimes \cdots \otimes v_{i_k}), S(u_1 \otimes \cdots \otimes u_k)\right)\mathbb{1}. \quad (1.47)$$

By Lemma 1.54, since τ is weakly non-degenerate on V, $\tau^{\otimes k}$ is weakly non-degenerate on $S^k V$. Since elements of the form $S_k(u_1 \otimes \cdots \otimes u_k)$ generate $S^k V$, there must exist at least one element of $S^k V$ of that form such that the coefficient in front of $\mathbb{1}$ in (1.47) is non-zero. Therefore, $\mathbb{1} \in \mathfrak{I}$ and we are done. $\square$

1.4 States and quasifree states on $\mathcal{A}(\boldsymbol{M})$

There is a plethora of states on $\mathcal{A}(\boldsymbol{M})$, this section is devoted to them. We first establish on some general properties of states on $\mathcal{A}(\boldsymbol{M})$ and next focus on a special class of states called *quasifree* or *Gaussian states*. They mimic the Fock representation of the so-called *Minkowski vacuum* and they are completely determined from the two-point function by means of a prescription generalizing the well known Wick procedure which also guarantees essential selfadjointness of the field operators $\hat{\phi}_\omega$ since they are regular according to comment (AKG5) after Definition 1.32. Next section is devoted to dicuss some general properties of states on $\mathcal{A}(\boldsymbol{M})$ and, in particular, to introduce the notion of *n-point function*.

1.4.1 n-point functions of a state

We start form the observation that the generic element of $\mathcal{A}(\boldsymbol{M})$ is always of the form[11]

$$a = c_{(0)}\mathbb{1} + \sum_{i_1} c^{i_1}_{(1)}\phi(f^{(1)}_{i_1}) + \sum_{i_1,i_2} c^{i_1 i_2}_{(2)}\phi(f^{(2)}_{i_1})\phi(f^{(2)}_{i_2}) + \cdots + \sum_{i_1,\ldots,i_n} c^{i_1\cdots i_n}_{(n)}\phi(f^{(n)}_{i_1})\cdots\phi(f^{(n)}_{i_n}), \quad (1.48)$$

where n is arbitrarily large but finite, $c^{i_1\cdots i_k}_{(k)} \in \mathbb{C}$ and $f^{(j)}_k \in C^\infty_c(M)$, with all sums arbitrary but finite. Due to (1.48), if $\omega\colon \mathcal{A}(\boldsymbol{M}) \to \mathbb{C}$ is a state, its action on a generic element of $\mathcal{A}(\boldsymbol{M})$

[11] As already observed, the term $c_{(0)}\mathbb{1}$ can be omitted since it is a special case of $\sum_{i_1,i_2} c^{i_1 i_2}_{(2)}\phi(f^{(2)}_{i_1})\phi(f^{(2)}_{i_2})$ in view of the commutation relations.

is known as soon as the full class of the so-called n-**point functions** of ω are known. We mean the maps:

$$C_c^\infty(M) \times \cdots \times C_c^\infty(M) \ni (f_1, \ldots, f_n) \ \mapsto \ \omega(\phi(f_1) \cdots \phi(f_n)) \stackrel{\text{def}}{=} \omega_n(f_1, \ldots, f_n)$$

At this point, the multilinear functionals $\omega_n(f_1, \ldots, f_n)$ are not yet forced to satisfy any continuity properties (in fact we have not even discussed any topologies on $\mathcal{A}(\boldsymbol{M})$ and how the states should respect it). However, in the sequel we will also deal with cases where ω_n is continuous in the usual test function topology on $\mathcal{D}(M) := C_0^\infty(M) + iC_0^\infty(M)$, after having naturally extended the considered multilinear functionals to complex functions. Then, by the Schwartz kernel theorem [44], we can write, as it is anyway customary, the n-point function in terms of its distributional kernel:

$$\omega_n(f_1, \ldots, f_n) = \int_{\boldsymbol{M}^n} \omega_n(x_1, \ldots, x_n) f_1(x_1) \cdots f_n(x_n) \, \mathrm{dvol}_{\boldsymbol{M}^n} \, .$$

It is worth stressing that a choice of a family of multilinear functionals ω_n – or also a family of corresponding integral kernels ω_n if any – $n = 1, 2, \ldots$, extends by linearity and the rule $\omega(\mathbb{1}) := 1$ to a normalized linear functional on all of $\mathcal{A}(\boldsymbol{M})$. However, this functional generally does *not* determine a state, because the positivity requirement $\omega(a^*a) \geq 0$ may not be valid. Nevertheless, if two states have the same set of n-point functions they necessarily coincide in view of (1.48).

Remark 1.55. As defined above, the n-point functions $\omega_n(f_1, \ldots, f_n)$ need not be symmetric in their arguments. However, they do satisfy some relations upon permutation of the arguments. The reason is that the products $\phi(f_1) \cdots \phi(f_n)$ and $\phi(f_{\sigma(1)}) \cdots \phi(f_{\sigma(n)})$, for any permutation $\sigma : \{1, \ldots, n\} \to \{1, \ldots, n\}$, are not completely independent in $\mathcal{A}(\boldsymbol{M})$. It is easy to see that the CCR $*$-algebra is **filtered**, namely that $\mathcal{A}(\boldsymbol{M}) = \bigcup_{n=0}^\infty \mathcal{A}_n(\boldsymbol{M})$, where each linear subspace $\mathcal{A}_n(\boldsymbol{M})$ consists of linear combinations of $\mathbb{1}$ and products of no more than n generators $\phi(f)$, $f \in C_0^\infty(M)$. The product $\phi(f_1) \cdots \phi(f_n)$ belongs to $\mathcal{A}_n(\boldsymbol{M})$, as does $\phi(f_{\sigma(1)}) \cdots \phi(f_{\sigma(n)})$. The commutation relation $[\phi(f), \phi(g)] = iE(f,g)\mathbb{1}$ then implies that the product $\phi(f_1) \cdots \phi(f_n)$ and the same product with any two f_i's swapped, hence also $\phi(f_{\sigma(1)}) \cdots \phi(f_{\sigma(n)})$ for any permutation σ, coincide "up to lower order terms," or more precisely coincide in the quotient $\mathcal{A}_n(\boldsymbol{M})/\mathcal{A}_{n-1}(\boldsymbol{M})$. Thus, without loss of generality, the coefficients $c_{(n)}^{i_1 \cdots i_n}$ in (1.48) can be taken to be, for instance, fully symmetric in their indices. So, in order to fully specify a state, it would be sufficient to specify only the fully symmetric part of each n-point function $\omega_n(f_1, \ldots, f_n)$. ∎

There are some further elementary technical properties of ω_2 and E that we list below. Item (b) will be useful when defining *Gaussian states.*

Proposition 1.56. *Consider a state $\omega : \mathcal{A}(\boldsymbol{M}) \to \mathbb{C}$ and define $P := \Box_{\boldsymbol{M}} + V$. The* **two-point function***, ω_2, enjoys the following properties*

(a) *for* $f, g \in C_c^\infty(M)$*:*

$$\omega_2(Pf, g) = \omega_2(f, Pg) = 0\,, \tag{1.49}$$

$$\omega_2(f, g) - \omega_2(g, f) = iE(f, g)\,, \tag{1.50}$$

$$\omega_2(f, g) = \overline{\omega_2(g, f)}\,, \tag{1.51}$$

$$Im(\omega_2(f, g)) = \frac{1}{2}E(f, g)\,, \quad Re(\omega_2(f, g)) = \frac{1}{2}\left(\omega_2(f, g) + \omega_2(g, f)\right)\,, \tag{1.52}$$

$$\frac{1}{4}|E(f, g)|^2 \leq \omega_2(f, f)\omega_2(g, g)\,. \tag{1.53}$$

(b) $\mu : \mathsf{Sol} \times \mathsf{Sol} \to \mathbb{R}$ *such that*

$$\mu(\psi, \psi') := Re(\omega_2(f, f')) \quad \text{where } \psi, \psi' \in Sol \text{ and } f, f' \in C_c^\infty(M) \text{ satisfy } \psi = Ef,\ \psi' = Ef'$$

is a well-defined real scalar product on Sol*.*

Proof. (a) The first identity trivially arises from $\omega_2(Pf, g) = \omega(\phi(Pf)\phi(g)) = 0$ and $\omega_2(f, Pg) = \omega(\phi(f)\phi(Pg)) = 0$ in view of the definition of $\phi(h)$. Next,

$$\omega_2(f, g) - \omega_2(g, f) = \omega([\phi(f), \phi(g)]) = \omega(iE(f, g)\mathbb{1}) = iE(f, g)\omega(\mathbb{1}) = iE(f, g)\,.$$

To go on, observe that, from the GNS construction and $\pi_\omega(\phi(f)) = \pi_\omega(\phi(f)^*) \subset \pi_\omega(\phi(f))^\dagger$,

$$\omega_2(f, g) = \langle\Psi_\omega|\hat{\phi}_\omega(f)\hat{\phi}_\omega(f)\Psi_\omega\rangle = \langle\hat{\phi}_\omega(f)\Psi_\omega|\hat{\phi}_\omega(f)\Psi_\omega\rangle = \overline{\langle\hat{\phi}_\omega(f)\Psi_\omega|\hat{\phi}_\omega(f)\Psi_\omega\rangle} = \overline{\omega_2(g, f)}$$

where $\hat{\phi}_\omega(h) := \pi_\omega(\phi(f))$. At this juncture, the first identity in (1.52) then follows immediately since $E(f, g)$ is real and the second is obvious.
Using the GNS representation again and the Cauchy-Schwartz inequality, we find that

$$|\omega_2(f, g)| = |\langle\hat{\phi}_\omega(f)\Psi_\omega|\hat{\phi}_\omega(f)\Psi_\omega\rangle| \leq |\langle\hat{\phi}_\omega(f)\Psi_\omega|\hat{\phi}_\omega(f)\Psi_\omega\rangle|^{1/2}\,|\langle\hat{\phi}_\omega(g)\Psi_\omega|\hat{\phi}_\omega(g)\Psi_\omega\rangle|^{1/2}$$

namely

$$|\omega_2(f, g)|^2 \leq \omega_2(f, f)\omega_2(g, g)\,.$$

So that, in particular

$$|Im(\omega_2(f, g))|^2 \leq \omega_2(f, f)\omega_2(g, g)$$

and thus, due to (1.52), we end up with (1.53).
(b) First of all, due to (1.49), $\omega(f, g)$ only depends on the associated $\psi_f, \psi_g \in \mathsf{Sol}$ due to Proposition 1.38. By direct inspection, noticing that $f \mapsto \psi_f$ is linear, one sees that μ is bilinear and symmetric for the second identity in (1.52). In summary, $\mu : \mathsf{Sol} \times \mathsf{Sol} \to \mathbb{R}$ is a well-defined symmetric bilinear form. It also holds $\mu(\psi, \psi) = \omega_2(f, f) \geq 0$. What remains to be proved is that $\mu(\psi, \psi) = 0$ implies $\psi = 0$. If $\mu(\psi, \psi) = 0$, (1.53) yields $E(g, f) = 0$ for every $g \in C_c^\infty(M)$. At this juncture (1.15) and Lemma 3.66 imply $f = 0$ and thus $\psi = Ef = 0$ as wanted. $\square$

1.4.2 Quasifree states, also known as Gaussian states

This section is devoted to examine the most elementary relevant facts about quasifree states on $\mathcal{A}(\boldsymbol{M})$ and their representations. We start with the basic definition.

Definition 1.57. [Quasifree states] An algebraic state $\omega : \mathcal{A}(\boldsymbol{M}) \to \mathbb{C}$ is said to be **quasifree** or, equivalently, **Gaussian** if its n-point functions agree with the so-called **Wick procedure**, in other words they satisfy the following pair of requirements for all choices of $f_k \in C_c^\infty(M)$,

$$\omega_n(f_1, \ldots, f_n) = 0 \qquad \text{for } n = 1, 3, 5, \ldots; \tag{1.54}$$

$$\omega_n(f_1, \ldots, f_n) = \sum_{\text{partitions}} \omega_2(f_{i_1}, f_{i_2}) \cdots \omega_2(f_{i_{n-1}}, f_{i_n}), \quad \text{for } n = 2, 4, 6, \ldots. \tag{1.55}$$

For the case of n even, the *partitions* refers to the class of all possible decomposition of set $\{1, 2, \ldots, n\}$ into $n/2$ pairwise disjoint subsets of 2 elements

$$\{i_1, i_2\}, \{i_3, i_4\} \ldots \{i_{n-1}, i_n\}$$

with $i_{2k-1} < i_{2k}$ for $k = 1, 2, \ldots, n/2$. ■

We will prove later that quasifree states exist in a generic curved spacetime for a minimally coupled massive scalar field, i.e., $P := \Box_{\boldsymbol{M}} + m^2$, for a constant $m^2 > 0$. Instead we intend to clarify here the structure of the GNS representation of quasifree states, proving that it is a so-called *Bosonic Fock representation*. This Hilbert space structure is constructed upon an initial Hilbert space called the *one-particle Hilbert space*. Next section concerns that basic structure from an abstract point of view.

1.4.3 One-particle structure

We know that $\mathcal{A}(\boldsymbol{M})$ is actually isomorphic to a CCR $*$-algebra constructed over a symplectic space like $\mathcal{A}(\mathsf{Sol}, \sigma)$. As a consequence, assigning a state on the former is the same as assigning a state on the latter. We can therefore assume a very general perspective, where we deal with a generic $\mathcal{A}(V, \tau)$.

The so-called *one-particle Hilbert space* is constructed out of a generic CCR algebra $\mathcal{A}(V, \tau)$ when a *real* scalar product μ is defined on the real vector space V. The one-particle space is the first non-trivial building block necessary to construct the GNS representation of a quasifree state when $\mathcal{A}(V, \tau) = \mathcal{A}(\mathsf{Sol}, \sigma)$.

Proposition 1.58. [One-particle structure] *Consider a symplectic vector space (V, τ). The following facts are valid.*

(a) *If a real scalar product $\mu : V \times V \to \mathbb{R}$ satisfies*

$$\frac{1}{4}|\tau(x, y)|^2 \leq \mu(x, x)\mu(y, y) \quad \forall x, y \in V \tag{1.56}$$

then there exists a pair (K,H)*, called* **one-particle structure** *associated to* (V,τ,μ) *where* H *is a complex Hilbert space and* $K\colon V\to H$ *is a map satisfying*

(i) K *is* $\mathbb{R}$ *linear and* $\overline{K(V)+i\mathsf{K}(V)}=\mathsf{H}$ *(though* $\mathsf{K}(V)$*, as a real subspace of* H*, need not be dense by itself),*

(ii) $\langle \mathsf{K}x|\mathsf{K}y\rangle=\mu(x,y)+\frac{i}{2}\tau(x,y)$ *for all* $x,y\in V$*.*

K *satisfying (i) and (ii) is necessarily injective.*

(b) *A pair* $(\mathsf{H}',\mathsf{K}')$ *satisfies (i) and (ii) in (a) if and only if there is complex Hilbert space isomorphism* $S:\mathsf{H}\to\mathsf{H}'$ *with* $S\mathsf{K}=\mathsf{K}'$*.*

(c) *If* (K,H) *is as in (a), then* $\mathsf{K}(V)$ *is dense in* H *if and only if*

$$\mu(x,x)=\sup_{V\ni y\neq x}\frac{1}{4}\frac{|\tau(x,y)|^2}{\mu(y,y)}\,,\quad \forall x\in V\,. \tag{1.57}$$

Proof. We follow here the proof of Proposition 3.1 in [48] with obvious re-adaptations.
(a) First of all we observe that K, if any, is injective since (ii) implies $||\mathsf{K}x||^2=\mu(x,x)$ and $\mu(x,x)=0$ implies $x=0$ since μ is a scalar product.
Let us move on to the existence issue. We can complete V with respect to the norm $||\cdot||_\mu:=\sqrt{\mu(\cdot,\cdot)}$ to the real Hilbert space $(\mathcal{R},\langle\cdot|\cdot\rangle_{\mathcal{R}})$ which therefore admits V as dense subspace. An easy application of the Riesz lemma to inequality (1.56), together with the standard extension procedure of bounded operators on a dense domain, imply that there exists a unique bounded operator $A:\mathcal{R}\to\mathcal{R}$ such that:

$$\frac{1}{2}\tau(\phi_1,\phi_2)=\langle\phi_1|A\phi_2\rangle_{\mathcal{R}}\,,\quad\forall\phi_1,\phi_2\in V\,.$$

Since σ is antisymmetric, we also have $A^\dagger=-A$. Inequality (1.56) now implies

$$|\langle\psi|A\phi\rangle_{\mathcal{R}}|\leq||\psi||_{\mathcal{R}}||\phi||_{\mathcal{R}}\,,\quad\forall\psi,\phi\in\mathcal{R}.$$

In turn, using $\psi=A\phi$, we obtain $||A\phi||_{\mathcal{R}}\leq||\phi||_{\mathcal{R}}$. We observe *en passant* here that the validity of (1.57) implies

$$||\phi||_{\mathcal{R}}=\sup_{V\ni\psi\neq0}\frac{|\langle\phi|A\psi\rangle_{\mathcal{R}}|}{||\psi||_{\mathcal{R}}}=\frac{|\langle A\phi|\psi\rangle_{\mathcal{R}}|}{||\psi||_{\mathcal{R}}}=||A\phi||_{\mathcal{R}}\,,\quad\forall\phi\in V.$$

By density $||A\phi||_{\mathcal{R}}=||\phi||_{\mathcal{R}}$ for every $\phi\in\mathcal{R}$ so that A is injective. However, in the general case A may have a non-trivial kernel. If the dimension of this kernel is finite and odd, we add an extra dimension by defining $\hat{\mathcal{R}}:=\mathcal{R}\oplus\mathbb{R}$ and defining $\hat{A}:=A\oplus0$. Otherwise $\hat{\mathcal{R}}:=\mathcal{R}$ and $\hat{A}:=A$ in the following. Next, we convert the real Hilbert space $\hat{R}$ to a complex Hilbert space $\mathcal{H}$ an operator J on $\hat{\mathcal{R}}$ such that $[J,\hat{A}]=0$, $J^\dagger=-J$, $J^2=-I$ and $J|\hat{A}|=\hat{A}$ – where $|\hat{A}|:=\sqrt{\hat{A}^\dagger\hat{A}}$ denotes the operator. To obtain such a J we decompose

$$\hat{\mathcal{R}}=(Ker\hat{A})^\perp\oplus Ker\hat{A}\,,$$

and – relative to this decomposition – set

$$J := U \oplus j \ ,$$

where U is the partial isometry in the polar decomposition $\hat{A} = U|\hat{A}|$ and $j : Ker\hat{A} \to Ker\hat{A}$ is any operator satisfying $j^\dagger = j$ and $j^2 = I$. (Such a j is guaranteed to exist since, by construction, the dimension of $Ker\hat{A}$ either is even or infinite.) Then J satisfies the required properties, and $\hat{\mathcal{R}}$ may now be made into a complex Hilbert space $\hat{\mathcal{H}}$ by defining for all $\phi_1, \phi_2, \phi \in \hat{\mathcal{R}}$

$$\begin{aligned} \langle \phi_1 | \phi_2 \rangle_{\hat{\mathcal{H}}} &:= \langle \phi_1 | \phi_2 \rangle_{\hat{\mathcal{R}}} + i \langle \phi_1 | J \phi_2 \rangle_{\hat{\mathcal{R}}} \\ i\phi &:= -J\phi \ . \end{aligned}$$

Since $[J, \hat{A}] = 0$ and $\hat{A}^\dagger = -\hat{A}$, we see that $i\hat{A}$ is self-adjoint on $\hat{\mathcal{H}}$, and that $|\hat{A}|$ on $\hat{\mathcal{H}}$ is the same map as $|\hat{A}|$ on $\hat{\mathcal{R}}$. One can easily construct a complex conjugation C on $\hat{\mathcal{H}}$ which satisfies $[C, |\hat{A}|] = 0$. (In particular, using the multiplication operator version (see, e.g., [61]) of the spectral theorem, C can be chosen as the ordinary complex conjugation in the L^2 space where $|\hat{A}|$ is a multiplicative operator.) Next we define $\mathcal{H}' := \hat{\mathcal{H}} \oplus \hat{\mathcal{H}}$ and define the map $\mathsf{K} : V \to \mathcal{H}'$ by

$$\mathsf{K}\phi := \sqrt{\frac{1}{2}(|\hat{A}| + I)}\phi \oplus C\sqrt{\frac{1}{2}(I - |\hat{A}|)}\phi \ .$$

Note that this formula simplifies considerably in the case where (1.57) holds, since in that case. $\hat{A} = A$ is isometric as previously stressed and thus $|\hat{A}| = I$.
Finally define

$$\mathsf{H} := \overline{Ran(\mathsf{K}) + iRan(\mathsf{K})} \quad \text{in } \mathcal{H}' \ .$$

It can be easily verified that (K, H) thus defined satisfies all of the conditions of the proposition, and thus existence is proven.
(b) If an isomorphism $S : \mathsf{H} \to \mathsf{H}'$ for $(\mathsf{H}', \mathsf{K}')$ as in (b) exists then $(\mathsf{H}', \mathsf{K}')$ satisfies (i) and (ii) in (a) trivially. Let us prove the converse fact and suppose that $(\mathsf{H}', \mathsf{K}')$ satisfies (i) and (ii) in (a). Since K and K' are injective, we can define a $\mathbb{R}$-linear map $S_0 : \mathsf{K}(V) \to \mathsf{K}'(V)$ by imposing

$$S_0 \mathsf{K} x := \mathsf{K}' x \ , \quad \forall x \in V \ .$$

The map S_0 is trivially isometric because $||S_0 \mathsf{K} x||^2_{H'} = \mu(x, x) = ||\mathsf{K} x||^2$ so that it is also injective, but is also surjective since the inverse map $S'_0 : \mathsf{K}'(V) \to \mathsf{K}(V)$ is nothing but

$$S'_0 \mathsf{K}' x := \mathsf{K} x \ , \quad \forall x \in V \ .$$

Observe that the polarization identity proves that, since S_0 is isometric, it also preserves the scalar products. We can now apply the following lemma (Lemma 5.1 in [47]) for $M := \mathsf{K}(V)$ and $M' := \mathsf{K}'(V)$.

Lemma 1.59. *Let H, H' be a pair of complex Hilbert spaces and let $M \subset \mathsf{H}$, $M' \subset \mathsf{H}'$ a pair of real subspaces such that $M + iM$ is dense in H and $M' + iM'$ is dense in H'. If $S_0 : M \to M$*

is a bijective linear map such that $\langle S_0 x|S_0 y\rangle_{\mathsf{H}'} = \langle x|y\rangle_{\mathsf{H}}$ for every $x, y \in M$, then S_0 extends to a unique complex Hilbert space isomorphism $S : \mathsf{H} \to \mathsf{H}'$.

$S : \mathsf{H} \to \mathsf{H}'$ satisfies the statement in (b).
(c) (ii) in (a) implies the identity

$$1 - \frac{1}{2}\frac{\tau(x,y)}{\sqrt{\mu(x,x)}\sqrt{\mu(y,y)}} = \frac{1}{2}\left|\left|\frac{iKx}{||Kx||} - \frac{Ky}{||Ky||}\right|\right|^2 \quad \forall x, y \in V\,.$$

just by expanding the right-hand side and taking (ii) into account. As a consequence

$$\frac{1}{4}\frac{|\tau(x,y)|^2}{\mu(y,y)} = \left|1 - \frac{1}{2}\left|\left|\frac{i\mathsf{K}x}{||\mathsf{K}x||} - \frac{\mathsf{K}y}{||\mathsf{K}y||}\right|\right|^2\right|^2 \mu(x,x) \quad \forall x, y \in V\,. \tag{1.58}$$

If identity (1.57) is true for a given non-vanishing $x \in V$, since (1.56) is valid, there must be a sequence $V \ni y_n$ such that $\frac{1}{4}\frac{|\tau(x,y_n)|^2}{\mu(y_n,y_n)} \to \mu(x,x)$. This sequence must be satisfy

$$||i\mathsf{K}x - \mathsf{K}z_n|| \to 0 \quad \text{for } n \to +\infty \text{ and } z_n := ||\mathsf{K}x||\tfrac{y_n}{||\mathsf{K}y_n||} \in V.$$

This fact easily implies that every vector in the dense complex subspace $\mathsf{K}(V) + i\mathsf{K}(V)$ can be approximated with arbitrary precision in the norm topology by using vectors of $\mathsf{K}(V)$. Therefore $\mathsf{K}(V)$ is dense in H. Suppose *vice versa* that $\mathsf{K}(V)$ is dense in H. Therefore, if $x \in V$ and $Kx \neq 0$ (the other case is trivial), there must be a sequence $y_n \in V$ such that

$$||i\mathsf{K}x - \mathsf{K}y_n|| \to 0$$

In particular $||\mathsf{K}y_n|| \to ||\mathsf{K}x||$, so that

$$\left|\left|i\frac{\mathsf{K}x}{||\mathsf{K}x||} - \frac{\mathsf{K}y_n}{||\mathsf{K}y_n||}\right|\right| \to 0$$

is true. This fact proves (1.57) when taking (1.58) and (1.56) into account. □

1.4.4 The Fock space structure of quasifree states

As we are about discussing, quasifree states are all induced by the real scalar produts on $\mathcal{A}(\mathsf{\mathbf{Sol}}, \sigma)$ which satisfies a certain inequality corresponding to the analogue satisfied by the-two point function of every state. In addition, the GNS Hilbert space of a quasifree state is a *Bosonic Fock space* [10]. We recall the basic definition and properties of this type of structure for the reader.

Let us consider a complex Hilbert space $(\mathsf{H}, \langle\cdot|\cdot\rangle)$ and its **algebraic tensor product** of n copies of it:

$$\mathsf{H}^{\otimes_A n} := \mathsf{H} \otimes_A \cdots (\text{n times}) \cdots \otimes_A \mathsf{H}\,.$$

The elements of this space are, by definition, *finite* linear combinations of elementary tensor products

$$u_1 \otimes \cdots \otimes u_n\,, \quad \text{with } u_k \in \mathsf{H} \text{ if } k = 1, \ldots, n\,.$$

The **Hilbert tensor product** of n copies of H is indicated by

$$\mathsf{H}^{\otimes n} := \mathsf{H} \otimes \cdots (\text{n times}) \cdots \otimes \mathsf{H}$$

and is defined [61] as the Hilbert completion of the algebraic tensor product with respect to the Hermitian scalar product uniquely induced by

$$\langle u_1 \otimes \cdots \otimes u_n | v_1 \otimes \cdots \otimes v_n \rangle := \prod_{j=1}^{n} \langle u_j | v_j \rangle \quad u_j, u_j \in \mathsf{H}\,.$$

Remark 1.60. Note that, with this procedure, if $N \subset \mathsf{H}$ is a Hilbert basis of H, then $\{u_1 \otimes \cdots \otimes u_n \mid u_k \in N, \quad k = 1, \ldots, n\}$ is a Hilbert basis of $\mathsf{H}^{\otimes n}$. ■

Let $\mathcal{P}_n$ be the **permutation group of n elements** , that is the group of all the bijective maps $\sigma : \{1, \ldots, n\} \to \{1, \ldots, n\}$ with respect to the composition of functions. These maps are $n!$ as is well known. There exists an operator $S_n \in \mathfrak{B}(\mathsf{H}^{n\otimes})$ completely defined by the following requirement (extending it by linearity and finally taking its continuous extension to the whole $\mathsf{H}^{\otimes n}$)

$$S_n(u_1 \otimes \cdots \otimes u_n) := \frac{1}{n!} \sum_{\sigma \in \mathcal{P}_n} u_{\sigma(1)} \otimes \cdots \otimes u_{\sigma(n)}\,, \tag{1.59}$$

From (1.59) and extending the result by linearity and continuity, it easy to see that

$$S_n = S_n^\dagger\,, \quad S_n S_n = S_n\,.$$

As a consequence, S_n is an orthogonal projector. The closed subspace of $\mathsf{H}^{\otimes n}$

$$S^n \mathsf{H} := S_n(\mathsf{H}^{\otimes n})\,, \tag{1.60}$$

is said the space of the **symmetric n-vectors**. By definition $S^0\mathsf{H} := \mathsf{H}^{\otimes 0} := \mathbb{C}$.

If $\{(\mathsf{H}_k, \langle\cdot|\cdot\rangle_k\}_{k\in\mathbb{N}}$ is a countable family of Hilbert spaces[12], the **Hilbert sum** of them

$$\bigoplus_{n\in\mathbb{N}} \mathsf{H}_n$$

is [61] the Hilbert space obtained as the completion of the vector space of the sequences

$$\oplus_{n\in\mathbb{N}} u_n := (u_0, u_1, \ldots u_k, \ldots)\,, \quad u_j \in \mathsf{H}_j \tag{1.61}$$

[12] Countability is not necessary actually.

with a finite (but arbitrary large) number of non-vanishing components $u_k \in \mathsf{H}_k$, with respect to the Hermitian scalar product

$$\langle \oplus_{n\in\mathbb{N}} u_n | \oplus_{n\in\mathbb{N}} v_n \rangle := \sum_{n\in\mathbb{N}} \langle u_n | v_n \rangle_n \,.$$

Note that the addends H_k are pairwise orthogonal closed subspaces of the Hilbert sum, this obviously implies in particular that the sum is *direct*.

Definition 1.61. [Bosonic Fock space] If H is a complex Hilbert space, the **Bosonic Fock space** – also called **symmetric Fock space** – generated by H is the Hilbert sum

$$\mathcal{F}_+(\mathsf{H}) := \bigoplus_{n=0}^{+\infty} S^n \mathsf{H} \,. \tag{1.62}$$

Furthermore

(a) H is called the **one-particle subspace** of $\mathcal{F}_+(\mathsf{H})$.

(b) $\Psi_0 := 1 \in \mathbb{C} = S^0\mathsf{H}$ is called the **vacuum vector** of the Fock space.

(c) A n**-particle vector** Ψ_n is a vector of the form $\Psi_n = S_n(u_1 \otimes \cdots \otimes u_n) \in S^n\mathsf{H}$.

(d) The **finite particle-number space** is the dense subspace $\mathcal{F} \subset \mathcal{F}_+(\mathsf{H})$ made of finite linear combinations of n-particle vectors with arbitrary values $n = 0, 1, \ldots$. ■

The symmetric Fock space is equipped with a pair of operators of utmost relevance in Quantum Field Theory but also in Quantum Statistical Mechanics [10, 11]. To present the definition we need a couple of auxiliary operators.

(i) For $x \in \mathsf{H}$ and $n = 0, 1, \ldots$, the linear operator $A^+(x) : \mathsf{H}^{\otimes_A n} \to \mathsf{H}^{\otimes_A (n+1)}$ is defined as the unique linear extension of

$$A^+(x)(u_1 \otimes \cdots \otimes u_n) := \sqrt{n+1}\,(x \otimes u_1 \otimes \cdots \otimes u_n) \,. \tag{1.63}$$

(ii) For $x \in \mathsf{H}$ and $n = 1, 2, \ldots$, the linear operator $A(x) : \mathsf{H}^{\otimes_A n} \to \mathsf{H}^{\otimes_A (n-1)}$ is defined as the unique linear extension of

$$A(x)(u_1 \otimes \cdots \otimes u_n) := \sqrt{n}\,\langle x | u_n \rangle\,(u_1 \otimes \cdots \otimes u_{n-1}) \,. \tag{1.64}$$

With these definitions we can move on to define the *creation* and *annihilation operators*. These are nothing but a symmetrized version of $A^+(x)$ and $A(x)$.

Definition 1.62. [Creation and annihilation operators] Let us consider the symmetric Fock space $\mathcal{F}_+(\mathsf{H})$ built upon the one-particle space H. If $x \in \mathsf{H}$, the following operators are defined.

(a) The **creation operator** is the operator

$$a^+(x) : \mathcal{F} \to \mathcal{F}_+(\mathsf{H})$$

defined as the unique linear extension of

$$a^+(x) : S^n\mathsf{H} \ni S_n(u_1 \otimes \cdots \otimes u_n) \mapsto S_{n+1}A^+(x)S_n(u_1 \otimes \cdots \otimes u_n) \in S^{n+1}\mathsf{H} \tag{1.65}$$

for $n = 0, 1, \ldots$.

(b) The **annihilation operator** is the operator

$$a(x) : \mathcal{F} \to \mathcal{F}_+(\mathsf{H})$$

defined as the unique linear extension of

$$a(x) : S^n\mathsf{H} \ni S_n(u_1 \otimes \cdots \otimes u_n) \mapsto S_{n-1}A(x)S_n(u_1 \otimes \cdots \otimes u_n) \in S^{n-1}\mathsf{H} \tag{1.66}$$

for $n = 1, 2, \ldots$. By definition $a(x)\restriction_{S^0\mathsf{H}} = 0$. ■

Remark 1.63.

(1) Notice that $\mathsf{H} \ni x \mapsto a(x)$ is antilinear whereas $\mathsf{H} \ni x \mapsto a^+(x)$ is linear.

(2) It holds in particular

$$a(x)\Psi_0 = 0 \quad \forall x \in \mathsf{H}\,. \tag{1.67}$$

This identity plays a crucial role in many proofs. ■

The elementary properties of $a(x)$ and $a^+(x)$ are listed in the following proposition.

Proposition 1.64. *The creation and annihilation operators $a(x)^+$ and $a(x)$ in the symmetric Fock space $\mathcal{F}_+(\mathsf{H})$ enjoy the following properties.*

(a) *The common dense domain $\mathcal{F}$ is invariant:*

$$a(x)(\mathcal{F}) \subset \mathcal{F} \quad \textit{and} \quad a^+(x)(\mathcal{F}) \subset \mathcal{F}\,, \quad \textit{for every } x \in \mathsf{H}.$$

(b) *It holds*

$$a^+(x_1)\cdots a^+(x_n)\Psi_0 = \sqrt{n!}\, S_n(x_1 \otimes \cdots \otimes x_n)$$

so that, in particular,

$$\mathcal{F} = \textit{Span}_{\mathbb{C}}\{a^+(x_1)\cdots a^+(x_n)\Psi_0 \mid \textit{where } x_1, \ldots, x_n \in \mathsf{H} \textit{ and } n = 0, 1, 2, \ldots\}\,.$$

(c) *Each of $a(x)$ and $a^*(x)$ is a restriction of the adjoint of the other:*

$$a(x) \subset (a^+(x))^\dagger \quad \textit{and} \quad a^+(x) \subset (a(x))^\dagger \quad \textit{for every } x \in \mathsf{H}. \tag{1.68}$$

In other words

$$\langle\Psi|a(x)\Phi\rangle = \langle a^+(x)\Psi|\Phi\rangle \quad \textit{and} \quad \langle\Psi|a^+(x)\Phi\rangle = \langle a(x)\Psi|\Phi\rangle \quad \textit{if } \Psi, \Phi \in \mathcal{F} \textit{ and } x \in \mathsf{H}. \tag{1.69}$$

(d) *The* **Bosonic commutation relations** *are valid*

$$[a(x), a(y)] = [a^+(x), a^+(y)] = 0\,, \quad [a(x), a^+(y)] = \langle x|y\rangle I\restriction_{\mathcal{F}} \quad \text{if } x, y \in \mathsf{H}. \tag{1.70}$$

(e) *If* $x \in \mathsf{H}$ *and* $\chi_n \in S^n\mathsf{H} \cap \mathcal{F}$ *(not necessarily of the form* $S_n(u_1 \otimes \cdots \otimes u_n)$*)*

$$||a(x)\chi_n|| \leq \sqrt{n+1}||x||||\chi_n||\,, \quad ||a^+(x)\chi_n|| \leq \sqrt{n+1}||x||||\chi_n||\,. \tag{1.71}$$

Proof. Everything follows per direct inspection form Definition 1.62. For detailed proofs see [11]. □

Theorem 1.65. [Quasifree states and their Fock representations] *Consider the* $*$*-algebra* $\mathcal{A}(\boldsymbol{M})$ *associated to a real scalar KG field. Suppose that* μ *is a real scalar product on* **Sol** *which verifies* (1.56) *with respect to its symplectic form* σ*:*

$$\frac{1}{4}|\sigma(\psi, \psi')|^2 \leq \mu(\psi, \psi)\mu(\psi', \psi') \quad \forall \psi, \psi' \in \textbf{Sol}\,.$$

The following hold.
(a) *There exists a state* ω *on* $\mathcal{A}(\boldsymbol{M})$ *such that*

$$\omega_2(f, g) = \mu(Ef, Eg) + \frac{i}{2}E(f, g)\,, \quad \forall f, g \in C_c^\infty(M)\,. \tag{1.72}$$

(b) *The GNS structure* $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ *consists of the following:*

(i) $\mathcal{H}_\omega = \mathcal{F}_+(\mathsf{H})$ *referring to the one-particle structure* (K, H) *of* μ *in Proposition 1.58;*

(ii) $\Psi_\omega = \Psi_0$ *the vacuum vector of the Fock space;*

(iii) $\mathcal{D}_\omega = \mathcal{F}_\omega \subset \mathcal{F}$*, where*

$$\mathcal{F}_\omega := Span_{\mathbb{C}}\left\{a^+(KEf_1)\cdots a^+(KEf_n)\Psi_0 \mid f_1, \ldots, f_n \in C_0^\infty(M) \text{ and } n = 0, 1, 2, \ldots.\right\}\,. \tag{1.73}$$

(iv) π_ω *is uniquely determined by*

$$\pi_\omega(\phi(f)) := \hat{\phi}_\omega(f) := a(KEf)\restriction_{\mathcal{F}_\omega} + a^+(KEf)\restriction_{\mathcal{F}_\omega} \quad \forall f \in C_c^\infty(M)\,. \tag{1.74}$$

(c) ω *is quasifree.*

(d) ω *is regular, meaning that* $\hat{\phi}_\omega(f)$ *is essentially self-adjoint on* $\mathcal{D}_\omega$*.*

Proof. (a) and (b). As a preliminary step of the proof we construct the generators of the GNS representation of the state ω we shall define later. To this end, taking the properties of the creation and annihilation operators into account as stated in Proposition 1.64, we start with the family of operators

$$a(\mathsf{K}\psi) + \ a^+(\mathsf{K}\psi) : \mathcal{F} \to \mathcal{F}_+(\mathsf{H}) \quad \forall \psi \in \textbf{\textsf{Sol}}\,,$$

and we define

$$\hat{\Phi}_\omega(\psi) := a(\mathsf{K}\psi)\restriction_{\mathcal{F}_\omega} + a^+(\mathsf{K}\psi)\restriction_{\mathcal{F}_\omega} \ . \tag{1.75}$$

It is clear that, due to the very definition of a and a^+, $\mathcal{F}_\omega$ is an invariant space for all operators $\hat{\Phi}_\omega(\psi) \in \mathscr{L}(\mathcal{F}_\omega)$. These operators satisfy the relations for the generators of $\mathcal{A}(\textbf{\textsf{Sol}}, \sigma)$ (isomorphic $\mathcal{A}(\boldsymbol{M})$ stated in Definition 1.46 for the symplectic space $(\textbf{\textsf{Sol}}, \sigma)$: $\mathbb{R}$-linearity, Hermiticity, Commutation Relations. The first one is trivially valid because $a(\mathsf{K}\psi)$ and $a^+(\mathsf{K}\psi)$ are $\mathbb{R}$ linear in $\psi = \mathsf{K}Ef$ and, in turn, $\mathbf{K}$ and is $\mathbb{R}$-linear. Regarding the commutation relations of the operators, (a) Proposition 1.64 yields

$$[\hat{\Phi}_\omega(\psi), \hat{\Phi}_\omega(\psi')] = (\langle \mathsf{K}\psi|\mathsf{K}\psi'\rangle - \langle \mathsf{K}\psi'|\mathsf{K}\psi\rangle)I\restriction_{\mathcal{F}_\omega} = i\sigma(\psi, \psi')I\restriction_{\mathcal{F}_\omega}\,,$$

where we also used (ii) (a) Proposition 1.58. Let us pass to the Hermiticity condition. Due to (c) of the same proposition, we also have that

$$\langle \Psi|\hat{\Phi}_\omega(\psi)\Phi\rangle = \langle \hat{\Phi}_\omega(\psi)\Psi|\Phi\rangle \quad \forall \Psi, \Phi \in \mathcal{F}_\omega\,.$$

We shall prove below that $\mathcal{F}_\omega$ is dense in $\mathcal{F}_+(\mathsf{H})$. As a consequence

$$\hat{\Phi}_\omega(\psi) = \hat{\Phi}_\omega(\psi)^\dagger\restriction_{\mathcal{F}_\omega}\,, \tag{1.76}$$

which is the wanted Hermiticity condition when interpreting $\hat{\Phi}_\omega(\psi)$ as the image of a representation of $\Phi(\psi) \in \mathcal{A}(\textbf{\textsf{Sol}}, \sigma)$.

Lemma 1.66. *$\mathcal{F}_\omega$ is dense in $\mathcal{F}_+(\mathsf{H})$ and furthermore*

$$\mathcal{F}_\omega = \mathit{Span}_\mathbb{C}\left\{\hat{\Phi}_\omega(\psi_1)\ldots\hat{\Phi}_\omega(\psi_n)\Psi_0 \mid \psi_1, \ldots, \psi_n \in \textbf{\textsf{Sol}} \text{ with } n = 0, 1, 2, \ldots\right\}. \tag{1.77}$$

More precisely,

$$\mathit{Span}_\mathbb{C}\left\{\hat{\Phi}_\omega(\psi_k)\cdots\hat{\Phi}_\omega(\psi_1)\Psi_0 \mid \psi_1, \ldots, \psi_k \in \textbf{\textsf{Sol}},\ k = 0, 1, \ldots, n\right\}$$

$$= \mathit{Span}_\mathbb{C}\left\{a^+(\mathsf{K}\psi'_k)\cdots a^+(\mathsf{K}\psi'_1)\Psi_0 \mid \psi'_1, \ldots, \psi'_k \in \textbf{\textsf{Sol}},\ k = 0, 1, \ldots, n\right\}$$

for $n = 0, 1, \ldots$.

Proof. In view of the Fock space structure, it is sufficient to prove that $\mathcal{F}_\omega \cap S^n\mathsf{H}$ is dense in $S^n\mathsf{H}$ for every $n = 0, 1, \ldots$. The thesis is true in the obvious case $n = 0$. We prove that it holds for every n using an inductive argument. Suppose that $\mathcal{F}_\omega \cap S^n\mathsf{H}$ is dense in $S^n\mathsf{H}$ and we want to prove that it happens for $n+1$ as well. If $\Psi_n = a^+(x_1)\cdots a^+(x_n)\Psi_0$ and $x \in \mathsf{H}$, consider $\chi_n \in \mathcal{F}_\omega \cap S^n\mathsf{H}$ and $\psi, \psi' \in \textbf{\textsf{Sol}}$. Exploiting (1.71), we have the inequality, where $(a^+_{\mathsf{K}\psi} + ia^+_{\mathsf{K}\psi'})\chi_n \in \mathcal{F}_\omega \cap S^{n+1}\mathsf{H}$ by construction,

$$||(a^+_{\mathsf{K}\psi} + ia^+_{\mathsf{K}\psi'})\chi_n - a^+_x\Psi_n|| \leq ||a^+_{\mathsf{K}\psi+i\mathsf{K}\psi'-x}\chi_n|| + ||a^+_x(\Psi_n - \chi_n)||$$

$$\leq \sqrt{n+1}\left(||\mathsf{K}\psi + i\mathsf{K}\psi' - x||||\chi_n|| + ||x||||\Psi_n - \chi_n||\right).$$

Since $\mathsf{K}(\textbf{\textsf{Sol}}) + i\mathsf{K}(\textbf{\textsf{Sol}})$ is dense in H and by inductive hypothesis $||\Psi_n - \chi_n||$ can be made arbitrarily small by suitably choosing $\chi_n \in \mathcal{F}_\omega \cap S^n\mathsf{H}$, we conclude that every vector $a^+_x\Psi_n \in S^{n+1}\mathsf{H}$ can be approximated with arbitrary precision by vectors in $\mathcal{F}_\omega \cap S^{n+1}\mathsf{H}$. Since the finite span of vectors $a^+_x\Psi_n \in S^{n+1}\mathsf{H}$ is dense in $\mathcal{F}_\omega \cap S^{n+1}\mathsf{H}$ (according to (b) Proposition 1.64), we have established that $\mathcal{F}_\omega \cap S^{n+1}\mathsf{H}$ is dense in $S^{n+1}\mathsf{H}$ and thus $\mathcal{F}_\omega$ is dense in $\mathcal{F}_+(\mathsf{H})$.
The proof of the second statement is again of inductive nature. We intend to prove that

$$\mathrm{Span}_{\mathbb{C}}\left\{a^+(\mathsf{K}\psi'_k)\cdots a^+(\mathsf{K}\psi'_1)\Psi_0 \mid \psi'_1, \ldots, \psi'_k \in \textbf{\textsf{Sol}},\, k = 0, 1, \ldots, n\right\}$$

$$= \mathrm{Span}_{\mathbb{C}}\left\{\hat{\Phi}_\omega(\psi_k)\cdots\hat{\Phi}_\omega(\psi_1)\Psi_0 \mid \psi_1, \ldots, \psi_k \in \textbf{\textsf{Sol}},\, k = 0, 1, \ldots, n\right\}$$

for $n = 0, 1, 2, \ldots$. The identity is evidently valid for $n = 0, 1$ so that we pass to prove that, if it is true for $n-1$, then it must be valid for n. Just in view of the definition of $\hat{\Phi}_\omega(\psi)$ the inclusion hold

$$\mathrm{Span}_{\mathbb{C}}\left\{\hat{\Phi}_\omega(\psi_k)\cdots\hat{\Phi}_\omega(\psi_1)\Psi_0 \mid \psi_1, \ldots, \psi_k \in \textbf{\textsf{Sol}},\, k = 0, 1, \ldots, n\right\}$$

$$\subset \mathrm{Span}_{\mathbb{C}}\left\{a^+(\mathsf{K}\psi'_k)\cdots a^+(\mathsf{K}\psi'_1)\Psi_0 \mid \psi'_1, \ldots, \psi'_k \in \textbf{\textsf{Sol}},\, k = 0, 1, \ldots, n\right\}$$

for every n. We want to prove the converse inclusion. The inductive hypothis gives

$$a^+(\mathsf{K}\psi'_{n-1})\cdots a^+(\mathsf{K}\psi'_1)\Psi_0 = C_0\Psi_0 + \cdots + \sum_{i_1,\ldots,i_{n-1}} C_{i_1\cdots i_{n-1}}\hat{\Phi}_\omega(\psi_{i_{n-1}})\ldots\hat{\Phi}_\omega(\psi_{i_1})\Psi_0$$

where only a finite number of coefficients $C_{i_1\ldots i_k}$ does not vanish. Since $a^+(\mathsf{K}\psi'_n) = \hat{\Phi}_\omega(\psi'_{i_n}) - a(\mathsf{K}\psi'_n)$, the identity holds

$$a^+(\mathsf{K}\psi'_n)a^+(\mathsf{K}\psi'_{n-1})\cdots a^+(\mathsf{K}\psi'_1)\Psi_0 =$$

$$\hat{\Phi}_\omega(\psi'_{i_n})\Psi_0 + \cdots + \sum_{i_1,\ldots,i_{n-1}} C_{i_1\cdots i_{n-1}}\hat{\Phi}_\omega(\psi'_{i_n})\hat{\Phi}_\omega(\psi_{i_{n-1}})\ldots\hat{\Phi}_\omega(\psi_{i_1})\Psi_0$$

$$+0 + \cdots - \sum_{i_1,\ldots,i_{n-1}} C_{i_1\cdots i_{n-1}}a(\mathsf{K}\psi'_n)\hat{\Phi}_\omega(\psi_{i_{n-1}})\ldots\hat{\Phi}_\omega(\psi_{i_1})\Psi_0\,.$$

The first line in the right hand side belongs to

$$\mathrm{Span}_{\mathbb{C}}\left\{\hat{\Phi}_\omega(\psi_k)\cdots\hat{\Phi}_\omega(\psi_1)\Psi_0 \mid \psi_1, \ldots, \psi_k \in \textbf{\textsf{Sol}},\, k = 0, 1, \ldots, n\right\}$$

as wanted. The second line is made of vectors in spaces $S^m\mathsf{H}$ with $m \leq n-1$, thus our inductive hypothesis can be applied and we conclude that it belongs to

$$\mathrm{Span}_{\mathbb{C}}\left\{\hat{\Phi}_\omega(\psi_k)\cdots\hat{\Phi}_\omega(\psi_1)\Psi_0 \mid \psi_1,\ldots,\psi_k \in \mathsf{Sol},\ k=0,1,\ldots,n-1\right\}.$$

In summary, we established that the vector $a^+(\mathsf{K}\psi'_n)a^+(\mathsf{K}\psi'_{n-1})\cdots a^+(\mathsf{K}\psi'_1)\Psi_0$ necessarily belongs to

$$\mathrm{Span}_{\mathbb{C}}\left\{\hat{\Phi}_\omega(\psi_k)\cdots\hat{\Phi}_\omega(\psi_1)\Psi_0 \mid \psi_1,\ldots,\psi_k \in \mathsf{Sol},\ k=0,1,\ldots,n\right\}$$

proving the thesis. $\square$

We are in a position to prove (a) and (b). First of all consider the unital $*$-algebra of operators $\mathcal{F}_\omega \to \mathcal{F}_\omega$

$$\mathcal{B} := \mathrm{Span}_{\mathbb{C}}\left\{I\restriction_{\mathcal{F}_\omega}, \hat{\Phi}_\omega(\psi_1)\ldots\hat{\Phi}_\omega(\psi_n) \mid \psi_1,\ldots,\psi_n \in \mathsf{Sol} \text{ with } n=1,2,\ldots\right\}$$

which we re-write in terms of the field operators $\hat{\Phi}_\omega(\psi)$ labeled by elements of Sol:

$$\mathcal{B} := \mathrm{Span}_{\mathbb{C}}\left\{I\restriction_{\mathcal{F}_\omega}, \hat{\Phi}_\omega(\psi_1)\ldots\hat{\Phi}_\omega(\psi_n) \mid \psi_1,\ldots,\psi_n \in \mathsf{Sol} \text{ with } n=1,2,\ldots\right\}$$

$\mathcal{F}_\omega$ is a dense invariant domain in common for all these operators and the $*$ operation is here defined as $a^* := a^\dagger\restriction_{\mathcal{F}_\omega}$. According to the universal property of $\mathcal{A}(\boldsymbol{M},\sigma)$ stated in Definition 1.8, the map

$$\mathcal{A}(\boldsymbol{M},\sigma) \ni \Phi(\psi) \mapsto \hat{\Phi}_\omega(\psi)$$

extends to a $*$-algebra homomorphism (which is also injective due to Corollary 1.51 and surjective in view of the fact that operators $\hat{\Phi}_\omega(\psi)$ are generators of $\mathcal{B}$). In summary we have a $*$-representation $\pi^\omega : \mathcal{A}(\mathsf{Sol},\sigma) \to \mathscr{L}(\mathcal{F}_\omega)$ such that

$$\pi^\omega(\Phi(\psi)) = \hat{\Phi}_\omega(\psi) \quad \forall \psi \in \mathsf{Sol}\,. \tag{1.78}$$

If we define

$$\omega(a) := \langle \Psi_0 | \pi^\omega(a)\Psi_0\rangle\,, \quad \forall a \in \mathcal{A}(\mathsf{Sol},\sigma) \tag{1.79}$$

the map $\mathcal{A}(\mathsf{Sol},\sigma) \ni a \mapsto \omega(a)$ is linear, positive and normalized and thus it defines a state on $\mathcal{A}(\mathsf{Sol},\sigma)$. On the other hand, the quadruple $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega) := (\mathcal{F}_+(\mathsf{H}), \mathcal{F}_\omega, \pi^\omega, \Psi_0)$ satisfies the requirements for a GNS structure of the state ω according to the discussion above. To conclude, since $\mathcal{A}(\boldsymbol{M})$ is isomorphic to $\mathcal{A}(\mathsf{Sol},\sigma)$ according to (c) Proposition 1.49, the $*$ isomorphism being uniquely determined by $\phi(f) \mapsto \Phi(Ef)$ if $f \in C_c^\infty(M)$, the above GNS representation, written in terms of generators $\phi(f)$ satisfies all conditions in (b). The two-point function ω_2 satisfies (1.72). Indeed using the fact that (H,K) is the one particle structure of $\mathcal{F}_+(\mathsf{H})$ and taking (1.20) into account:

$$\omega_2(f,g) = \langle \Psi_0 | \hat{\phi}_\omega(\mathsf{K}Ef)\hat{\phi}_\omega(\mathsf{K}Eg)\Psi_0\rangle = \langle a^+(\mathsf{K}Ef)\Psi_0 | a^+(\mathsf{K}Eg)\Psi_0\rangle = \langle \mathsf{K}Ef | \mathsf{K}Eg\rangle$$

$$= \mu(Ef,Eg) + \frac{i}{2}\sigma(Ef,Eg) = \mu(Ef,Eg) + \frac{i}{2}E(f,g)\,.$$

(c) Let us focus on the generic n-point function

$$\omega_n(f_1, \ldots, f_n) = \langle \Psi_0 | (a(\mathsf{K}\psi_1) + \; a^+(\mathsf{K}\psi_1)) \cdots (a(\mathsf{K}\psi_1) + \; a^+(\mathsf{K}\psi_1))\Psi_0 \rangle \;,$$

where $\psi_n := Ef_n$. Expanding the products we end up with a sum of terms

$$\langle \Psi_0 | a^{(+)}(\mathsf{K}\psi_n) \cdots a^{(+)}(\mathsf{K}\psi_1)\Psi_0 \rangle \;.$$

This number is zero unless the number N_+ of operators $a^+(\mathsf{K}\psi_j)$ is equal to the number N_- of operators $a(\mathsf{K}\psi_j)$, and $N_+ + N_- = n$. This is an immediate consequence of the fact that, on the one hand Ψ_0 is orthogonal to every $S^k\mathsf{H}$ with $k > 0$, on the other hand

$$a^{(+)}(\mathsf{K}\psi_n) \cdots a^{(+)}(\mathsf{K}\psi_1)\Psi_0 \in S^{N_+ - N}\mathsf{H} \quad \text{if } N_+ \geq N_-$$

$$a^{(+)}(\mathsf{K}\psi_n) \cdots a^{(+)}(\mathsf{K}\psi_1)\Psi_0 = 0 \quad \text{if } N_+ < N_-$$

in view of the definition of a and a^+. In particular, if n is odd, the condition $N_+ = N_-$ cannot be satisfied. Therefore only the n-point functions with n even may not vanish in agreement with (1.54). We end up to consider only the case of n even and, in the expansion of $\omega_n(f_1, \ldots, f_n)$ only the addends $\langle \Psi_0 | a^{(+)}(\mathsf{K}\psi_n) \cdots a^{(+)}(\mathsf{K}\psi_1)\Psi_0 \rangle$ where the number of elements a^+ is equal to the number of factors a and $\psi_k = Ef_k$. At this juncture one can apply *Wick's contraction theorem* [11] for creation and annihilation operators: the value of a specific term $\langle \Psi_0 | a^{(+)}(\mathsf{K}\psi_n) \cdots a^{(+)}(\mathsf{K}\psi_1)\Psi_0 \rangle$ (with n even and $N_+ = N_-$) is a sum of addends, each addends is the product of all possible contractions between an operator $a(\mathsf{K}\psi_h)$ and an operator $a^+(\mathsf{K}\psi_k)$ in order to exhaust all possible such couples of the specific sequence $a^{(+)}(\mathsf{K}\psi_n) \cdots a^{(+)}(\mathsf{K}\psi_1)$. There are many ways to choose these couples and this arbitrariness gives rise to several addends each made of a product of $n/2$ factors. In each addend, every contraction produces a factor $\langle \Psi_0 | a(\mathsf{K}\psi_h) a^+(\mathsf{K}\psi_k)\Psi_0 \rangle$. With the help of commutation relations (1.70) one finds

$$\langle \Psi_0 | a(\mathsf{K}\psi_h) a^+(\mathsf{K}\psi_k)\Psi_0 \rangle = \langle \Psi_0 | \hat{\phi}_\omega(\mathsf{K}\psi_h) \hat{\phi}_\omega(\mathsf{K}\psi_k)\Psi_0 \rangle = \omega_2(f_h, f_k) \;.$$

Collecting all possible contributions (1.55) arises easily.

(d) The operators $\hat{\phi}_\omega(f) = \hat{\Phi}_\omega(Ef)$ are symmetric because they are Hermitian and defined on the domain $\mathcal{D}_\omega = \mathcal{F}_\omega$ which is dense. The vectors $\chi_n \in S^n\mathsf{H} \cap \mathcal{F}_\omega$ with n arbitrary are analytic for $\hat{\Phi}_\omega(f)$ and thus, since their finite linear combinations are dense in the Hilbert space, $\hat{\phi}_\omega(f) = \hat{\Phi}_\omega(f)$ is essentially self-adjoint as a consequence of *Nelson's criterion* [62]. Analyticity can be established as follows. Taking advantage of (1.71) and (1.75), it is not difficult to prove the estimate

$$||\hat{\Phi}^k_\omega(\psi)\chi_n|| \leq 2^k ||\mathsf{K}\psi||^k \sqrt{(k+n)!}||\chi_n|| \;, \quad \text{if } \chi_n \in S^n\mathsf{H} \cap \mathcal{F}_\omega. \tag{1.80}$$

From it, for $t > 0$

$$\sum_{k=0}^{+\infty} \frac{t^k}{k!} ||\hat{\Phi}^k_\omega(\psi)\chi_n|| \leq ||\chi_n|| \sum_{k=0}^{+\infty} (2||\mathsf{K}\psi||t)^k \frac{\sqrt{(k+n)!}}{k!} < +\infty$$

since the convergence radius of the last power series is $+\infty$ as it easy arises from the Stirling approximation, the claim follows. $\square$

To close the loop, we prove that, not only there are quasifree states constructed out of real scalar products $\mu : \mathsf{Sol} \times \mathsf{Sol} \to \mathbb{R}$ as in Theorem 1.65, but every quasifree state ω is constructed with that procedure if μ is defined by ω_2 as in (b) Proposition 1.56.

Proposition 1.67. *Suppose that $\omega : \mathcal{A}(\boldsymbol{M}) \to \mathbb{C}$ is a quasifree state according to the general Defintion 1.57. Then ω coincides with the quasifree state constructed out of the real scalar product $\mu(\psi, \psi') := Re(\omega_2(f_\psi, f_{\psi'}))$ where $\psi = Ef_\psi$ and $\psi' = Ef_{\psi'}$ with $\psi, \psi' \in \mathsf{Sol}$.*

Proof. The bilinear map μ is a well-defined real scalar product on Sol as established by (b) Proposition 1.56. Inequality (1.53) in (a) of the same proposition proves that (1.56) is satisfied for $\tau = \sigma$. Let ω_μ be the quasifree state on $\mathcal{A}(\boldsymbol{M})$ associated to μ according to Theorem 1.65. By construction ω and ω_μ have the same n-functions due to the very definition of quasifree state and the fact that the 2-point functions coincide by construction. Hence $\omega = \omega_\mu$. □

Remark 1.68. The proof of Proposition 1.67 more generally proves that every state ω defines an associated quasifree state ω_G out of its 2-point function ω_2. It holds $\omega_G = \omega$ if and only if ω is quasifree. ■

1.4.5 Quasifree pure states

We pass to study conditions which assure that a quasifree state ω on $\mathcal{A}(\boldsymbol{M})$ is pure. To tackle this issue we need some preliminary results valid for a generic Bosonic Fock space $\mathcal{F}_+(\mathsf{H})$.

Definition 1.69. Consider a Bosonic Fock space $\mathcal{F}_+(\mathsf{H})$. The **Bosonic field operator** associated to $x \in \mathsf{H}$ is

$$F(x) := a(x) + a^+(x) : \mathcal{F} \to \mathcal{F}_+(\mathsf{H}) \tag{1.81}$$

The dense subspace $\mathcal{F} \subset \mathcal{F}_+(\mathsf{H})$ being defined in (d) Definition 1.61. ■

These operators admit $\mathcal{F}$ as common invariant and dense domain and are symmetric (all that according to the properties in Proposition 1.64 of a and a^+).
Using linearity of $a^\dagger(x)$ and antilinearity of $a(x)$ in the variable $x \in \mathsf{H}$, one easily finds

$$a(x) = \frac{1}{2}(F(x) - iF(ix)) , \quad a^+(x) = \frac{1}{2}(F(x) + iF(ix)) . \tag{1.82}$$

Lemma 1.70. *In the Bosonic Fock space $\mathcal{F}_+(\mathsf{H})$ the operator $F(x)$ is essentially selfadjoint for every $x \in \mathsf{H}$.*

Proof. Use the same argument used in the proof of (d) Theorem 1.65: the vectors $\Phi_n \in S^{n+1}\mathsf{H} \cap \mathcal{F}$, for $n = 0, 1, \ldots$, are analytic for $F(x)$ and their finite span is dense. □

Another technical fact needs.

Lemma 1.71. *In the Bosonic Fock space $\mathfrak{F}_+(\mathsf{H})$ with zero-particle vector Ψ_0,*

$$Span_{\mathbb{C}}\{F(x_k)\cdots F(x_1)\Psi_0 \mid x_1,\ldots,x_k \in \mathsf{H},\ k=0,1,\ldots,n\}$$

$$= Span_{\mathbb{C}}\left\{a^+(x'_k)\cdots a^+(x'_1)\Psi_0 \mid x'_1,\ldots,x'_k \in \mathsf{H},\ k=0,1,\ldots,n\right\}$$

for $n = 0,1,\ldots$.

Proof. Easily follows from (1.81) and (1.82). □

These facts have an important consequence for the CCR algebra $\mathcal{A}(\mathsf{H},\tau)$, where H is viewed as a real vector space equipped with the weakly non-degenerate (real) symplectic form $\tau : \mathsf{H}\times\mathsf{H} \to \mathbb{R}$ defined as

$$\tau(x,y) := 2Im(\langle x|y\rangle)\,, \forall x,y \in \mathsf{H}\,. \tag{1.83}$$

Notice that τ is weakly non degenerate, since $Im\langle x|y\rangle = 0$ for every $y \in \mathsf{H}$ implies $||x||^2 = Im\langle x|ix\rangle = 0$. According to the universal property of $\mathcal{A}(\mathsf{H},\tau)$ stated in Definition 1.8, this unital $*$ algebra is concretely represented by the unique (necessarily faithful) $*$ algebra representation $\pi_\mathsf{H} : \mathcal{A}(\mathsf{H},\tau) \to \mathscr{L}(\mathfrak{F})$ on $\mathfrak{F}_+(\mathsf{H})$ which satisfies $\pi_\mathsf{H}(\Phi(x)) := F(x)$ for $x \in \mathsf{H}$. At this juncture, the following lemma is valid.

Lemma 1.72. *The $*$ representation $\pi_\mathsf{H} : \mathcal{A}(\mathsf{H},\tau) \to \mathscr{L}(\mathfrak{F})$ is weakly irreducible. More strongly, if $A \in \mathfrak{B}(\mathfrak{F}_+(\mathsf{H}))$ satisfies*

$$\langle \Phi'_m|AF(x)\Phi_n\rangle = \langle F(x)\Phi'_m|A\Phi_n\rangle \quad \textit{for every } \Phi_n \in S^{n+1}\mathsf{H}\cap\mathfrak{F},\ \Phi'_m \in S^m\mathsf{H}\cap\mathfrak{F},\ n,m=0,1,\ldots$$

then $A = cI$ for some $c \in \mathbb{C}$.

Proof. Suppose that $A \in \pi'_{\mathsf{H}w}$, or more weakly $\langle \Phi'_m|AF(x)\Phi_n\rangle = \langle F(x)\Phi'_m|A\Phi_n\rangle$ for every $\Phi_n \in S^n\mathsf{H}\cap\mathfrak{F}$, $\Phi'_m \in S^m\mathsf{H}\cap\mathfrak{F}$, $n,m = 0,1,\ldots$. The identities (1.82) and (anti) linearity imply $\langle \Phi'_m|Aa^+(x)\Phi_n\rangle = \langle a(x)\Phi'_m|A\Phi_n\rangle$. At this juncture, iterating this identity and taking advantage of Lemma 1.71, we also have

$$\langle a^+(x_m)\cdots a^+(x_1)\Phi_0|Aa^+(y_n)\cdots a^+(y_1)\Phi_0\rangle = \langle a(y_1)\cdots a(y_n)a^+(x_m)\cdots a^+(x_1)\Phi_0|A\Phi_0\rangle$$

$$= \langle \Phi_0|A\Phi_0\rangle\langle a(y_1)\cdots a(y_n)a^+(x_m)\cdots a^+(x_1)\Phi_0|\Phi_0\rangle\,.$$

The last identity is, in fact, trivially true if $n \neq m$ because both sides vanish separately. In the case $n = m$, we have necessarily

$$a(y_1)\cdots a(y_n)a^+(x_n)\cdots a^+(x_1)\Phi_0 = c_{x_1,\ldots,x_n y_1,\ldots,y_n}\Psi_0$$

for some constant $c_{x_1,\ldots,x_n y_1,\ldots,y_n} \in \mathbb{C}$ and the considered identity still holds for

$$c_{x_1,\ldots,x_n y_1,\ldots,y_n} = \langle a(y_1)\cdots a(y_n)a^+(x_n)\cdots a^+(x_1)\Phi_0|\Phi_0\rangle\,.$$

In summary $A - \langle \Phi_0|A\Phi_0\rangle I \in \mathfrak{B}(\mathfrak{F}_+(\mathsf{H}))$ is zero in a dense set and thus $A = \langle \Phi_0|A\Phi_0\rangle I$. □

We are in a position to state and prove an important result.

Theorem 1.73. *A quasifree state ω induced by the scalar product $\mu : \mathsf{Sol} \times \mathsf{Sol} \to \mathbb{R}$ as in Theorem 1.65 is pure if and only if*

$$\overline{\mathsf{K}(\mathsf{Sol})} = \mathsf{H}\,. \tag{1.84}$$

According to (c) Proposition 1.58, this condition is equivalent to:

$$\mu(\psi,\psi) = \frac{1}{4}\sup_{\phi\neq 0}\frac{|\sigma(\psi,\phi)|^2}{\mu(\phi,\phi)}\,. \tag{1.85}$$

In this case the $*$-algebra representation π_ω is also irreducible.

Proof. Taking Proposition 1.24 into account, it is sufficient to prove that $\overline{\mathsf{K}(\mathsf{Sol})} = \mathsf{H}$ is equivalent to weak irreducibility of π_ω.
Suppose that $\overline{\mathsf{K}(\mathsf{Sol})} = \mathsf{H}$ but π_ω is not weakly irreducible. Then there is $A \in \mathfrak{B}(\mathcal{F}_+(\mathsf{H}))$, not of the form cI, such that $\chi_n \in S^n\mathsf{H}\cap\mathcal{F}$, $\chi'_m \in S^m\mathsf{H}\cap\mathcal{F}$, $n,m = 0,1,\ldots$

$$\langle\chi'_m|A\hat{\Phi}_\omega(\psi)\chi_n\rangle = \langle\hat{\Phi}_\omega(\psi)\chi'_m|A\chi_n\rangle$$

for every $\chi_n \in S^n\mathsf{H}\cap\mathcal{F}_\omega$, $\chi'_m \in S^m\mathsf{H}\cap\mathcal{F}_\omega$, $n,m = 0,1,\ldots$ and $\psi \in \mathsf{Sol}$ in particular. The written identity can be re-phrased to

$$\langle\chi'_m|AF(\mathsf{K}\psi)\chi_n\rangle = \langle F(\mathsf{K}\psi)\chi'_m|A\chi_n\rangle$$

Taking advantage of (1.71), we easily have

$$||F(\mathsf{K}\psi)\chi_n - F(x)\chi_n|| \leq \sqrt{n+1}||\mathsf{K}\chi_n - x||||\chi_n||\,.$$

Since $\mathsf{K}(Sol)$ is dense in H, we conclude that, for every $x \in \mathsf{H}$,

$$\langle A^\dagger\chi'_m|F(x)_0\chi_n\rangle = \langle A^\dagger F(x)_0\chi'_m|\chi_n\rangle\,,$$

where $F(x)_0 := F(x)\restriction_{\mathcal{F}_\omega}$. Observe that $F(x)_0$ is symmetric and the vectors $\chi_n \in S^n\mathsf{H}\cap\mathcal{F}_\omega \subset S^n\mathsf{H}\cap\mathcal{F}$ are analytic of it (as proved in the proof of Lemma 1.72) and their span is dense for Lemma 1.66. Therefore $F(x)_0$ is essentially selfadjoint. Since $F(x)^\dagger$ is a selfadjoint extension of it, we conclude that $F(x)_0^\dagger = F(x)^\dagger$. The above identity can be re-written

$$\langle F(x)_0^\dagger A^\dagger\chi'_m|\chi_n\rangle = \langle A^\dagger F(x)_0\chi'_m|\chi_n\rangle\,,$$

Using density of linear combinations of vectors χ'_n in $S^n\mathsf{H}\cap\mathcal{F}$, the result extends to

$$\langle F(x)_0^\dagger A^\dagger\chi'_m|\Phi_n\rangle = \langle A^\dagger F(x)_0\chi'_m|\Phi_n\rangle\,,$$

for every $\Phi_n \in S^n\mathsf{H}\cap\mathcal{F}$ and $\chi'_m \in S^m\mathsf{H}\cap\mathcal{F}_\omega$. In turn, since $F(x)_0^\dagger = F(x)^\dagger$ is selfadjoint, and Φ_m belongs both to the of $F(x) \subset F(x)^\dagger$,

$$\langle\chi'_m|AF(x)\Phi_n\rangle = \langle F(x)_0\chi'_m|A\Phi_n\rangle\,,$$

for every $\chi'_m \in S^m\mathsf{H} \cap \mathcal{F}_\omega$. This identity finally implies

$$\langle \chi'_m | AF(x)\Phi_n \rangle = \langle \chi'_m | F(x)^\dagger A\Phi_n \rangle \,,$$

and thus, by continuity and density

$$\langle \Phi'_m | AF(x)\Phi_n \rangle = \langle \Phi'_m | F(x)^\dagger A\Phi_n \rangle \,,$$

and finally

$$\langle \Phi'_m | AF(x)\Phi_n \rangle = \langle F(x)\Phi'_m | A\Phi_n \rangle \,,$$

for every $\Phi_n \in S^n\mathsf{H} \cap \mathcal{F}$, $\Phi'_m \in S^m\mathsf{H} \cap \mathcal{F}$, $n, m = 0, 1, \ldots$. Lemma 1.72 implies that $A = cI$ contrarily to the hypothesis. We established that $\overline{\mathsf{K}(\mathbf{Sol})} = \mathsf{H}$ implies that π_ω is weakly irreducible.
To conclude, we now prove that if $\overline{\mathsf{K}(\mathbf{Sol})} \subsetneq \mathsf{H}$ then π_ω is weakly reducible. Under this hypothesis, let $x_0 \in \overline{\mathsf{K}(\mathbf{Sol})}^\perp \setminus \{0\}$ and define the strongly-continuous one-parameter group $A_t := e^{i\overline{F(tx_0)}} = e^{it\overline{F(x_0)}} \in \mathfrak{B}(\mathcal{F}_+(\mathsf{H}))$, $t \in \mathbb{R}$. There must be a value $t_0 \in \mathbb{R} \setminus \{0\}$ such that $A_{t_0} \neq cI$ for $c \in \mathbb{C}$. If this value did not exist,

$$\langle e^{-it\overline{F(x_0)}}\Phi_0 | F(y)\Phi_0 \rangle = \langle \Phi_0 | e^{it\overline{F(x_0)}} F(y)\Phi_0 \rangle = \langle \Phi_0 | F(y) e^{it\overline{F(x_0)}}\Phi_0 \rangle = \langle F(y)\Phi_0 | e^{it\overline{F(x_0)}}\Phi_0 \rangle \,.$$

Stone's theorem would imply $\langle F(x_0)\Phi_0 | F(y)\Phi_0 \rangle = \langle F(y)\Phi_0 | F(x_0)\Phi_0 \rangle$. Namely, $\langle x_0 | y \rangle = \langle y | x_0 \rangle$. Taking $y = ix_0$, we find $x_0 = 0$ that was excluded. Redefining x_0 if necessary, we define $A := e^{iF(x_0)} \neq cI$.
Since $F(\mathsf{K}\psi)\Phi_n$ is analytic for $F(x_0)$, if $\Phi_n \in S^n\mathsf{H} \cap \mathcal{F}$,

$$AF(\mathsf{K}\psi)\Phi_n = e^{i\overline{F(x_0)}}\Phi_n = \sum_{k=0}^{+\infty} \frac{i^k}{k!} F(x_0)^k F(\mathsf{K}\psi)\Phi_n = \sum_{k=0}^{+\infty} F(\mathsf{K}\psi) \frac{i^k}{k!} F(x_0)^k \Phi_n = \overline{F(\mathsf{K}\psi)} A\Phi_n$$

namely

$$AF(\mathsf{K}\psi)\Phi_n = F(\mathsf{K}\psi)^\dagger A\Phi_n \,.$$

Above we used the fact that $F(\mathsf{K}\psi)^\dagger = \overline{F(\mathsf{K}\psi)}$ is trivially closed and

$$F(\mathsf{K}\psi)F(x_0) - F(x_0)F(\mathsf{K}\psi) = i\tau(x_0, \mathsf{K}\psi) = 2iIm\langle \mathsf{K}\psi | x_0 \rangle I\restriction_{\mathcal{F}} = 0 \,.$$

For $\Phi'_m \in S^m\mathsf{H} \cap \mathcal{F}$, we therefore have

$$\langle \Phi'_m | AF(\mathsf{K}\psi)\Phi_n \rangle = \langle F(\mathsf{K}\psi)\Phi'_m | A\Phi_n \rangle \,.$$

The identity can be specialized to

$$\langle \chi'_m | A\hat{\Phi}_\omega(\psi)\chi_n \rangle = \langle \hat{\Phi}_\omega(\psi)\chi'_m | A\chi_n \rangle$$

for every $\chi'_m \in S^m\mathsf{H} \cap \mathcal{F}_\omega$ and $\chi_n \in S^n\mathsf{H} \cap \mathcal{F}_\omega$. Iterating the procedure, replacing χ_n for $\hat{\Phi}_\omega(\psi')\chi_n$ and so on, we end up with

$$\langle \chi'_m | A\hat{\Phi}_\omega(\psi_n) \cdots \hat{\Phi}_\omega(\psi_1)\chi_n \rangle = \langle \hat{\Phi}_\omega(\psi_1) \cdots \hat{\Phi}_\omega(\psi_n)\chi'_m | A\chi_n \rangle$$

and thus

$$\langle \chi' | A\pi_\omega(a)\chi\rangle = \langle \pi_\omega(a)\chi' | A\chi\rangle \,, \quad \text{for every } \chi, \chi' \in \mathcal{D}_\omega = \mathcal{F}_\omega \text{ and } a \in \mathcal{A}(\textsf{Sol}, \sigma).$$

We proved that the weak commutant $\pi'_{\omega w}$ is non trivial and thus the representation is weakly reducible by definition. $\square$

1.4.6 The so-called Minkowski vacuum

In four-dimensional Minkowski spacetime $\boldsymbol{M} := \mathbb{M}$, for $P := \Box_{\mathbb{M}} + m^2$, with $m^2 > 0$ constant, a distinguished real scalar product μ on **Sol** can easily be defined as follows in a Minkowski reference frame with coordinates $(t, \vec{x}) \in \mathbb{R} \times \mathbb{R}^3$. Consider a solution of KG equation $\psi \in$ **Sol**. Let us define the associated function $\phi_\psi \in \mathcal{S}(\mathbb{R}^3)$ (the Schwartz test function space) obtained by the smooth compactly supported Cauchy data of ψ on the Cauchy surface defined by $t = 0$:

$$\phi_\psi(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-i\vec{x}\cdot\vec{k}} \left(\sqrt{\frac{E(\vec{k})}{2}} \psi(0, \vec{x}) + i \frac{1}{\sqrt{2E(\vec{k})}} \frac{\partial \psi}{\partial t}(0, \vec{x}) \right) d\vec{x} \,, \tag{1.86}$$

where $E(\vec{k}) := \sqrt{\vec{k}^2 + m^2}$ (we assume here $m > 0$) physically represents the energy of the particle with wavefunction ψ. With this definition, by standard properties of the Fourier transform, the initial solution ψ can be represented as:

$$\psi(t, \vec{x}) = \int_{\mathbb{R}^3} \frac{\overline{\phi_\psi(\vec{k})} e^{-(i\vec{x}\cdot\vec{k} - itE(\vec{k}))} + \phi_\psi(\vec{k}) e^{i\vec{x}\cdot\vec{k} - itE(\vec{k})}}{(2\pi)^{3/2}\sqrt{2E(\vec{k})}} d\vec{k} \tag{1.87}$$

This integral formula is often called the *decomposition of ψ into modes of positive and negative energy.* In particular, ϕ_ψ is the **positive-energy part** of ψ.

As already stated, since $\psi(0, \cdot)$ and $\frac{\partial \psi}{\partial t}(0, \cdot)$ are smooth and compactly supported (thus of Schwartz type), the associated function ϕ_ψ is of Schwartz type and, in particular, $\phi_\psi \in L^2(\mathbb{R}^3, d\vec{k})$. Therefore

$$\mu_{\mathbb{M}}(\psi, \psi') := Re \int_{\mathbb{R}^3} \overline{\phi_\psi(\vec{k})} \phi_{\psi'}(\vec{k}) d\vec{k} \tag{1.88}$$

is a well-defined real bilinear form on **Sol** that is non negative. If $\langle \cdot | \cdot \rangle$ is the scalar product of $L^2(\mathbb{R}^3, d\vec{k})$, the identity

$$\langle \phi_\psi | \phi_{\psi'} \rangle = \mu(\psi, \psi') + \frac{i}{2} \sigma(\psi, \psi')$$

can be proved immediately out of (1.86) by elementary properties of the Fourier transform. This identity and the Cauchy-Schwarz inequality immediately imply that

$$\frac{1}{4} |\sigma(\psi, \psi')|^2 = |Im(\langle \phi_\psi | \phi_{\psi'} \rangle)|^2 \leq |\langle \phi_\psi | \phi_{\psi'} \rangle|^2 \leq \langle \phi_\psi | \phi_\psi \rangle \langle \phi_{\psi'} | \phi_{\psi'} \rangle = \mu(\psi, \psi)\mu(\psi', \psi') \,,$$

in particular μ is a scalar product on **Sol**, i.e., $\mu(\psi, \psi) = 0$ implies $\mu = 0$ in view of weak non-degenerateness of σ. Furthermore, Proposition 1.58 and Theorem 1.65 entail that there is a one-particle structure $(\mathsf{H}_{\mathbb{M}}, \mathsf{K}_{\mathbb{M}})$ associated to μ and a corresponding quasifree state $\omega_{\mathbb{M}}$. This quasifree state is known as the **Minkowski vacuum**. Up to Hilbert space isomorphisms, the associated one-particle structure $(\mathsf{H}_{\mathbb{M}}, \mathsf{K}_{\mathbb{M}})$ is

$$\mathsf{H}_{\mathbb{M}} = L^2(\mathbb{R}^3, d\vec{k}) \,, \quad \mathsf{K}_{\mathbb{M}} : \textsf{\textbf{Sol}} \ni \psi \mapsto \phi_\psi \in L^2(\mathbb{R}^3, d\vec{k}) \tag{1.89}$$

with ϕ_ψ defined in (1.86). That is because, the following result holds, where we also see that $\omega_{\mathbb{M}}$ is pure.

Proposition 1.74. *Consider the* $\mathbb{R}$*-linear map* $\mathsf{K}_{\mathbb{M}} : \textsf{\textbf{Sol}} \ni \psi \mapsto \phi_\psi \in L^2(\mathbb{R}^3, d\vec{k})$ *where* ϕ_ψ *is defined in (1.86) and* $m > 0$*. Then* $\overline{\mathsf{K}_{\mathbb{M}}(\textsf{\textbf{Sol}})} = L^2(\mathbb{R}^3, d\vec{k})$*. So that,*

- **(a)** *the one-particle structure* $(\mathsf{H}_{\mathbb{M}}, \mathsf{K}_{\mathbb{M}})$ *of Minkowski vacuum* $\omega_{\mathbb{M}}$ *is (1.89);*
- **(b)** $\omega_{\mathbb{M}}$ *is pure.*

Proof. The map $\mathsf{K}_{\mathbb{M}}$ can be rearranged to

$$\sqrt{2E}\phi_\psi = E\mathcal{F}(\psi) + \mathcal{F}(i\pi) \,, \tag{1.90}$$

where ψ and π are *arbitrary* $C_c^\infty(\mathbb{R}^3)$ functions, thus real valued, whereas the function in the left-and side is a Schwartz complex function. We consider the two transformations described by the two integrals separately. We start by observing that $C_c^\infty(\mathbb{R}^3, \mathbb{C})$ is dense in the Schwartz space $\mathcal{S}(\mathbb{R}^3)$ with respect to its natural topology. Since the Fourier transform $\mathcal{F} : \mathcal{S}(\mathbb{R}^3) \to \mathcal{S}(\mathbb{R}^3)$ is a homeomorphism of this space, $\mathcal{F}(C_c^\infty(\mathbb{R}^3, \mathbb{C}))$ is still dense in $C_c^\infty(\mathbb{R}^3, \mathbb{C})$. We consider the two real subspaces

$$\mathcal{S}(\mathbb{R}^3)_\pm := \{f \in \mathcal{S}(\mathbb{R}^3) \mid f(\vec{k}) = \pm\overline{f(-\vec{k})} \,, \ \vec{k} \in \mathbb{R}^3\} \,.$$

The direct decomposition holds $\mathcal{S}(\mathbb{R}^3) = \mathcal{S}(\mathbb{R}^3)_+ + \mathcal{S}(\mathbb{R}^3)_-$ since $f(\vec{k}) = \frac{1}{2}(f(\vec{k}) + \overline{f(-\vec{k})}) + \frac{1}{2}(f(\vec{k}) - \overline{f(-\vec{k})})$. At this juncture, from the elementary properties of the Fourier transform, we have that $\mathcal{F}(C_c^\infty(\mathbb{R}^3))$ is dense in $\mathcal{S}(\mathbb{R}^3)_+$ and $\mathcal{F}(iC_c^\infty(\mathbb{R}^3))$ is dense in $\mathcal{S}(\mathbb{R}^3)_-$. These two spaces are in fact the ranges of the two integral transforms in the right-hand side of (1.90). If $f \in \mathcal{S}(\mathbb{R}^3)_+$, there is a sequence $\mathcal{F}(C_c^\infty(\mathbb{R}^3)) \ni \hat{\psi}_n \to f$ in the Schwartz topology. As a consequence, we also have $E\hat{\psi}_n \to Ef$ in the same topology, where $E := E(\vec{k})$, since the latter smooth function $(m > 0)$ is polynomially bounded. We can finally argue that, if $g \in \mathcal{S}(\mathbb{R}^3)_+$ then $E^{-1}g \in \mathcal{S}(\mathbb{R}^3)_+$ and thus $E\hat{\psi}_n^g \to EE^{-1}g = g$ for a suitable sequence in $\psi_n^g \in \mathcal{F}(C_c^\infty(\mathbb{R}^3))$. Analogously, we have that, if $h \in \mathcal{S}(\mathbb{R}^3)_-$ then $i\hat{\pi}_n^h \to h$ for a suitable sequence $i\pi_n^h \in \mathcal{F}(iC_c^\infty(\mathbb{R}^3))$. To go on, choose $f \in \mathcal{S}(\mathbb{R}^3)$ and decompose it as $f_+ + f_-$ respectively in $\mathcal{S}(\mathbb{R}^3)_+$ and $\mathcal{S}(\mathbb{R}^3)_-$. According to the previous results, there is a sequence $E\hat{\psi}_n + i\hat{\pi}_n \to f$ in the Schwartz topology, where $\pi_n, \psi_n \in C_c^\infty(\mathbb{R}^3)$ and $\hat{\psi}_n = \mathcal{F}(\psi_n)$, $\hat{\pi}_n = \mathcal{F}(\pi_n)$. Consequently also $E^{-1/2}(E\hat{\psi}_n + i\hat{\pi}_n) \to E^{-1/2}f$ in the

Schwartz topology, but as before $E^{-1/2}f$ is a generic function of $\mathcal{S}(\mathbb{R}^3)$. Hence, if $\phi \in \mathcal{S}(\mathbb{R}^3)$, there is a sequence $(E^{1/2}\hat{\psi}_n + iE^{-1/2}\hat{\pi}_n) \to \phi$ in the Schwartz topology. Since the Schwartz space is dense in $L^2(\mathbb{R}^3, d\vec{k})$, the result immediately extends to the case of $\phi \in L^2(\mathbb{R}^3, d\vec{k})$. To conclude, take $\phi \in L^2(\mathbb{R}^3, d\vec{k})$ and assume that $\langle \phi | \mathsf{K}_{\mathbb{M}}\psi\rangle = 0$ for every $\psi \in \mathsf{Sol}$. if we prove that $\phi = 0$ the thesis is established. We have

$$0 = \langle \phi | \mathsf{K}_{\mathbb{M}}(\psi_n)\rangle = \frac{1}{\sqrt{2}}\langle \phi | E^{1/2}\hat{\psi}_n + iE^{-1/2}\hat{\pi}_n\rangle \,,$$

where we can prepare the sequence $\psi_n \in \mathsf{Sol}$ such that $E^{1/2}\hat{\psi}_n + iE^{-1/2}\hat{\pi}_n \to \phi$ in L^2. We conclude that $\phi = 0$ ending the proof because we proved that $\overline{\mathsf{K}_{\mathbb{M}}(\mathsf{Sol}) + i\mathsf{K}_{\mathbb{M}}(\mathsf{Sol})} = \overline{\mathsf{K}_{\mathbb{M}}(\mathsf{Sol})} = L^2(\mathbb{R}^3, d\vec{k})$ so that the uniqueness part of Proposition 1.58 entails that the one-particle structure of Minkowski vacuum is (1.89). The state is pure due to (e) Theorem 1.73. $\square$

Developing further the theory, we find the standard QFT free theory for a real scalar field in Minkowski spacetime. $\mathsf{H}_{\mathbb{M}}$ is the Hilbert space of the states of one particle associated to the field. These particles are called Klein-Gordon particles. These particles are electrically uncharged, their spin is 0, and they have mass m.

Remark 1.75. In spite of the Poincaré non-invariant approach we pursued to construct the above structure, the pictured procedure leads to a Poincaré invariant structure as we shall see later. ■

Let us consider the two-point function $\omega_{\mathbb{M}2} : C_c^\infty(\mathbb{M}) \times C_c^\infty(\mathbb{M}) \to \mathbb{C}$. The integral kernel of $\omega_{\mathbb{M}2}(f, g)$ in this case is a proper distribution of $\mathcal{D}'(\mathbb{R}^4 \times \mathbb{R}^4)$ and reads

$$\omega_{\mathbb{M}2}(x, y) = w\text{-}\lim_{\epsilon \to 0^+} \frac{m^2}{(2\pi)^2} \frac{K_1\left(m\sqrt{(|\vec{x}-\vec{y}|^2 - (t_x - t_y - i\epsilon)^2)}\right)}{m\sqrt{|\vec{x}-\vec{y}|^2 - (t_x - t_y - i\epsilon)^2}} \tag{1.91}$$

where the *weak* limit is understood in the standard distributional sense and the branch cut in the complex plane to uniquely define the analytic functions appearing in (1.91) is assumed to stay along the negative real axis. In view of the definition of quasifree state Definition 1.57, all the n-point functions of $\omega_{\mathbb{M}}$ are distributions of $\mathcal{D}'((\mathbb{R}^4)^n)$.

Another equivalent expression for $\omega_{\mathbb{M}2}(x, y)$ is given in terms of Fourier transformation of distributions,

$$\omega_{\mathbb{M}2}(x, y) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^4} e^{-ip(x-y)}\theta(p^0)\delta(p^2 + m^2)d^4p \,. \tag{1.92}$$

where $px = p^0x^0 - \sum_{j=1}^3 p^jx^j$ is the Minkowski scalar product. The above formula is convenient for showing the following important property of $\omega_{\mathbb{M}2}(x, y)$ when interpreting it as the kernel of a map $C_c^\infty(\mathbb{R}^4; \mathbb{C}) \to \mathcal{D}'(\mathbb{R}^4)$ according to the *Schwartz-kernel theorem*.

Proposition 1.76. *If $f \in C_c^\infty(\mathbb{R}^4, \mathbb{C})$, then $\omega_{\mathbb{M}2}(x, f)$ and $\omega_{\mathbb{M}2}(f, y)$ are smooth.*

Proof. Let $\hat{f}(p) = \int_{\mathbb{R}^4} e^{ipy} f(y)\, d^4y$. Since $f \in C_c^\infty(\mathbb{R}^4, \mathbb{C})$, $\hat{f}$ must be a Schwartz function. Then, since $\omega_{\mathbb{M}2}(f, y) = \overline{\omega_{\mathbb{M}2}(y, f)}$, it is enough to consider

$$\begin{aligned}
\omega_{\mathbb{M}2}(x, f) &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^4} d^4p\, e^{-ipx} \theta(p^0) \delta(p^2 + m^2) \int_{\mathbb{R}^4} d^4y\, f(y) e^{ipy} \\
&= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\vec{k}\, e^{-ip_{\vec{k}}x} \frac{\hat{f}(p_{\vec{k}})}{\sqrt{\vec{k}^2 + m^2}} \,,
\end{aligned}$$

where $p_{\vec{k}} = \left(\sqrt{\vec{k}^2 + m^2}, \vec{k}\right)$. Since $\hat{f}$ is Schwartz, so is the above integrand. It is then easy to see from this integral representation that $\omega_{\mathbb{M}2}(x, f)$ is smooth. □

1.5 Quasifree states in curved spacetime

In this section we prove that every globally hyperbolic spacetime admits quasifree states starting from a simplified case provided by a *stationary* spacetime. We investigate the various implications of this fact. Finally we discuss unitary equivalence of different GNS representations of quasifree states on a given spacetime.

1.5.1 Quasifree states in stationary spacetimes

We start with an important definition.

Definition 1.77. A spacetime $(\boldsymbol{M}, g, \mathfrak{o})$ is said to be **stationary** if it admits a (smooth) future-directed timelike Killing vector ζ. Furthermore

(1) A stationary spacetime $(\boldsymbol{M}, g, \mathfrak{o}, \zeta)$ of dimension $n+1$ is called **static** if, for every $p \in M$, there is a spacelike smooth n-dimensional embedded submanifold normal to ζ in a neighborhood of p.

(1) A static spacetime $(\boldsymbol{M}, g, \mathfrak{o}, \zeta)$ is called **ultrastatic** if $g(\zeta, \zeta) = 1$ everywhere in M. ■

Remark 1.78. If a spacetime admits a timelike smooth vector field, up to a sign, it is future-directed, so that this hypothesis may be omitted. We keep it just for convenience. ■

Reinforcing the hypotheses on ζ we have the following important technical result.

Proposition 1.79. *Let $(\boldsymbol{M}, g, \mathfrak{o}, \zeta)$ be a stationary spacetime of dimension $n+1$ such that*

(i) the spacetime is globally hyperbolic,

(ii) the Killing vector ζ is complete*, i.e., its integral lines have parameter t which ranges in the whole real line.*

If $\Sigma \subset M$ is a spacelike smooth Cauchy surface, then there is a diffeomorphism $\Gamma : \mathbb{R} \times \Sigma \to M$ which satisfies the following facts.

(a) $\frac{\partial}{\partial t}$ *in $\mathbb{R} \times \Sigma$ and ζ in M correspond trough $d\Gamma$. Here $t \in \mathbb{R}$ is the integral parameter of the integral lines of ζ itself with origin at Σ.*

(b) $\Sigma_t := \Gamma(\{t\} \times \Sigma) \subset M$*, is a spacelike smooth Cauchy surface for every $t \in \mathbb{R}$.*

(c) *In every local chart adapted to the product $\mathbb{R} \times \Sigma$ with coordinates $(t, x^1, \ldots, x^n)$, so that $x^1, \ldots, x^n$ are local coordinates on Σ, the metric coefficients satisfy $\frac{\partial g_{ab}}{\partial t} = 0$.*

Proof. (a) and (b). First of all, from (ii), we have that ζ generates a (global!) one-parameter group $\{\chi_t^{(\zeta)}\}_{t\in\mathbb{R}}$ of diffeomorphisms of M. These diffeomorphisms are actually isometries of (M, g) since ζ is Killing. If Σ is a spacelike smooth Cauchy surface of $\boldsymbol{M}$, then every integral line of ζ meets Σ exactly once. Since every event of the spacetime is met by exactly one integral line starting from Σ, where we assume $t = 0$, the map

$$\Gamma : \mathbb{R} \times \Sigma \ni (t, p) \mapsto \chi_t^{(\zeta)}(p) \in M$$

is smooth and bijective and, by construction, $t \in \mathbb{R}$ is the integral parameter of ζ with origin fixed on Σ. We are assuming here the product structure of smooth manifolds on $\mathbb{R} \times \Sigma$. By construction, $\Sigma_t := \Gamma(\{t\} \times \Sigma) = \chi_t^{(\zeta)}(\Sigma)$ is a n-dimensional smooth embedded submanifold of M because $\chi_t^{(\zeta)}$ is a diffeomorphism.. Since $\chi_t^{(\zeta)}$ is an isometry, Σ_t is a spacelike smooth Cauchy surface as Σ is. To conclude, we prove that $d\Gamma_{(t,p)} : T_{(t,p)}(\mathbb{R} \times \Sigma) \to T_{\Gamma(t,p)}M$ is everywhere non singular so that Γ must be a diffeomorphism. By construction $d\Gamma_{(t,p)}$ sends bijectively the n-dimensional tangent space $T_{(t,p)}(\{t\} \times \Sigma)$ to the n-dimensional subspace $T_{(t,\chi_t^{(\zeta)}(p))}\Sigma_t \subset T_{\Gamma(t,p)}M$. On the other hand $d\Gamma_{(t,p)}$ maps the vector $\left.\frac{\partial}{\partial t}\right|_{(t,p)} \in T_{(t,p)}(\{t\} \times \Sigma)$ to $\zeta_{\chi_t^{(\zeta)}(p)} \in T_{\Gamma(t,p)}M$. $\left.\frac{\partial}{\partial t}\right|_{(t,p)}$ is by construction linearly independent from the vectors in $T_{(t,p)}(\{t\} \times \Sigma)$, on the other hand $\zeta_{\chi_t^{(\zeta)}(p)}$ is timelike and thus linearly independent form the vectors in $T_{(t,\chi_t^{(\zeta)}(p))}\Sigma_t \subset T_{\Gamma(t,p)}M$, since they are spacelike. We established that $d\Gamma$ is everywhere one-to-one, i.e., non singular, so that Γ is a diffeomorphism.
(c) In every local chart with coordinates $(t, x^1, \ldots, x^n)$ adapted to this product, so that $x^1, \ldots, x^n$ are local coordinates on Σ, $\chi_\tau^{(\zeta)} : (t, x^1, \ldots, x^n) \mapsto (t + \tau, x^1, \ldots, x^n)$ so that the ζ-Lie derivative $\mathscr{L}_\zeta$ corresponds to the standard t-derivative. Since $\chi_\tau^{(\zeta)}$ is an isometry $\mathscr{L}_\zeta g = 0$, in coordinates, just reads $\frac{\partial g_{ab}}{\partial t} = 0$ proving (c). □

Remark 1.80. An interesting issue is to provide sufficient conditions for that a spacetime decomposed as $\mathbb{R} \times \Sigma$, such that Σ is a spacelike smooth co-dimension 1 submanifold and $\frac{\partial}{\partial t}$ is a timelike Killing vector, where t the natural variable of the factor $\mathbb{R}$, is globally hyperbolic and Σ is a Cauchy surface. Thys type of conditions are discussed in [45] ■

If we add some further technical conditions on ζ and Σ, a natural *pure quasifree* state ω_ζ exists for the Klein-Gordon field ϕ. The idea, originally due to Ashtekar and Magnon [1] (see also Kay in [45] for a similar but technically different approach), is quickly discussed in a more modern approach in [79, §4.3]. It is based on the following overall structure induced by ζ.

Proposition 1.81. *Let $(\boldsymbol{M}, g, \mathfrak{o}, \zeta)$ be a stationary globally hyperbolic spacetime of dimension $n+1$ where ζ is complete. If Σ is a spacelike smooth Cauchy surface. Consider the space* Sol *associated to $P := \Box_{\boldsymbol{M}} + m^2$, for a constant $m^2 \geq 0$ and its complexification*

$$\mathsf{Sol}_{\mathbb{C}} = \mathsf{Sol} + i\mathsf{Sol}\,.$$

The sesquilinear form ($\mathbf{n}_\Sigma$ being the future-oriented unit normal vector to Σ)

$$(\psi|\psi')_T := \int_\Sigma T_{ab}(\overline{\psi}, \psi') n^a_\Sigma \zeta^b \, d\Sigma\,, \quad \psi, \psi' \in \mathsf{Sol}_{\mathbb{C}} \tag{1.93}$$

constructed out of the stress-energy tensor

$$T_{ab}(\overline{\psi}, \psi') := \frac{1}{2}\left(\nabla_a\overline{\psi}\nabla_b\psi' + \nabla_b\overline{\psi}\nabla_a\psi'\right) - \frac{1}{2}g_{ab}\left(\nabla^c\overline{\psi}\nabla_c\psi' - m^2\overline{\psi}\psi'\right) \tag{1.94}$$

satisfies the following properties.

(a) *$(\cdot|\cdot)_T$ does not depend on the choice of the spacelike smooth Cauchy surface Σ.*

(b) *$(\cdot|\cdot)_T$ is invariant under the action on $\mathsf{Sol}_{\mathbb{C}}$ of the one-parameter group of isometries $\chi^{(\zeta)}$ generated by ζ:*
$$(\psi|\psi')_T = (\psi \circ \chi^{(\zeta)}_{-t}|\psi' \circ \chi^{(\zeta)}_{-t})\,, \quad \forall t \in \mathbb{R}\,, \tag{1.95}$$
where $\chi^{(\zeta)}$ leaves $\mathsf{Sol}_{\mathbb{C}}$ invariant as well.

(c) *$(\psi|\psi)_T \geq 0$ for $\psi \in \mathsf{Sol}_{\mathbb{C}}$. Furthermore, $(\cdot|\cdot)_T$ is an Hermitian scalar product on $\mathsf{Sol}_{\mathbb{C}}$ if either $m^2 > 0$, or $m^2 \geq 0$ and Σ is not compact.*

Proof. (a) In view of the Killing equation $\nabla_a\zeta_b + \nabla_b\zeta_a = 0$, the conservation law $\nabla_a T^{ab}(\overline{\psi}, \psi) = 0$, which holds as an immediate consequence of KG equations for ψ and ψ', and the symmetry property $T^{ab}(\overline{\psi}, \psi') = T^{ba}(\overline{\psi}, \psi')$, we have $\nabla_a(T^{ab}(\overline{\psi}, \psi')\zeta_b) = 0$. At this juncture, in view of the known support properties of the solutions ψ and ψ' (see the proof of Theorem 1.36), we can apply the divergence identity in Theorem 3.71 to the divergence-free vector field $J^a := T^{ab}(\overline{\psi}, \psi')\zeta_b$. This should be done for a suitably constructed relatively-compact cylinder in M, with bases contained in the two different spacelike smooth Cauchy surfaces Σ and Σ', proving that the integral of $J^a n_a$ on these two surfaces coincide. Thus establishing that $(\psi|\psi')$ does not depend on the choice of the Cauchy surface.
(b) In our hypotheses, as discussed at the beginning of this section, M is isometric to $\mathbb{R} \times M$ and, under this isometry, in every local chart adapted to the product $(t, x^1, \ldots, x^n)$ where $t \in \mathbb{R}$ is also the integral parameter of ζ, the coefficients of the metric do not depend on t. Furthermore, the action of $\chi^{(\zeta)}$ on smooth functions f defined on $\mathbb{R} \times \Sigma \ni (t, p)$ takes the form $f \circ \chi^{(\zeta)}_{-\tau}(t, p) = f(t - \tau, p)$. Writing down the Klein-Gordon equation with $P = \Box_{\boldsymbol{M}} + m^2$ (where

m^2 is constant!) in local coordinates adapted to the product structure as above, it is immediate to prove that ψ solves the Klein-Gordon equation if and only if $\psi \circ \chi^{(\zeta)}_{-\tau}$ does. Therefore Sol and $\mathsf{Sol}_{\mathbb{C}}$ are invariant under the action of these isometries and we established the second statement in (b). Let us pass to the invariance of the Hermitian form $(\cdot|\cdot)_T$. Using a partition of the unity subordinated to adapted local charts as above to compute the integral in (1.93), taking advantage of the t-independence of the metric coefficients and the action of $\chi^{(\zeta)}$ as illustrated above, we easily obtain that $(\psi \circ \chi^{(\zeta)}_{-t}|\psi' \circ \chi^{(\zeta)}_{-t})_T$ coincides with $(\psi|\psi')_T$ computed on the Cauchy surface $\Sigma_t := \{t\} \times \Sigma$. The required invariance property of $(\cdot|\cdot)_T$ therefore holds due to (a).
(c) Since the form $(\cdot|\cdot)_T : \mathsf{Sol}_{\mathbb{C}} \times \mathsf{Sol}_{\mathbb{C}} \to \mathbb{C}$ is sesquilinear by construction, we have to prove that $(\psi|\psi)_T \geq 0$ and $(\psi|\psi)_T = 0$ implies $\psi = 0$. Take $p \in \Sigma$ and consider the two timelike future-oriented unit vectors $n_+ := \frac{\zeta}{\sqrt{g(\zeta,\zeta)}}$ and $n_- := n_\Sigma$ evaluated at p. We can arrange a local chart around p such that, exactly at p, the metric is represented in canonical form $g_{ab} = \eta_{ab}$ and $n_\pm := \alpha e_0 \pm \beta e_1$. As a matter of fact e_0 is the unit vector parallel to $\frac{\zeta}{\sqrt{g(\zeta,\zeta)}} + n_\Sigma$ and e_1 is the unit vector orthogonal to e_0 and parallel to $\frac{\zeta}{\sqrt{g(\zeta,\zeta)}} - n_\Sigma$. Here $\alpha > 0$ and $\alpha^2 - \beta^2 = 1$, since $n_\pm$ are future-oriented timelike unit vectors as e_0 is. At this juncture observe that, exactly at p,

$$T_{ab}(\overline{\psi},\psi) n^a_\Sigma \zeta^b = \sqrt{g(\zeta,\zeta)} T_{ab}(\overline{\psi},\psi) n^a_+ n^b_- = \sqrt{g(\zeta,\zeta)} \left(\alpha^2 T_{00}(\overline{\psi},\psi) - \beta^2 T_{11}(\overline{\psi},\psi)\right) . \tag{1.96}$$

A direct computation that uses (1.85) proves that

$$T_{00}(\overline{\psi},\psi) = \frac{1}{2}\left[|\partial_0\psi|^2 + |\partial_1\psi|^2 + \left(\sum_{k=2}^{3} |\partial_k\psi|^2 + m^2|\psi|^2\right)\right] \tag{1.97}$$

while

$$T_{11}(\overline{\psi},\psi) = \frac{1}{2}\left[|\partial_0\psi|^2 + |\partial_1\psi|^2 - \left(\sum_{k=2}^{3} |\partial_k\psi|^2 + m^2|\psi|^2\right)\right] .$$

It is now evident that

$$|T_{11}(\overline{\psi},\psi)| \leq T_{00}(\overline{\psi},\psi) \tag{1.98}$$

Furthermore, since $\alpha^2 - \beta^2 = 1$, we also have

$$\frac{T_{ab}(\overline{\psi},\psi)}{\sqrt{g(\zeta,\zeta)}} n^a_\Sigma \zeta^b = \left(\alpha^2 T_{00}(\overline{\psi},\psi) - \beta^2 T_{11}(\overline{\psi},\psi)\right) \geq (\alpha^2 - \beta^2) T_{00}(\overline{\psi},\psi) = T_{00}(\overline{\psi},\psi) \geq 0 .$$

In summary,

$$\frac{T_{ab}(\overline{\psi},\psi)}{\sqrt{g(\zeta,\zeta)}} n^a_\Sigma \zeta^b \geq T_{00}(\overline{\psi},\psi) \geq 0 . \tag{1.99}$$

As a consequence $(\psi|\psi)_T \geq 0$. To conclude, let us consider the case $(\psi|\psi)_T = 0$. Using the fact that the measure on Σ has strictly positive Radon-Nikodym derivative with respect to the Lebesgue measure in local coordinates, one immediately has that $(\psi|\psi) = 0$ implies $T_{ab}(\overline{\psi},\psi) n^a_\Sigma \zeta^b = 0$ at every $p \in \Sigma$. We conclude from (1.99) that $T_{00}(\overline{\psi},\psi) = 0$. (1.97) implies in particular the all derivatives $\partial_a \psi$ vanish everywhere on Σ, and also $\psi = 0$ thereon if $m^2 > 0$. In particular $\nabla_{\mathbf{n}_\Sigma}\psi = 0$ and ψ is constant on Σ (since the derivatives along local coordinates on Σ vanish as well), thus $\psi\restriction_\Sigma = 0$ if Σ is *not* compact because the support of $\psi\restriction_\Sigma$ is compact. In conclusion, in all considered cases, the Cauchy data of $\psi \in \mathsf{Sol}$ are trivial (for both the real and imaginary part of ψ). According to the existence and uniqueness Theorem 3.59 (for the real and imaginary parts of ψ), the only possible solution of $P\psi = 0$ with these Cauchy data is $\psi = 0$. $\square$

To construct a pure state associate to ζ we still need some technical results. First of all, we can complete the complex space $\mathsf{Sol}_{\mathbb{C}}$ with Hermitian scalar product $(\cdot|\cdot)_T$ obtaining a complex Hilbert space H_0. The Killing vector ζ defines an operator

$$\mathsf{Sol}_{\mathbb{C}} \ni \psi \mapsto U_t\psi := \psi \circ \chi_t^{(\zeta)} \tag{1.100}$$

for every choice of $t \in \mathbb{R}$. The physical meaning of U_t is the *time evolution* according to the Killing flow. Conversely U_t represent the *time translation* along the Killing flow.

Evidently U_t is isometric (in view of the previous proposition) and surjective, since U_{-t} is its inverse. As usual, since $\mathsf{Sol}_{\mathbb{C}}$ is dense in H_0, every operator U_t uniquely extends by continuity to a unitary operator we shall indicate with the same symbol. By construction, the family $\{U_t\}_{t\in\mathbb{R}}$ is a one-parameter group of unitary operators on H_0.

Proposition 1.82. *Let $(\boldsymbol{M}, g, \mathfrak{o}, \zeta)$ be a stationary globally hyperbolic spacetime, where ζ is complete, equipped with the Hermitian scalar product $(\cdot|\cdot)_T : \mathsf{Sol}_{\mathbb{C}} \times \mathsf{Sol}_{\mathbb{C}} \to \mathbb{C}$ as in Proposition 1.81. Assume that $m^2 > 0$, or $m^2 \geq 0$ and there is a compact spacelike smooth Cauchy surface Σ.*

In the complex Hilbert space $(\mathsf{H}_T, (\cdot|\cdot)_T)$, obtained by completing $\mathsf{Sol}_{\mathbb{C}}$ with respect to the said scalar product, consider the one-parameter group of unitary operators $U := \{U_t\}_{t\in\mathbb{R}}$ associated to ζ and induced by (1.100). The following holds.

(a) *U is strongly continuous and thus it admits a selfadjoint generator $H : D(H) \to \mathsf{H}_T$ such that $U_t = e^{-itH}$ if $t \in \mathbb{R}$;*

(b) *$\mathsf{Sol}_{\mathbb{C}} \subset D(H)$ is invariant under U and it is a core for H;*

(c) *It holds*

$$H\psi = i\zeta(\psi)\,, \quad \forall \psi \in \mathsf{Sol}_{\mathbb{C}}$$

so that, in particular, $\mathsf{Sol}_{\mathbb{C}}$ is invariant under H as well.

Proof. (a) With the same argument used in the proof of (c) Proposition 1.27, since $\mathsf{Sol}_{\mathbb{C}}$ is dense in H_T, strong continuity is equivalent to

$$(\psi|U_t\psi)_T \to (\psi|\psi)_T \quad \text{if } t \to 0\text{, for every } \psi \in \mathsf{Sol}_{\mathbb{C}}.$$

In other words

$$\int_\Sigma T_{ab}(\overline{\psi}, \psi \circ \chi_t^{(\zeta)}) n_\Sigma^a \zeta^b \, d\Sigma \to \int_\Sigma T_{ab}(\overline{\psi}, \psi) n_\Sigma^a \zeta^b \, d\Sigma \quad \text{if } t \to 0, \text{ for every } \psi \in \mathsf{Sol}_\mathbb{C}. \tag{1.101}$$

This fact is true because, by construction $T_{ab}(\overline{\psi}, \psi \circ \chi_t^{(\zeta)}) \to T_{ab}(\overline{\psi}, \psi)$ pointwise on Σ. Furthermore, taking $t \in [-\epsilon, \epsilon]$ with $\epsilon > 0$, there is a compact $K \subset \Sigma$ which includes the supports of all $\psi \circ \chi_t^{(\zeta)}$ as one easily proves in view of the support properties in M of $\psi \in \mathsf{Sol}_\mathbb{C}$, referred to the region between two Cauchy surfaces $\Sigma_{-\epsilon}$ and Σ_ϵ (adopting the notation of Proposition 1.79 and using the diffeomorphism between M and $\mathbb{R} \times \Sigma$). Therefore there is a constant C such that $|T_{ab}(\overline{\psi}, \psi \circ \chi_t^{(\zeta)})_{(t,p)}| \leq C < +\infty$ for $(t,p) \in [-\epsilon, \epsilon] \times K$ because the considered function is continuous. The dominated convergence theorem, restricting the integration to K, implies the (1.101) is valid since K has finite measure it being compact.
(b) and (c). By construction $\mathsf{Sol}_\mathbb{C}$ is invariant under U, as a consequence of the general theory of strongly continuous groups, $\mathsf{Sol}_\mathbb{C}$ is a core for the selfadjoint generator H of U [62]. With the same argument as before, using coordinates adapted to the product structure $\mathbb{R} \times \Sigma$, so that $\zeta(\psi) = \frac{\partial \psi}{\partial t}$ locally, and the Lagrange theorem, one sees that

$$||it^{-1}(U_t\psi - \psi)) - i\zeta(\psi)||^2 = ||t^{-1}(U_t\psi - \psi)) - \zeta(\psi)||^2$$

$$= \int_\Sigma T_{ab}\left(t^{-1}(\overline{\psi} \circ \chi_t^{(\zeta)} - \overline{\psi}) - \zeta(\overline{\psi}), \overline{\psi} \circ t^{-1}(\psi \circ \chi_t^{(\zeta)} - \psi) - \zeta(\psi)\right) n_\Sigma^a \zeta^b \, d\Sigma \to 0 \quad \text{for } t \to 0.$$

This fact proves (c). $\square$

Proposition 1.83. *With the same hypotheses as in Proposition 1.82, explicitly assuming $m^2 > 0$, define the complexified version of symplectic form (1.22)*

$$\sigma(\overline{\psi}, \psi') := \int_S (\overline{\psi} \nabla_{\boldsymbol{n}_S} \psi' - \psi' \nabla_{\boldsymbol{n}_S} \overline{\psi}) \, dS, \tag{1.102}$$

where S is any spacelike smooth Cauchy surface of $\boldsymbol{M}$ (σ does not depend on this choice). The following holds.

(a) *If*

$$g(\zeta, \zeta) \geq c_1^2 > 0 \quad \textit{uniformly in } M \textit{ for some constant } c_1 \in \mathbb{R} \tag{1.103}$$

and there is a spacelike smooth Cauchy surface Σ such that

$$g(\zeta, \mathbf{n}_\Sigma) \leq c_2 < +\infty \quad \textit{uniformly in } \Sigma \textit{ for some constant } c_2 \in \mathbb{R}, \tag{1.104}$$

then there is a constant $C > 0$ such that

$$|\sigma(\overline{\psi}, \psi')|^2 \leq C(\psi|\psi)_T(\psi'|\psi')_T \quad \forall \psi, \psi' \in \mathsf{Sol}_\mathbb{C}\,. \tag{1.105}$$

(b) *Referring to the Hilbert space* $(\mathsf{H}_T, (\cdot|\cdot)_T)$ *as in Proposition 1.82,*

$$\sigma(\overline{\psi}, H\psi') = -2i(\psi|\psi')_T \quad \forall \psi, \psi' \in \mathsf{Sol}_{\mathbb{C}} \tag{1.106}$$

where H *is the selfadjoint generator of* $\{U_t\}_{t\in\mathbb{R}}$ *as in Proposition 1.82.*

(c) *The spectrum* $\sigma(H)$ *of the selfadjoint operator* H *satisfies*

$$\sigma(H) \subset \mathbb{R} \setminus (-\delta, \delta)$$

for some $\delta > 0$.

(d) *Ran*$(H) = \mathsf{H}_T$ *and the inverse operator of* $H^{-1} : \mathsf{H}_T \to D(H)$ *is a selfadjoint element of* $\mathfrak{B}(\mathsf{H}_T)$.

Remark 1.84. Since ζ and $\mathbf{n}_\Sigma$ are timelike and future directed, the *inverse Cauchy-Schwartz inequality* holds: $g(\zeta, \mathbf{n}_\Sigma)^2 \geq g(\zeta,\zeta)g(\mathbf{n}_\Sigma, \mathbf{n}_\Sigma) = g(\zeta,\zeta)1$. As a consequence the further automatic restrictions are valid $g(\zeta,\zeta) < c_2^2$ (everywhere in M) and $g(\zeta, \mathbf{n}_\Sigma) \geq c_1$ (on Σ). ■

Proof. (a) If Σ is as in the hypothesis, observe that

$$|\sigma(\overline{\psi}, \psi')| \leq \int_\Sigma (|\overline{\psi}\nabla_{\boldsymbol{n}_\Sigma}\psi'| + |\psi'\nabla_{\boldsymbol{n}_\Sigma}\overline{\psi}|)\, d\Sigma.$$

As a consequence of the Cauchy Schwarz inequality,

$$|\sigma(\overline{\psi}, \psi')|^2 \leq \int_\Sigma |\psi|^2\, d\Sigma \int_\Sigma |\nabla_{\boldsymbol{n}_\Sigma}\psi'|^2\, d\Sigma + \int_\Sigma |\psi'|^2\, d\Sigma \int_\Sigma |\nabla_{\boldsymbol{n}_\Sigma}\psi|^2\, d\Sigma\,. \tag{1.107}$$

At this juncture, using $m^2 > 0$, we have the estimate

$$\int_\Sigma |\psi|^2\, d\Sigma = \frac{2c_2}{m^2}\int_\Sigma \frac{g(\zeta, n_\Sigma)}{c_2}\frac{m^2}{2}|\psi|^2\, d\Sigma \leq \frac{2c_2}{m^2}\int_\Sigma \frac{m^2}{2}|\psi|^2\, d\Sigma \leq \frac{2c_2}{m^2}\int_\Sigma T_{ab}(\overline{\psi}, \psi)n_\Sigma^a\zeta^b\, d\Sigma$$

$$= \frac{2c_2}{m^2}(\psi|\psi)_T\,.$$

To estimate the other type of integral in (1.107), we adopt the same coordinate system around $p \in \Sigma$, which is pseudo orthonormal exactly at p, and we use the same notations as in the proof of (c) Proposition 1.81.

$$|\nabla_{\boldsymbol{n}_\Sigma}\psi|^2 = |\nabla_{\mathbf{n}_-}\psi|^2 \leq (|\alpha\partial_0\psi| + |\beta\partial_1\psi|)^2 \leq 2\alpha^2|\partial_0\psi|^2 + 2\beta^2|\partial_1\psi|^2 \leq 2\alpha^2(|\partial_0\psi|^2 + |\partial_1\psi|^2) \leq 4\alpha^2 T_{00}.$$

Taking advantage of (1.99),

$$\int_\Sigma |\nabla_{\boldsymbol{n}_\Sigma}\psi|^2 d\Sigma \leq 4\int_\Sigma \alpha^2 \frac{T_{ab}(\overline{\psi}, \psi)}{\sqrt{g(\zeta,\zeta)}} n_\Sigma^a \zeta^b d\Sigma\,, \tag{1.108}$$

where, from the definition of $n_\pm$,

$$\alpha^2 = \frac{1}{2}\left(1 + \frac{g(\zeta, n_\sigma)}{\sqrt{g(\zeta,\zeta)}}\right) \quad \Rightarrow \frac{4\alpha^2}{\sqrt{g(\zeta,\zeta)}} = 2\frac{1}{\sqrt{g(\zeta,\zeta)}}\left(1 + \frac{g(\zeta, n_\sigma)}{\sqrt{g(\zeta,\zeta)}}\right) \leq \frac{2(c_1+c_2)}{c_1^2}\,.$$

Inserting in (1.108), we have

$$\int_\Sigma |\nabla_{\boldsymbol{n}_\Sigma}\psi|^2 d\Sigma \leq \frac{2(c_1+c_2)}{c_1^2}(\psi|\psi)_T\,.$$

Collectiong everything in (1.107) we have the thesis

$$|\sigma(\overline{\psi}, \psi')|^2 \leq \frac{8c_2}{m^2}\frac{c_1+c_2}{c_1^2}(\psi|\psi)_T(\psi'|\psi')_T\,.$$

Since both sides are independent from the choice of Σ, this estimate holds for every choice of Σ.
(b) Since $H\psi = i\zeta(\psi)$ if $\psi \in \mathsf{Sol}_\mathbb{C}$ and using a trivial complexification procedure, the thesis is equivalent to

$$\sigma(\psi', \zeta(\psi)) = -2(\psi'|\psi)_T\,, \quad \forall \psi, \psi' \in \mathsf{Sol}\,. \tag{1.109}$$

In turn, this identity is equivalent to

$$\sigma(\psi, \zeta(\psi)) = -2(\psi|\psi)_T\,, \quad \forall \psi \in \mathsf{Sol}\,. \tag{1.110}$$

In fact, replacing in (1.110), first ψ for $\psi'+\psi$, and next for ψ for $\psi'-\psi$, using $(\psi|\psi')_T = (\psi'|\psi)_T$ if $\psi', \psi \in \mathsf{Sol}$ as well as $\mathbb{R}$-bilinearity of both sides of (1.109) and antisymmetry of σ, we easily have that (1.109) is valid if (1.110) holds. At this point we prove (1.110) to conclude. Consider $\psi \in \mathsf{Sol}$. A lenghty but elementary computation, where we take advantage of the Killing identity for ζ: $\nabla_a\zeta_b + \nabla_b\zeta_b = 0$, its immediate consequence $\nabla_a\zeta^a = 0$, the fact that $\nabla_a\nabla_b\psi = \nabla_b\nabla_a\psi$, and the Klein-Gordon equation $\nabla_a\nabla^a\psi = -m^2\psi$, shows that

$$\psi n^a\nabla_a(\zeta^b\nabla_b\psi) - (\zeta^b\nabla_b\psi)n^a\nabla_a\psi = -2n^a\zeta^b(\nabla_a\psi)(\nabla_b\psi) + n^a\zeta_a(\nabla_b\psi)\nabla^b\psi - n^a\zeta_a m^2\psi\psi$$
$$+n^a\nabla_b(\psi\zeta^b\nabla_a\psi - \psi\zeta_a\nabla^b\psi)\,.$$

Integrating both sides, we have

$$\sigma(\psi, \zeta(\psi)) = -2(\psi|\psi)_T + \int_\Sigma n_a\nabla_b(\psi\zeta^b\nabla^a\psi - \psi\zeta^a\nabla^b\psi)d\Sigma$$

To evaluate the integral, consider a local chart of $M \equiv \mathbb{R}\times\Sigma$, adapted to this product structure. Let $(t, x^1, \ldots, x^b) = (x^0, x^1, \ldots, x^b)$ be the coordinates of this chart where $x^1, \ldots x^n$ are coordinates on the spacelike smooth Cauchy surface Σ. In components: $n_a = \frac{\delta^0_a}{\sqrt{g^{00}}}$, $d\Sigma = \sqrt{|\det h|}dx^1\cdots dx^n$, where $h := [g_{ab}]_{a,b=1,\ldots,n}\restriction_\Sigma$. At this juncture

$$n_a\nabla_b(\psi\zeta^b\nabla^a\psi - \psi\zeta^a\nabla^b\psi)d\Sigma$$

$$
= \frac{\delta_a^0}{\sqrt{g^{00}}\sqrt{|\det g|}} \left(\frac{\partial}{\partial x^b} \sqrt{|\det g|} (\psi \zeta^b \nabla^a \psi - \psi \zeta^a \nabla^b \psi) \right) \sqrt{|\det h|} dx^1 \cdots dx^n \, .
$$

Cramer's rule gives $\det h = g^{00} \det g$, so that

$$
n_a \nabla_b (\psi \zeta^b \nabla^a \psi - \psi \zeta^a \nabla^b \psi) d\Sigma
$$

$$
= \frac{1}{\sqrt{|\det h|}} \left(\frac{\partial}{\partial x^b} \sqrt{|\det h|} \frac{1}{\sqrt{g^{00}}} (\psi \zeta^b \nabla^0 \psi - \psi \zeta^0 \nabla^b \psi) \right) \sqrt{|\det h|} dx^1 \cdots dx^n
$$

$$
= \frac{1}{\sqrt{|\det h|}} \sum_{\beta=1}^{n} \left(\frac{\partial}{\partial x^\beta} \sqrt{|\det h|} \frac{1}{\sqrt{g^{00}}} (\psi \zeta^\beta \nabla^0 \psi - \psi \zeta^0 \nabla^\beta \psi) \right) \sqrt{|\det h|} dx^1 \cdots dx^n \, .
$$

In summary

$$
\sigma(\psi, \zeta(\psi)) = -2(\psi|\psi)_T + \int_\Sigma \mathrm{div}_\Sigma J \, \mathrm{dvol}_\Sigma \tag{1.111}
$$

where div_Σ is the divergence for the vector fields on Σ defined with respect to the metric h induced by g on Σ and J is the vector field on Σ defined in coordinates by, where the covariant derivative is the one associated to g,

$$
J^\beta := \frac{1}{\sqrt{g^{00}}} (\psi \zeta^\beta \nabla^0 \psi - \psi \zeta^0 \nabla^\beta \psi) \, , \quad \beta = 1, \ldots, n \, .
$$

(We stress that changing local chart adapted to the product $\mathbb{R} \times \Sigma$, the components ^{0} remain untouched so that the above expression of J does not depend on the used adapted chart and defines a well defined smooth vector field on Σ.) Since the support of ψ is compact on Σ (which may be compact itself), the divergence theorem implies that the integral vanishes and the proof of (b) is over.

(c) and (d). From (a) and (b), if $\psi \in \mathsf{Sol}_\mathbb{C}$:

$$
(\psi|\psi)_T^2 = |\sigma(\overline{\psi}, H\psi)_T|^2 \leq C(\psi|\psi)_T (H\psi|H\psi)_T
$$

for some constant $C > 0$, so that

$$
||H\psi|| \geq \frac{1}{\sqrt{C}} ||\psi|| \, , \quad \psi \in \mathsf{Sol}_\mathbb{C} \, .
$$

Since H is closed and the closure of its restriction to $\mathsf{Sol}_\mathbb{C}$ is H itself because $\mathsf{Sol}_\mathbb{C}$ is a core, the inequality above is valid for every $\psi \in D(H)$:

$$
||H\psi|| \geq \frac{1}{\sqrt{C}} ||\psi|| \, , \quad \psi \in D(H) \, .
$$

In particular $Ker(H) = \{0\}$, so that $\overline{Ran(H)} = Ker(H)^\perp = \mathsf{H}_T$. Actually, the inequality above, using the fact that H is cloded because is selfadjoint, immediately implies that $Ran(H) = \mathsf{H}_T$.

$H^{-1} : \mathsf{H}_T \to \mathsf{H}_T$ is well defined, $||H^{-1}|| \leq \frac{1}{\sqrt{C}}$ so that $\sigma(H^{-1}) \subset [-C^{-1/2}, C^{-1/2}]$, and $H^{-1} = \int_{\sigma(H)} \lambda^{-1} dP^{(H)}(\lambda)$ form spectral calculus and the uniqueness property of the inverse operator. As a consequence, the spectrum of H must be included in the compact $[-\sqrt{C}, \sqrt{C}]$: if $\lambda_0 \in \sigma(H)$ stays outside $[-C^{-1/2}, C^{-1/2}]$, then there is an open set $E \ni \lambda_0$ such that $P^{(H)}_E \neq 0$. At this juncture, $\psi \in P^{(H)(\mathsf{H}_T)}_E \setminus \{0\}$ violates the condition $\sigma(H^{-1}) \subset [-C^{-1/2}, C^{-1/2}]$ as easily follows from $H^{-1} = \int_{\sigma(H)} \lambda^{-1} dP^{(H)}(\lambda)$.

□

Remark 1.85. According its proof, identity (1.110) is generally valid also if ζ is not timelike and its parameter is not the coordinate t of the foliation $M \equiv \mathbb{R} \times \Sigma$ which, however, aways exists due to Theorem 3.55 when the spacetime is globally hyperbolic and Σ is a Cauchy surface. If $\boldsymbol{M} := (M, g, \mathfrak{o})$ is globally hyperbolic and X is a smooth Killing vector field, the noticeable identity therefore holds for the smooth real solutions ψ with compact Cauchy data of the Klein-Gordon equation $\Box_{\boldsymbol{M}}\psi + m^2\psi = 0$ with constant $m^2 \in \mathbb{R}$:

$$\int_\Sigma (\psi \nabla_{\boldsymbol{n}_\Sigma} X(\psi) - X(\psi)\nabla_{\boldsymbol{n}_\Sigma}\psi)\, d\Sigma = -2 \int_\Sigma T_{ab}(\psi,\psi) n^a_\Sigma X^b \, d\Sigma \,,$$

Σ being any spacelike smooth Cauchy surface. The value of each integral does not depend on the choice of Σ. Above,

$$T_{ab}(\psi,\psi) := \frac{1}{2}\left(\nabla_a\psi\nabla_b\psi + \nabla_b\psi\nabla_a\psi\right) - \frac{1}{2} g_{ab}\left(\nabla^c\psi\nabla_c\psi - m^2\psi\psi\right)$$

is the standard stress-energy tensor of the Klein-Gordon field. ■

We are ready to state and prove the crucial theorem about the existence of quasifree states in stationary globally hyperbolic spacetimes.

Theorem 1.86. *Let $(\boldsymbol{M}, g, \mathfrak{o}, \zeta)$ be a stationary globally hyperbolic spacetime. Suppose that the following holds.*

(1) The timelike Killing vector ζ is complete.

(2) $g(\zeta,\zeta) \geq c_1^2 > 0$ uniformly in M.

(3) $g(\zeta, \mathbf{n}_\Sigma) \leq c_2 < +\infty$ uniformly on a spacelike smooth Cauchy surface Σ.

Referring to a real Klein-Gordon field with operator $P := \Box_{\boldsymbol{M}} + m^2$, where $m^2 > 0$ is constant, and the associated CCR algebra $\mathcal{A}(\boldsymbol{M})$ the following facts are valid.

(a) *There is a quasifree state ω_ζ on $\mathcal{A}(\boldsymbol{M})$ whose one-particle structure is generated, according Theorem 1.65 and Proposition 1.58, by the real scalar product $\mu_\zeta : \mathsf{Sol} \times \mathsf{Sol} \to \mathbb{R}$*

$$\mu_\zeta(\psi,\psi') := 2Re\left(\frac{1}{\sqrt{H}}P_+\psi \middle| \frac{1}{\sqrt{H}}P_+\psi'\right)_T \quad \psi,\psi' \in \mathsf{Sol}\,. \tag{1.112}$$

Above,

(i) $(\cdot|\cdot)_T$ *is the Hermitian scalar product (1.93) on* $\mathsf{Sol}_{\mathbb{C}} = \mathsf{Sol} + i\mathsf{Sol}$ *induced by the stress-energy tensor and* ζ*.*

(ii) H *is the selfadjoint generator – in the Hilbert space* H_T *obtained by* $(\cdot|\cdot)_T$*-completing* $\mathsf{Sol}_{\mathbb{C}}$ *– of the strongly continuous one-parameter group of unitaries defined in (1.100):*

$$\mathsf{Sol}_{\mathbb{C}} \ni \psi \mapsto U_t\psi = e^{-itH}\psi := \psi \circ \chi_t^{(\zeta)} .$$

(iii) $P_+ : \mathsf{H}_T \to \mathsf{H}_T$ *is the positive spectral projector of* H*.*

(b) *The one-particle structure of* ω_μ*, up to isomorphisms, is* (H, K) *where*

(i) H *is the completion of* $P_+(\mathsf{H}_T)$ *with respect to the Hermitian scalar product*

$$\langle x|y\rangle := 2(x|H^{-1}y)_T, \quad \textit{for } x, y \in \mathsf{H}_T;$$

(ii) K *is the restriction* $P_+\restriction_{\mathsf{Sol}}: \mathsf{Sol} \to P_+(\mathsf{H}_T) \subset \mathsf{H}$*.*

(c) ω_ζ *is pure.*

Remark 1.87. Minkowski spacetime is stationary (more precisely ultrastatic) where the preferred unit Killing vector ζ is the vector field $\zeta := \frac{\partial}{\partial t}$ with respect to any Minkowski frame with coordinates $x^0 = t, x^1, \ldots, x^n$. $P_+\psi$ entering the right hand side of (1.112) contains "positive frequencies" or "positive energies" only, since P_+ projects on the positive part of the spectrum of the energy H. It easy to see that the state ω_ζ coincides with the Minkowski vacuum in Minkowski spacetime when $\zeta = \partial_t$ Therefore the procedure described in the theorem above is a generalization of the Minkowski vacuum. Notice that, up to now, there is a quasifree state ω_ζ for every choice of ζ as said above. Actually, as we shall discuss later, all these states coincide: the Minkowski quasifree vacuum is unique. ■

Proof. (a) Let us define $C : \mathsf{Sol}_{\mathbb{C}} \ni \psi \mapsto \overline{\psi} \in \mathsf{Sol}_{\mathbb{C}}$. Since $\mathsf{Sol}_{\mathbb{C}}$ is dense in H_T, This antilinear map uniquely continuously extend to am antiunitary operator $C : \mathsf{H}_T \to \mathsf{H}_T$ such that $CC = I$. Since, trivially, $\overline{U_t\psi} = U_t\overline{\psi}$ for $\psi \in \mathsf{Sol}_{\mathbb{C}}$, we have that $CU_t = U_tC$ so that $CH \subset -HC$ and thus $CHC \subset -HCC = -H$. However CHC is selfadjoint as it arises by direct inspection, using the fact that C is antiunitary, and thus CHC does not admit symmetric extensions. Hence $CHC \subset -H$ implies $CHC = -H$ because the latter is selfadjoint and thus symmetric. Since both sides of $CHC = -H$ are selfadjoint, they must have the same spectral measure: $P_E^{(CHC)} = P_E^{(-H)}$ which, in particular, implies

$$CP_+C = P_- , \tag{1.113}$$

where $P_+ := \int_{\sigma(H)\cap\{\lambda\in\mathbb{R}\,|\,\lambda\geq 0\}} dP^{(H)}$, $P_- := \int_{\sigma(H)\cap\{\lambda\in\mathbb{R}\,|\,\lambda\leq 0\}} dP^{(H)}$ are the spectral projectors onto the positive and negative parts of the spectrum of H, respectively. Notice that $P_+P_- = 0$ as $P_{\{0\}} = 0$ since the spectrum of H does not meet 0. Finally $P_+ + P_- = I$. (1.113) implies that μ_ζ is a well-beahved real scalar product on **Sol**. The only condition to be proved is that $\mu_\zeta(\psi,\psi) = 0$ imply $\psi = 0$. This is true because, $\mu(\psi,\psi) = 0$ implies $H^{-1/2}P_+\psi = 0$ and thus $H^{-1}P_+\psi = H^{-1/2}H^{-1/2}P_+\psi = 0$, so that $P_+\psi = HH^{-1}P_+\psi = 0$. Finally $P_-\psi = CP_+C\psi = CP_+\psi = 0$. In summary $\psi = P_+\psi + P_-\psi = 0$. We pass to prove that (1.56) is valid, so that a one-particle structure associated to μ_ζ and a quasifree state ω_ζ exist according to Proposition 1.58 and Theorem 1.65. To this end we prove that

$$2(H^{-1/2}P_+\psi|H^{-1/2}P_+\psi')_T = \mu_\zeta(\psi,\psi') + \frac{i}{2}\sigma(\psi,\psi') \,. \tag{1.114}$$

Since $2(H^{-1/2}\cdot|H^{-1/2}\cdot)_T$ is an Hermitian scalar product, the Cauchy-Schwarz inequality implies in particular

$$|Im2(H^{-1/2}x|H^{-1/2}y)_T|^2 \leq Re2(H^{-1/2}x|H^{-1/2}x)_T Re2(H^{-1/2}y|H^{-1/2}y)_T \,.$$

Using $x = P_+\psi$, $y = P_+\psi'$, the identity above yields (1.114). To conclude the proof of (a) we prove (1.114). By definition of μ_ζ

$$2(H^{-1/2}P_+\psi|H^{-1/2}P_+\psi')_T = \mu_\zeta(\psi,\psi') + iIm2(H^{-1/2}P_+\psi|H^{-1/2}P_+\psi')_T \,. \tag{1.115}$$

On the other hand

$$Im2(H^{-1/2}P_+\psi|H^{-1/2}P_+\psi')_T = 2Im(P_+\psi|H^{-1}P_+\psi')_T = -i[(P_+\psi|H^{-1}P_+\psi')_T - (P_+\psi'|H^{-1}P_+\psi)_T].$$

At this juncture, we observe that (1.82) entails for $\psi,\psi' \in$ **Sol**,

$$\sigma(\psi,\psi') = \sigma(\overline{\psi},\psi') = -2i(\psi|H^{-1}\psi')_T = -2i(P_+\psi|H^{-1}P_+\psi')_T - 2i(P_-\psi|H^{-1}P_-\psi')_T$$

where we used $P_+ + P_- = I$, $P_+P_- = 0$, $[P_\pm, H^{-1}] = 0$. Since $C\psi = \psi$ and $C\psi' = \psi'$, $P_-C = CP_+$, $CH^{-1}C = -H^{-1}$, and finally $(Cx|Cy)_T = \overline{(x|y)_T} = (y|x)_T$,

$$\sigma(\psi,\psi') = -2i[(P_+\psi|H^{-1}P_+\psi')_T + (P_-C\psi|H^{-1}P_-C\psi')_T]$$

$$= -2i[(P_+\psi|H^{-1}P_+\psi')_T - (P_+\psi'|H^{-1}P_+\psi)_T] = 2Im2(H^{-1/2}P_+\psi|H^{-1/2}P_+\psi')_T \,,$$

so that

$$\frac{1}{2}\sigma(\psi,\psi') = Im2(H^{-1/2}P_+\psi|H^{-1/2}P_+\psi')_T \quad \text{if } \psi,\psi' \in \textsf{\textbf{Sol}} \tag{1.116}$$

which, inserted in (1.115) proves (1.114) as wanted.
(b) $P_+($**Sol**$) + iP_+($**Sol**$) = P_+($**Sol** $+ i$**Sol**$) = P_+($**Sol**$_{\mathbb{C}})$ is evidently dense in $P_+(\mathsf{H}_T)$ in the topology of the scalar product $(\cdot|\cdot)_T$ just because **Sol**$_{\mathbb{C}}$ is dents in H_T and P_+ is continuos. *A fortiori*, $P_+($**Sol**$) + iP_+($**Sol**$) = P($**Sol** $+ i$**Sol**$)$ is dense in $P_+(\mathsf{H}_T)$ in the topology of the scalar product $\langle\cdot|\cdot\rangle = 2(\cdot|\cdot)_T$ since $H^{-1/2} \in \mathfrak{B}(\mathsf{H}_T)$, so it is also dense in the completion H of $P_+(\mathsf{H}_T)$. The identity $\langle P_+\psi|P_+\psi'\rangle = \mu_\zeta(\psi,\psi') + \frac{i}{2}\sigma(\psi,\psi')$ is (1.114) already established. Hence we can

apply the uniqueness part of Proposition 1.58 and the thesis arises.
(c). On account of Theorem 1.73, The thesis is equivalent to

$$\mu_\zeta(\psi,\psi') = \sup_{\textsf{Sol}\ni\psi'\neq 0} \frac{|\sigma(\psi,\psi')|^2}{4\mu_\zeta(\psi,\psi')}\,, \forall\psi\in\textsf{Sol}\,.$$

Since (1.114) is valid, it is sufficient to prove that, for every $\psi \in \textsf{Sol}$ there is a sequence of elements $\psi_n \in \textsf{Sol}$ such that

$$\lim_{n\to+\infty} \frac{|\sigma(\psi,\psi_n)|^2}{4\mu_\zeta(\psi_n,\psi_n)} = \mu_\zeta(\psi,\psi)\,.$$

If $\psi \in \textsf{Sol}$, consider a sequence $\textsf{Sol} \ni \psi_n \to \phi := i(P_+\psi - P_-\psi) \in \mathsf{H}_T$. Notice that the right-hand side satisfies $C\phi = \phi$ so that the said sequence does exist because $\textsf{Sol}_{\mathbb{C}}$ is dense in H_T and thus $\textsf{Sol}$ is dense in the real subspace of elements which satisfy $C\phi = \phi$. By construction $\mu_\zeta(\psi,\psi) = \mu_\zeta(\psi,\psi)$, furthermore, taking advantage of (1.116),

$$\frac{|\sigma(\psi,\psi_n)|^2}{4\mu_\zeta(\psi_n,\psi_n)} \to 4\frac{|Im(P_+\psi|H^{-1}(P_+i(P_+\psi-P_-\psi))_T|^2}{4\mu_\zeta(\psi,\psi)} = \frac{\mu_\zeta(\psi,\psi)^2}{\mu_\zeta(\psi,\psi)} = \mu_\zeta(\psi,\psi)\,.$$

The proof is over. □

The quasifree state ω_ζ on $\mathcal{A}(\boldsymbol{M})$ discussed in Theorem 1.86 is *invariant* under the action of ζ (which we assume to be complete) in the following sense. Just because ζ is a Killing field, the action of the one-parameter group of isometries $\{\chi^{(\zeta)}_t\}_{t\in\mathbb{R}}$ generated by ζ leaves $\textsf{Sol}$ ant its symplectic form σ invariant. This is equivalent to saying that when $\{\chi^{(\zeta)}_t\}_{t\in\mathbb{R}}$ acts on sooth functions it preserves $C^\infty_c(M)$ and E (the commutation relations of quantum fields are consequently preserved in particular). In view of Proposition 1.48, taking the isomorphism $\mathcal{A}(\textsf{Sol},\sigma) \cong \mathcal{A}(\boldsymbol{M})$ into account, a one-parameter group of $*$-algebra isomorphisms $\alpha^{(\zeta)}_t : \mathcal{A}(\boldsymbol{M}) \to \mathcal{A}(\boldsymbol{M})$ arises this way, completely defined by the requirement beyond the obvious $\alpha_t(\mathbb{1}) = \mathbb{1}$ if $t\in\mathbb{R}$ and

$$\alpha^{(\zeta)}_t(\phi(f)) := \phi\left(f\circ\chi^{(\zeta)}_{-t}\right)\,,\quad t\in\mathbb{R}\,,\quad f\in C^\infty_c(M)\,. \tag{1.117}$$

Here is the afore-mentioned invariance result.

Proposition 1.88. *Consider a stationary globally hyperbolic spacetime $(\boldsymbol{M},\zeta)$. The pure quasifree state $\omega_\zeta : \mathcal{A} \to \mathbb{C}$ constructed by the procedure in Theorem 1.86, for the complete future-directed timelike smooth satisfies*

$$\omega_\zeta \circ \alpha^{(\zeta)}_t = \omega_\zeta \quad \forall t\in\mathbb{R}\,. \tag{1.118}$$

Proof. Since the state is quasifree, it is sufficient to prove that its 2-point function satisfies

$$\omega_2(f \circ \chi_t^{(\zeta)}, g \circ \chi_t^{(\zeta)}) = \omega_2(f, g) \quad \forall t \in \mathbb{R}, \forall f, g \in C_0^\infty(M).$$

Since $\omega_2(f, g) = \langle P_+ Ef | P_+ Eg \rangle$ and $\chi_t^{(\zeta)}$ is an isometry and (b) Theorem 1.86 is valid,

$$\omega_2(f \circ \chi_t^{(\zeta)}, g \circ \chi_t^{(\zeta)}) = \langle P_+ \chi_t^{(\zeta)} Ef | P_+ \chi_t^{(\zeta)} Eg \rangle = 2(P_+ e^{-itH} Ef | H^{-1} P_+ e^{-itH} Eg)_T$$

$$= 2(e^{-itH} P_+ Ef | e^{-itH} H^{-1} P_+ Eg)_T = 2(P_+ Ef | H^{-1} P_+ Eg)_T = \langle P_+ Ef | P_+ Eg \rangle = \omega_2(f, g).$$

The proof is over. □

When passing to the GNS representation of ω_ζ, Proposition 1.27 implies that there is a one-parameter group of unitary operators which *implements* the one-paremeter group of isometries generated by ζ, namely

(i) $U_t^{(\zeta)} \Psi_{\omega_\zeta} = \Psi_{\omega_\zeta}$, $U_t^{(\zeta)}(\mathcal{D}_{\omega_\zeta}) = \mathcal{D}_{\omega_\zeta}$,

(ii) $U_t^{(\zeta)} \pi_{\omega_\zeta}(a) U_t^{(\zeta)*} := \pi_{\omega_\zeta}\left(\alpha_t^{(\zeta)}(a)\right)$ for all $t \in \mathbb{R}$ and $a \in \mathcal{A}(\boldsymbol{M})$.

Moreover we know that $\{U_t^{(\zeta)}\}_{t \in \mathbb{R}}$ is *strongly continuous* if and only if

$$\lim_{t \to 0} \omega_\zeta\left(a^* \alpha_t^{(\zeta)}(a)\right) = \omega_\zeta(a^* a) , \quad \forall a \in \mathcal{A}(\boldsymbol{M}) .$$

In the considered case this condition holds as the reader easily proves. In this case, Stone's theorem entails that there is a unique self-adjoint operator $H^{(\zeta)}$ with $e^{-itH^{(\zeta)}} = U_t^{(\zeta)}$ for every $t \in \mathbb{R}$ and $H^{(\zeta)} \Psi_\omega = 0$. In the considered case $\sigma(H^{(\zeta)}) \subset [0, +\infty)$.

Remark 1.89. The one-parameter group $U_t^{(\zeta)}$ associated with the time-like-Killing vector field ζ has the natural interpretation of **time evolution** with respect to the *notion of time* associated with ζ and, in case the group is strongly continuous $H^{(\zeta)}$ is the natural **Hamiltonian** operator associated with that evolution. However, for a generic time-oriented globally hyperbolic spacetime, no notion of Killing time is suitable and consequently, no notion of (unitary) time evolution is possible. Time evolution *à la Schroedinger* is not a good notion to be extended to QFT in curved spacetime. Observables do not evolve, they are localized in bounded regions of spacetime by means of the smearing procedure. Causal relations are encompassed by the *Time-slice axiom* which is a theorem for free fields (Proposition 1.40). ■

1.5.2 Existence of quasifree states in globally hyperbolic spacetimes

The result presented in the previous section has a well-known important consequence about the existence of quasifree states in curved spacetime. We present here a classic argument based on a so-called *deformation procedure.* There are other approaches [79], in particular a more sophisticated procedure of different nature, which uses *Moller operators* [64].

Theorem 1.90. [Existence of quasifree states] *Consider a globally hyperbolic spacetime $\boldsymbol{M}$ and assume that $P = \Box + m^2$ and $m^2 > 0$ is constant in the definition of $\mathcal{A}(\boldsymbol{M})$. There exist quasifree states on $\mathcal{A}(\boldsymbol{M})$.*

Proof. According to [65], it is always possible to smoothly deform M in the chronological past of a spacelike smooth Cauchy surface Σ of $\boldsymbol{M}$ obtaining an overall globally hyperbolic spacetime still admitting Σ as a Cauchy surface and such that the chronological past of Σ, $\boldsymbol{M}^-$, (in the deformed spacetime) has the following property. There is a second Cauchy surface Σ_1 in $\boldsymbol{M}^-$ whose chronological past $\boldsymbol{M}_1^-$ includes a smooth time-like Killing field ζ satisfying the sufficient requirements for defining and associate quasifree state ω_ζ on $\mathcal{A}(\boldsymbol{M}_1^-)$. More precisely $g(\zeta, \zeta) = 1$ and $\zeta = \mathbf{n}_{\Sigma_1}$. However, if $\boldsymbol{M}^+$ denotes the chronological future of Σ (in the original spacetime), Propositions 1.38 and 1.40 easily imply that $\mathcal{A}(\boldsymbol{M}^+) = \mathcal{A}(\boldsymbol{M}^-) = \mathcal{A}(\boldsymbol{M}_1^-)$. Therefore ω_ζ is a state on $\mathcal{A}(\boldsymbol{M}^+) = \mathcal{A}(\boldsymbol{M})$. Again Propositions 1.38 and 1.40 and the very definition of quasifree state easily prove that ω_ζ is quasifree on $\mathcal{A}(\boldsymbol{M})$ if it is quasifree on $\mathcal{A}(\boldsymbol{M}_1^-)$. $\Box$

1.5.3 States invariant under the action of spacetime symmetries

Abandoning the case of time-like Killing symmetries, every isometry $\gamma : \boldsymbol{M} \to \boldsymbol{M}$ which is also time-orientation preserving, not necessarily Killing and not necessarily time-like if Killing, induces a corresponding $*$ automorphism, $\beta^{(\gamma)}$ of $\mathcal{A}(\boldsymbol{M})$, via Proposition 1.48, completely defined by

$$\beta^{(\gamma)}(\phi(f)) := \phi(f \circ \gamma^{-1}) \,. \tag{1.119}$$

Indeed, since γ is a time-orientation preserving isometry, it must be

$$E(f \circ \gamma^{-1}, f' \circ \gamma^{-1}) = E(f, f') \quad \text{for all } f, f' \in C_c^\infty(M). \tag{1.120}$$

(1.120) corresponds to the preservation of the symplectic form of (Sol, σ) when passing to the elements $\psi := Ef \in \mathsf{Sol}$ associated to the smearing functions $f \in C_c^\infty(M)$. Taking the isomorphism $\mathcal{A}(\mathsf{Sol}, \sigma) \cong \mathcal{A}(\boldsymbol{M})$, induced by (1.33), into account, (1.119) completely defines a $*$ automorphism acoording to Proposition 1.48 if explicitly defining

$$\gamma\psi := E(f \circ \gamma^{-1}) = \psi \circ \gamma^{-1} \quad \text{when } \psi = Ef. \tag{1.121}$$

Some discrete symmetries can be represented in terms of anti-linear automorphisms, like the *time reversal* in Minkowski spacetime. Notice that it is an isometry but it reverses the time orientation. In this case (1.120) is replaced by

$$E(f \circ \gamma^{-1}, f' \circ \gamma^{-1}) = -E(f, f') \quad \text{for all } f, f' \in C_c^\infty(M) \tag{1.122}$$

Again (1.119) completely determines the anti-linear automorphism via Proposition 1.48.

If a state ω is invariant under $\beta^{(\gamma)}$, we can apply Proposition 1.27, in order to implement this symmetry unitarily in the GNS representation of ω.

Proposition 1.91. *Let $\omega : \mathcal{A}(\boldsymbol{M}) \to \mathbb{C}$ be a quasifree state invariant under the (anti) $*$ automorphism $\beta^{(\gamma)} : \mathcal{A}(\boldsymbol{M}) \to \mathcal{A}(\boldsymbol{M})$ induced by an isometry $\gamma : M \to M$ satisfying (1.120) (respectively (1.122).*
Consider the (anti) unitary operator $U^{(\beta^{(\gamma)})} : \mathcal{H}_\omega \to \mathcal{H}_\omega$ which implements $\beta^{(\gamma)}$ according to Proposition 1.48, so that
(i) $U^{(\beta^{(\gamma)})}\Psi_\omega = \Psi_\omega$, $U^{(\beta^{(\gamma)})}(\mathcal{D}_\omega) = \mathcal{D}_\omega$,
(ii) $U^{(\beta^{(\gamma)})}\pi_\omega(\phi(f))U^{(\beta)-1} := \pi_\omega\left(\phi(f \circ \gamma^{-1})\right)$ *for all* $f \in C_c^\infty(M)$.
Referring to the GNS Fock structure

$$\mathcal{H}_\omega = \mathcal{F}_+(H) = \oplus_{n=0}^{+\infty} S^n H,$$

$U^{(\beta^{(\gamma)})}$ *is completely determined by its restriction* $U_1^{(\beta^{(\gamma)})}$ *to the one-particle space* $H = S^1 H$

$$U^{(\beta^{(\gamma)})} = I \oplus U_1^{(\beta^{(\gamma)})} \oplus (U_1^{(\beta^{(\gamma)})} \otimes U_1^{(\beta^{(\gamma)})}) \oplus (U_1^{(\beta^{(\gamma)})} \otimes U_1^{(\beta^{(\gamma)})} \otimes U_1^{(\beta^{(\gamma)})}) \oplus \cdots \tag{1.123}$$

In particular $U^{(\beta^\gamma)}$ leaves separately invariant the spaces with fixed number of particles.

Proof. The proof can be done by induction, proving that

$$U^{(\beta^{(\gamma)})}\pi_\omega(\phi(f_1)) \cdots \pi_\omega(\phi(f_n))\Psi_\omega = \pi_\omega\left(\phi(f_1 \circ \gamma^{-1})\right) \cdots \pi_\omega\left(\phi(f_n \circ \gamma^{-1})\right)\Psi_\omega$$

for $n = 0, 1, 2, \ldots, N$ is equivalent to

$$U^{(\beta^{(\gamma)})}a^+(KEf_1) \cdots a^+(KEf_1)\Psi_\omega = a^+(U_1^{(\beta^{(\gamma)})}KEf_1) \cdots a^+(U_1^{(\beta^{(\gamma)})}KEf_1)\Psi_\omega$$

for $n = 0, 1, \ldots, N$. For $N \leq 1$ the thesis is trivially true. The second identity implies (1.123) on a dense domain. Therefore it is is true everywhere because all the involved operators are continuous. □

An important general definition is valid when we consider a one-parameter group of $*$ automorphisms with the physical meaning of time evolution as in the case of the group induced by a timelike Killing vector. However, mathematical speaking, this definition is general.

Definition 1.92. Consider a one-parameter group $\beta := \{\beta_t\}_{t\in\mathbb{R}}$ of $*$ automorphisms of the unital $*$ algebra $\mathcal{A}$ and suppose that a state $\omega : \mathcal{A} \to \mathbb{C}$ is β-invariant and satisfies

$$\lim_{t\to 0} \omega_\zeta\left(a^*\beta_t(a)\right) = \omega_\zeta(a^*a)\,, \quad \forall a \in \mathcal{A}\,. \tag{1.124}$$

Consider the one-parameter group $U^{(\beta)} := \{e^{-itH^{(\beta)}}\}_{t\in\mathbb{R}}$ which implements β, according to Proposition 1.27, in the GNS representation of ω. If

(i) $\sigma(H^{(\beta)}) \subset [0, +\infty)$

(ii) the cyclic vector Ψ_ω, up to phases, is the unique normalized vector in $\mathcal{H}_\omega$ with $H^{(\beta)}\Psi_\omega = 0$, then ω is called **ground state**. ■

In spite of having explicitly usied a specific GNS construction for ω, the written definition is actually invariant under change of the GNS structure compatible with ω as immediately arises from the uniqueness part of the GNS theorem.

Coming back to the CCR algebra $\mathcal{A}(\boldsymbol{M})$, a known result by Kay [46] establishes the following remarkable uniqueness result (actually proved for Weyl algebras and one-particle structures of quasifree states, but immediately adaptable to our CCR framework).

Proposition 1.93. [Uniqueness of pure invariant quasifree states] *Consider the CCR algebra $\mathcal{A}(\boldsymbol{M})$ for a real scalar Klein Gordon field with Klein-Gordon operator $P = \Box_{\boldsymbol{M}} + V$, $V \in C^\infty(M)$. Consider a one-parameter group γ of isometries $\gamma_t : M \to M$, $t \in \mathbb{R}$ (which necessarily satisfies (1.120)). Assume that a quasifree state $\omega : \mathcal{A}(\boldsymbol{M}) \to \mathbb{C}$ satisfies the following conditions.*

(i) ω is pure.

(ii) ω is invariant under a one-parameter group of $*$ automorphisms $\beta := \{\beta_t\}_{t\in\mathbb{R}}$ of $\mathcal{A}(\boldsymbol{M})$ induced by γ according to (1.119).

(iii) ω satisfies (1.124), thus giving rise to a strongly continuous unitary group $\{U_t^{(\beta)}\}_{t\in\mathbb{R}}$ implementing β in the GNS representation of ω.

Then ω is uniquely determined by β if the self-adjoint generator of $\{U_t^{(\beta)}\}_{t\in\mathbb{R}}$ restricted to the one-particle Hilbert space of ω satisfies

(a) it is positive

(b) its kernel is trivial.

1.5.4 Poincaré invariance and uniqueness of the quasifree Minkowski vacuum

Let us focus on the *Minkowski vacuum*, that is the quasifree state $\omega_{\mathbb{M}}$ on four dimensional Minkowski spacetime $\mathbb{M}$ defined in Section 1.5.2 by the two-point function (1.91). As a matter of fact, $\omega_{\mathbb{M}}$ turns out to be invariant under the natural action of *orthochronous proper Poincaré group* and that the corresponding unitary representation of this connected Lie (and thus topological) group is strongly continuous. In particular the self-adjoint generator of time displacements (with respect to every timelike direction), in the one-particle Hilbert space, satisfies the hypotheses of Proposition 1.93. As $\omega_{\mathbb{M}}$ is pure, it *is therefore the unique pure quasifree state invariant under the orthochronous proper Poincaré group.* $\omega_{\mathbb{M}}$ is a ground state with respect to any Minkowski time evolution and, by direct inspection, one easily sees that the state it is also invariant under the remaining discrete symmetries of Poincaré group T, P and PT which are consequently (anti-)unitarily implementable in the GNS Hilbert space. Finally, it turns out that the one-particle space is irreducible under the action of the orthochronous proper Poincaré group, thus determining an *elementary particle* in the sense of the *Wigner classification*, with mass m and zero spin.

1.5.5 Unitarily inequivalent quasifree states gravitationally produced

Let us start with the following definition.

Definition 1.94. Two states ω_1 and ω_2 on $\mathcal{A}(\boldsymbol{M})$ and the respective GNS representations are said to be **unitarily equivalent**[13] if there is an isometric surjective operator $U : \mathcal{H}_{\omega_1} \to \mathcal{H}_{\omega_2}$ such that $U\hat{\phi}_{\omega_1}(f)U^{-1} = \hat{\phi}_{\omega_2}(f)$ for every $f \in C_c^\infty(M)$. ■

Remark 1.95. Notice that it is not necessary that $U\Psi_{\omega_1} = \Psi_{\omega_2}$ and it generally does not happen. As a consequence $\mathcal{H}_{\omega_2}$ includes vector states *different from the Fock vacuum* which are however quasifree. ■

The question if a pair of states are unitarily equivalent naturally arises in the following situation. Consider a time-oriented globally hyperbolic spacetime $\boldsymbol{M}$ such that, in the future of a Cauchy surface Σ_+, the spacetime is stationary with respect to the Killing vector field ξ_+ and it is also stationary in the past of another Cauchy surface Σ_-, in the past of Σ_+, referring to another Killing vector field ξ_-. For instance we can suppose that $\boldsymbol{M}$ coincides to (a portion of) Minkowski spacetime in the two mentioned stationary regions and a gravitational curvature bump takes place between them. This way, two preferred quasifree states ω_+ and ω_- turn out to be defined on the whole algebra $\mathcal{A}(\boldsymbol{M})$, not only in the algebras of observables localized in the two respective static regions regions. The natural question is whether or not the GNS representations of ω_+ and ω_- are unitarily equivalent, so that, in particular, the state ω_- can be represented as a vector state $U\Psi_{\omega_-}$ in the Hilbert space $\mathcal{H}_{\omega_+}$ of the state ω_+. Notice that, even in the case the isometric surjective operator U exists making the representations unitarily equivalent, $U\Psi_{\omega_-} \neq \Psi_{\omega_+}$ in general, so that $U\Psi_{\omega_-}$ may have non-vanishing projection in the subspace containing states with n particles in $\mathcal{H}_{\omega_+}$. This phenomenon is physically interpreted as *creation of particles due to the gravitational field* and U has the natural interpretation of an *S matrix*.
The following crucial result holds for quasifree states [79].

Theorem 1.96. [Unitary equivalence of quasifree states] *If $\boldsymbol{M}$ is a globally hyperbolic spacetime, consider two quasifree states ω_1 and ω_2 on $\mathcal{A}(\boldsymbol{M})$ respectively induced by the scalar product μ_1 and μ_2 on* $\mathsf{Sol}(\boldsymbol{M})$ *and indicate by $\mathcal{R}_{\mu_1}$ and $\mathcal{R}_{\mu_2}$ the real Hilbert spaces obtained by respectively completing* Sol.
The states ω_1 and ω_2 may be unitarily equivalent only if they induce equivalent norms on Sol*,*

[13] It should be evident that the given definition does not depend on the particular GNS representation chosen for each state ω_i.

that is there are constants $C, C' > 0$ with

$$C\mu_1(x,x) \leq \mu_2(x,x) \leq C'\mu_1(x,x) \quad \forall x \in \textsf{\textbf{Sol}}\,.$$

When the condition is satisfied there is a unique bounded operator $Q : \mathcal{R}_{\mu_1} \to \mathcal{R}_{\mu_1}$ such that

$$\mu_1(x, Qy) = \mu_2(x,y) - \mu_1(x,y) \quad \forall x, y \in \textsf{\textbf{Sol}}\,.$$

In this case ω_1 and ω_2 are unitarily equivalent if and only if Q is trace class in $\mathcal{R}_{\mu_1}$.

In general, the said condition fails when ω_1 and ω_2 are stationary states associated with two stationary regions (in the past and in the future) of a spacetime, as discussed in the introduction of this section [79], [27, Ch.7]. It happens in particular when the Cauchy surfaces have infinite volume. In this case the states turn out to be unitarily inequivalent. On the other hand there is no natural preferred choice between ω_+ and ω_- and this fact suggests that the algebraic formulation is more useful in QFT in curved spacetime than the, perhaps more familiar, formulation in a Hilbert space.

Chapter 2

Hadamard states

2.1 Hadamard quasifree states in curved spacetime

The algebra of observables generated by the field $\phi(f)$ smeared with smooth functions is too small to describe important observables in QFT in curved spacetime. Maybe the most important is the stress energy tensor (obtained as a functional derivative of the action with respect to g^{ab}) that, for our Klein-Gordon field with $P = \Box_{\boldsymbol{M}} + m^2 + \xi R$ it reads, where G_{ab} is the standard Einstein tensor

$$T_{ab} := (1-2\xi)\nabla_a\phi\nabla_b\phi - 2\xi\phi\nabla_a\nabla_b\phi - \xi\phi^2 G_{\mu\nu} \\ + g_{ab}\left\{2\xi\phi^2 + \left(2\xi - \frac{1}{2}\right)\nabla^c\phi\nabla_c\phi + \frac{1}{2}m^2\phi^2\right\} . \tag{2.1}$$

It concerns products of fields evaluated at the same point of spacetime, like $\phi^2(x)$. This observable, as usual smeared with a function $f \in C_c^\infty(M)$, could be formally interpreted as

$$\phi^2(f) = \int_M \phi(x)\phi(y)f(x)\delta(x,y)\ \mathrm{dvol}_{\boldsymbol{M}} . \tag{2.2}$$

However this object does not belong to $\mathcal{A}(\boldsymbol{M})$. Beyond the fact that T_{ab} describe the local content of energy, momentum and stress of the field, the stress-energy tensor is of direct relevance for describing the back reaction on the quantum fields on the spacetime geometry through the semi-classical Einstein equation

$$G_{ab}(x) = 8\pi\omega(T_{ab}(x)) \tag{2.3}$$

or also, introducing a smearing procedure

$$\int_M G_{ab}(x)f(x)\ \mathrm{dvol}_{\boldsymbol{M}} = 8\pi\int_M \omega(T_{ab}(x))f(x)\ \mathrm{dvol}_{\boldsymbol{M}} ,$$

where $\omega(T_{ab}(x))$ has the interpretation of the (integral kernel of the) expectation value of the quantum observable T_{ab} with respect to some quantum state ω. Barring technicalities due to the appearance of derivatives, the overall problem is here to provide (2.2) with a precise mathematical meaning, which in fact, is equivalent to a suitable enlargement the algebra $\mathcal{A}(\boldsymbol{M})$.

2.1.1 Enlarging the observable algebra in Minkowski spacetime

In flat spacetime $\boldsymbol{M} = \mathbb{M}$, $P = \Box_{\mathbb{M}} + m^2$ ($m > 0$) for free QFT, at the level of *expectation values* and *quadratic forms* the above mentioned enlargement of the algebra is performed exploiting a *physically meaningful reference state*, the unique Poincaré invariant quasifree (pure) state introduced in Section 1.5.2 and discussed at the end of Section 1.5.3, $\omega_{\mathbb{M}}$. We call this state *Minkowski vacuum*.

Let us first focus on the elementary observable ϕ^2. We shall indicate it with $:\!\phi^2(x)\!:$ and we define it as a *Hermitian quadratic form* on $\mathcal{D}_{\omega_{\mathbb{M}}}$.

We start by defining the operator on $\mathcal{D}_{\omega_{\mathbb{M}}}$ for $f, g \in C_c^\infty(\mathbb{R}^4)$

$$:\!\hat{\phi}(f)\hat{\phi}(g)\!: := \hat{\phi}(f)\hat{\phi}(g) - \langle \Psi_{\omega_{\mathbb{M}}} | \hat{\phi}(x)\hat{\phi}(y)\Psi_{\omega_{\mathbb{M}}}\rangle I \tag{2.4}$$

(As usual $\hat{\phi}(f) := \hat{\phi}_{\omega_{\mathbb{M}}}(f)$ throughout this section.) Next, for $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$ we analyze its integral kernel, assuming that it exists, $\langle \Psi | :\!\hat{\phi}(x)\hat{\phi}(y)\!: \Psi\rangle$ which is symmetric since the antisymmetric part of the right-hand side of (2.4) vanishes in view of the commutation relations of the field. The explicit form of the distribution $\omega_{\mathbb{M}2}(x,y) = \langle \Psi_{\omega_{\mathbb{M}}} | \hat{\phi}(x)\hat{\phi}(y)\Psi_{\omega_{\mathbb{M}}}\rangle$ appears in (1.91). We prove below that the mentioned formal kernel $\langle \Psi | :\!\hat{\phi}(x)\hat{\phi}(y)\!: \Psi\rangle$ not only exists but it also is a jointly smooth function. Consequently we are allowed to define, for any $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$,

$$\langle \Psi | :\!\hat{\phi}^2\!: (f)\Psi\rangle := \int_{\mathbb{M}^2} \langle \Psi | :\!\hat{\phi}(x)\hat{\phi}(y)\!: \Psi\rangle f(x)\delta(x,y)\ \mathrm{dvol}_{\mathbb{M}^2}(x,y)\,. \tag{2.5}$$

Finally, the polarization identity uniquely defines $:\hat{\phi}^2: (f)$ as a symmetric quadratic form $\mathcal{D}_{\omega_{\mathbb{M}}} \times \mathcal{D}_{\omega_{\mathbb{M}}}$.

$$\begin{aligned}\langle \Psi' | :\!\phi^2\!: (f)\Psi\rangle := \frac{1}{4}\big(&\langle \Psi' + \Psi | :\!\phi^2\!: (f)(\Psi' + \Psi)\rangle - \langle \Psi' - \Psi | :\!\phi^2\!: (f)(\Psi' - \Psi)\rangle \\ &- i\langle \Psi' + i\Psi | :\!\phi^2\!: (f)(\Psi' + i\Psi) + i\langle \Psi' - i\Psi | :\!\phi^2\!: (f)(\Psi' - i\Psi)\rangle\big)\end{aligned} \tag{2.6}$$

There is no guarantee that an operator $:\!\phi^2\!: (f)$ really exists on $\mathcal{D}_{\omega_{\mathbb{M}}}$ satisfying (2.5)[1], however if it exists, since $\mathcal{D}_{\omega_{\mathbb{M}}}$ is dense and (2.6) holds, it is uniquely determined by the class of the expectation values $\langle \Psi | :\!\hat{\phi}^2\!: (f)\Psi\rangle$ on the states $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$. As promised, let us prove that the kernel defined in (2.5) is a smooth function. First of all, notice that, as a general result arising from the GNS construction, every $\Psi \in \mathcal{D}_\omega$ can be written as

$$\Psi = \sum_{n\geq 0, i_1, \ldots, i_n \geq 1} C^{(n)}_{i_1 \ldots i_n} \hat{\phi}(f^{(n)}_{i_1}) \cdots \hat{\phi}(f^{(n)}_{i_n})\Psi_{\omega_{\mathbb{M}}} \tag{2.7}$$

where only a finite number of coefficients $C^{(n)}_{i_1 \ldots i_n} \in \mathbb{C}$ is non-vanishing and the term in the sum corresponding to $n = 0$ is defined to have the form $c^0\Psi_{\omega_{\mathbb{M}}}$. We have

$$\begin{aligned}\langle \Psi | \hat{\phi}(x)\hat{\phi}(y)\Psi\rangle = &\sum_{n\geq 0, i_1, \ldots, i_n \geq 1}\ \sum_{m\geq 0, j_1, \ldots, j_n \geq 1} \overline{C^{(m)}_{j_1 \ldots j_n}} C^{(n)}_{i_1 \ldots i_n} \\ &\left\langle \Psi_{\omega_{\mathbb{M}}} \middle| \hat{\phi}(f^{(m)}_{j_m}) \cdots \hat{\phi}(f^{(m)}_{j_1})\hat{\phi}(x)\hat{\phi}(y)\hat{\phi}(f^{(n)}_{i_1}) \cdots \hat{\phi}(f^{(n)}_{i_n})\Psi_{\omega_{\mathbb{M}}}\right\rangle\,.\end{aligned} \tag{2.8}$$

[1]By Riesz lemma, it exists if an only if the map $\mathcal{D}_{\omega_{\mathbb{M}}} \ni \Psi' \mapsto \langle \Psi' | :\!\phi^2\!: (f)\Psi\rangle$ is continuous for every $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$

Taking advantage of the quasifree property of $\omega_{\mathbb{M}}$, hence using the expansion of n-point functions in terms of the 2-point function of Definition 1.57, we can re-arrange the right hand side of (2.8) as (all the sums are over finite terms)

$$\begin{aligned}\langle\Psi|\hat{\phi}(x)\hat{\phi}(y)\Psi\rangle = C^0_\Psi \omega_{\mathbb{M}2}(x,y) \\ + \sum_{m\geq 0, j\geq 1}\sum_{m'\geq 0, j'\geq 1} C^{(m)(m')}_{\Psi,j,j'}\omega_{\mathbb{M}2}(f^{(m)}_j, x)\omega_{\mathbb{M}2}(f^{(m')}_{j'}, y) \\ + \sum_{m\geq 0, j\geq 1}\sum_{n\geq 0, i\geq 1} C^{(m)(n)}_{\Psi,j,i}\omega_{\mathbb{M}2}(f^{(m)}_j, x)\omega_{\mathbb{M}2}(y, f^{(n)}_i) \\ + \sum_{n'\geq 0, i'\geq 1}\sum_{n\geq 0, i'\geq 1} C^{(n')(n)}_{\Psi,i',i}\omega_{\mathbb{M}2}(x, f^{(n')}_{i'})\omega_{\mathbb{M}2}(y, f^{(n)}_i)\,, \quad (2.9)\end{aligned}$$

with all sums finite and some C_Ψ-coefficients that depend on the state Ψ. We can be more specific about the first coefficient, in fact, according to the formula from Definition 1.57, we have $C^0_\Psi = \langle\Psi|\Psi\rangle$. Recall also, from Proposition 1.76, that $y \mapsto \omega_{\mathbb{M}2}(f, y)$ and $x \mapsto \omega_{\mathbb{M}2}(x, f)$ are smooth for any test function $f \in C^\infty_0(M)$. Hence, we can interpret Equation (2.9) as saying that

$$\langle\Psi|\,{:}\hat{\phi}(x)\hat{\phi}(y){:}\,\Psi\rangle = \langle\Psi|\hat{\phi}(x)\hat{\phi}(y)\Psi\rangle - \langle\Psi|\Psi\rangle\omega_{\mathbb{M}}(x,y) \in C^\infty(M\times M)\,. \quad (2.10)$$

More complicated operators, i.e. **Wick polynomials** and corresponding differentiated Wick polynomials, generated by **Wick monomials**, ${:}\hat{\phi}^n{:}\,(f)$, of arbitrary order n, can analogously be defined as quadratic forms, by means of a recursive procedure of subtraction of divergences. The stress energy operator is a differentiated Wick polynomial of order 2.
The procedure for defining ${:}\hat{\phi}^n{:}\,(f)$ as a quadratic form is as follows. First define recursively, where the tilde just means that the indicated element has to be omitted,

$$\begin{aligned}{:}\hat{\phi}(f_1){:} &:= \hat{\phi}(f_1) \\ {:}\hat{\phi}(f_1)\cdots\hat{\phi}(f_{n+1}){:} &:= {:}\hat{\phi}(f_1)\cdots\hat{\phi}(f_n){:}\,\hat{\phi}(f_{n+1}) \\ &\quad - \sum_{l=1}^{n} {:}\hat{\phi}(f_1)\cdots\widetilde{\hat{\phi}(f_l)}\cdots\hat{\phi}(f_n){:}\;\omega_{\mathbb{M}2}(f_l, f_{n+1})\,. \quad (2.11)\end{aligned}$$

These elements of $\mathcal{A}(\mathbb{M})$ turn out to be symmetric under interchange of $f_1, f_2, \dots f_n$ as it can be proved by induction[2]. By induction, it is next possible to prove that, for $n \geq 2$ and $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$, there is a *jointly smooth kernel*

$$\langle\Psi|\,{:}\hat{\phi}(x_1)\cdots\hat{\phi}(x_n){:}\,\Psi\rangle$$

which produces $\langle\Psi|\,{:}\hat{\phi}(f_1)\cdots\hat{\phi}(f_n){:}\,\Psi\rangle$ by integration. This result arises from (2.11) as a consequence of the fact that

(a) $\omega_{\mathbb{M}}$ is quasifree so that Definition 1.57 can be used to compute the said kernels,

(b) $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$ so that the expansion (2.7) can be used,

[2]Observe in particular that ${:}\hat{\phi}(f)\hat{\phi}(g){:} - {:}\hat{\phi}(g)\hat{\phi}(f){:} = iE(f,g)\mathbb{1} - \omega_{\mathbb{M}2}(iE(f,g)\mathbb{1})\mathbb{1} = 0$.

(c) the functions $F_k : x \mapsto \omega_{\mathbb{M}2}(x, f_k) = \overline{\omega_{\mathbb{M}2}(f_k, x)}$ are smooth when $f_k \in C_c^\infty(M)$ as was mentioned above.
Indeed, we have

$$\langle \Psi | :\hat{\phi}(x_1)\cdots\hat{\phi}(x_n): \Psi\rangle = \sum_{n\geq 0, i_1,\ldots,i_n\geq 1}\ \sum_{m\geq 0, j_1,\ldots,j_n\geq 1} \overline{C^{(m)}_{j_1\ldots j_n}} C^{(n)}_{i_1\ldots i_n}$$
$$\left\langle \Psi_{\omega_{\mathbb{M}}} | \, \hat{\phi}(f^{(m)}_{j_m})\cdots\hat{\phi}(f^{(m)}_{j_1}) :\hat{\phi}(x_1)\cdots\hat{\phi}(x_n): \hat{\phi}(f^{(n)}_{i_1})\cdots\hat{\phi}(f^{(n)}_{i_n})\Psi_{\omega_{\mathbb{M}}}\right\rangle \ . \tag{2.12}$$

after having expanded the normal product $:\hat{\phi}(g_1)\cdots\hat{\phi}(g_n):$ in the right-hand side, one can evaluate the various n-point functions arising this way by applying Definition 1.57. It turns out that all terms $\omega_{\mathbb{M}2}(x_i, x_j)$ always appear in a sum with corresponding terms $-\omega_{\mathbb{M}2}(x_i, x_j)$ arising by the definition (2.11) and thus give no contribution. The remaining factors are of the form $F_k(x_j)$ and thus are smooth.
We therefore are in a position to write the definition of $\langle\Psi| :\hat{\phi}^n: (f)\Psi\rangle$ if $\Psi \in \mathcal{D}_{\omega_{\mathbb{M}}}$

$$\langle\Psi| :\hat{\phi}^n: (f)\Psi\rangle = \int_{M^n} \langle \Psi | :\hat{\phi}(x_1)\cdots\hat{\phi}(x_n): \Psi\rangle f(x_1)\delta(x_1,\ldots x_n)\mathrm{dvol}_{\boldsymbol{M}^n} \tag{2.13}$$

Exactly as before, polarization extends the definition to a quadratic form on $\mathcal{D}_{\omega_{\mathbb{M}}} \times \mathcal{D}_{\omega_{\mathbb{M}}}$. There is no guarantee that operators fitting these quadratic forms really exist.

Remark 2.1. The definition (2.11) can be proved to be formally equivalent to the formal definition

$$:\hat{\phi}(x_1)\cdots\hat{\phi}(x_n): := \frac{1}{i^n}\frac{\delta^n}{\delta f(x_1)\cdots\delta f(x_n)}\bigg|_{f=0} e^{i\hat{\phi}(f)+\frac{1}{2}\omega_{\mathbb{M}2}(f,f)} \tag{2.14}$$

Though the exponential converges in the strong operator topology to a unitary operator, the **Weyl generator**, restricted to the dense domain $\mathcal{D}_{\omega_{\mathbb{M}}}$, $e^{i\hat{\phi}(f)}$ can be viewed here as a formal series and this series can be truncated at finite, sufficiently large, order in view of linearity of the exponent and $f = 0$. ■

2.1.2 Enlarging the observable algebra in curved spacetime

The discussed definition of Wick polynomials is *equivalent* in Minkowski spacetime to the more popular one based on the well known re-ordering procedure of creation and annihilation operators as can be proved by induction. Nevertheless this second approach is not natural in curved spacetime because, to be implemented, it needs the existence of a physically preferred reference state as Minkowski vacuum in flat spacetime, which in the general case it is not given. To develop a completely covariant theory another approach has been adopted, which generalises to curved spacetime the previously outlined definition of Wick polynomials based on a "divergence subtraction" instead of a re-ordering procedure. The idea is that, although it is not possible to uniquely assign each spacetime with a physically distinguishable state, it is possible to select a type of divergence in common with all physically relevant states is every spacetime. These preferred quasifree states with the same type of divergence "resembling" Minkowski vacuum in a generic spacetime are called *Hadamard states*. Minkowski vacuum belongs to this class and these states are remarkable also in view of their *microlocal features*, which revealed to be of crucial importance for the technical advancement of the theory, as we will describe later. Exploiting these distinguished states, it is possible to generalize the outlined approach in order to enlarge $\mathcal{A}(\boldsymbol{M})$, including other algebraic elements as the stress-energy tensor operator [59, 42]. Actually this is nothing but the first step to generalize the ultraviolet renormalization procedure to curved spacetime [79, 13, 12, 40, 41]. The rest of the chapter is devoted to discuss some elementary properties of Hadamard states.

Let us quickly remind some local features of (pseudo)Riemannian differential geometry [66, 57, 63], necessary to introduce the notion of Hadamard states from a geometric viewpoint. If (M, g) is a smooth Riemannian or Lorentzian manifold, an open set $C \subset M$ is said a **normal convex** neighborhood if there is a open set $W \subset TM$ with the form $W = \{(q, v) \,|\, q \in C, v \in S_q\}$ where $S_q \subset T_qM$ is a star-shaped open neighborhood of the origin, such that

$$exp\restriction_W : (q, v) \mapsto exp_q v$$

is a diffeomorphism onto $C \times C$. It is clear that C is connected and there is only one geodesic segment joining any pair $q, q' \in C$ if we require that it is completely contained in C. It is $[0, 1] \ni t \mapsto exp_q(t((exp_q)^{-1}q'))$. Moreover if $q \in C$ and we fix a basis $\{e_\alpha|_q\} \subset T_qM$,

$$t = t^\alpha e_\alpha|_q \mapsto exp_q(t^\alpha e_\alpha|_q)\ , \quad t \in S_q$$

defines a set of coordinates on C centered in q which is called the **normal Riemannian coordinate system** centered in q. In (M, g) as above, $\sigma(x, y)$ indicates the **squared (signed) geodesic distance** of x from y. With our signature $(+, -, \cdots, -)$, it is defined as

$$\sigma(x, y) := -g_x(exp_x^{-1}y, exp_x^{-1}y)\ .$$

$\sigma(x, y)$ turns out to be smoothly defined on $C \times C$ if C is a convex normal neighborhood where we also have $\sigma(x, y) = \sigma(y, x)$. The class of the convex normal neighborhoods of a point $p \in M$ is a fundamental system of neighborhoods of p [24, 4].
In Riemannian manifolds σ defined as above is everywhere nonnegative with the standard Euclidean choice of the signature.

In a convex neighborhood C of a spacetime $\boldsymbol{M}$, taking in particular advantage of several properties of σ, it is possible to define a local *approximate solution* of KG equation, technically called a *parametrix*, which has essentially the same short-distance singularity of the two point function of Minkowski vacuum. Its construction uses only the local geometry and the parameters defining the equation of motion but does not refers to particular states, which are global objects. The technical idea can be traced back to Hadamard [37] (and extensively studied by Riesz [72]) and it is therefore called *Hadamard parametrix*. In the rest of the chapter we only consider a four dimensional spacetime, essentially following [35]. A quick technical discussion on the general case (details and properties of the constructions strongly depend of the dimension of the spacetime) also in relation with heath kernel expansion, can be found in [59] (see also [29, 24, 32, 3] for more extended discussions also on different types of parametrices and their use in field theory). In a convex neighborhood C of a four dimensional spacetimes the **Hadamard parametrix** of order N of the two-point function has the form

$$H_\epsilon^{(N)}(x,y) = \frac{u(x,y)}{(2\pi)^2\sigma_\epsilon(x,y)} + \sum_{n=0}^{N} v_n \sigma^n \log\left(\frac{\sigma_\epsilon(x,y)}{\lambda^2}\right) \tag{2.15}$$

where $x, y \in C$, T is any local time coordinate increasing towards the future, $\lambda > 0$ a length scale and

$$\sigma_\epsilon(x,y) := \sigma(x,y) + 2i\epsilon(T(x) - T(y)) + \epsilon^2 \,, \tag{2.16}$$

finally, the cut in the complex domain of the log function is assumed along the negative axis in (2.15). Recursive differential equations (see the appendix A of [59] and also [72, 29, 24, 27, 58, 34]) determine $u = u(x,y)$ and all the **Hadamard coefficients** $v_n = v_n(x,y)$ in C as smooth functions, when assuming $u(x,x) = 1$ and $n = 0, 1, 2, \ldots$. These recurrence relations have been obtained by requiring that the sequence of the $H_0^{(N)}(x,y)$ defines a local, y-parametrized,"approximate solution" of the KG equation for $\sigma(x,y) \neq 0$ (with some further details we can say that the error with respect to a true solution is of order σ^N for each N). That solution would be exact in the $N \to \infty$ limit of the sequence provided the limit exists. The limit exists in the analytic case, but in the smooth general case the sequence diverges. However, as proved in [24, §4.3], if $\chi : \mathbb{R} \to [0,1]$ is a smooth function with $\chi(r) = 1$ for $|r| \leq 1/2$ and $\chi(r) = 0$ for $|r| > 0$ one can always find a sequence of numbers $0 < c_1 < c_2 < \cdots < c_n \to +\infty$ for that

$$v(x,y) := \sum_{n=0}^{\infty} v_n(x,y)\sigma(x,y)^n \chi(c_n\sigma(x,y)) \tag{2.17}$$

uniformly converges, with all derivatives, to a C^∞ function on $C \times C$. A parametrix H_ϵ

$$H_\epsilon(x,y) = \frac{u(x,y)}{(2\pi)^2\sigma_\epsilon(x,y)} + v(x,y)\log\left(\frac{\sigma_\epsilon(x,y)}{\lambda^2}\right) \tag{2.18}$$

arises this way. This parametrix distributionally satisfies KG equation in both arguments up to jointly smooth functions of x and y. In other words, there is a smooth function s defined in $C \times C$ such that if $f, g \in C_c^\infty(C)$ and defining $P := \Box_{\boldsymbol{M}} + m^2 + \xi R$,

$$\lim_{\epsilon\to 0^+} \int_{C\times C} H_\epsilon(x,y)(Pf)(x)g(y)\mathrm{dvol}_{M\times M} = \int_{C\times C} s(x,y)f(x)g(y)\mathrm{dvol}_{M\times M} \,. \tag{2.19}$$

The analog holds swapping the role of the test functions. We are in a position to state our main definition.

Definition 2.2. With $\boldsymbol{M}$ four dimensional, we say that a (not necessarily quasifree) state ω on $\mathcal{A}(\boldsymbol{M})$ and its two point function ω_2 are **Hadamard** if $\omega_2 \in \mathcal{D}'(M \times M)$ and every point of $\boldsymbol{M}$ admits an open normal neighborhood C where

$$\omega_2(x,y) - H_{0^+}(x,y) = w(x,y) \quad \text{for some} \quad w \in C^\infty(C \times C) \,. \tag{2.20}$$

Here 0^+ indicates the standard weak distributional limit as $\epsilon \to 0^+$ ("first integrate against test functions and next take the limit").

Remark 2.3.

(1) The given definition does not depend either on the choice of χ or the sequence of the c_n used in (2.17) since different choices simply change w as one may easily prove. Similarly, the definition does not depend on the choice of the local time function T used in the definition of σ_ϵ. This fact is far from being obvious and requires a more detailed analysis [48].

(2) Using the following result arising form recurrence relations determining the Hadamard coefficients, one finds that the distribution

$$\left(v(x,y) - \sum_{k=0}^{N} v_n(x,y)\sigma(x,y)^n\right) \ln \sigma_{0^+}(x,y)$$

is a function in $C^N(O \times O)$. Exploiting this result, it is not difficult to prove that the requirement (2.20) is equivalent to the following requirement:

$$\omega_2(x,y) - H^{(N)}_{0^+}(x,y) = w_N(x,y) \quad \text{for each } N \geq 1, \text{ with } \quad w_N \in C^N(C \times C)\,. \tag{2.21}$$

The equivalent definition of Hadamard state in [69] was, in fact, nothing but Definition 2.2 with (2.20) replaced by (2.21).

(3) Minkowski vacuum $\omega_{\mathbb{M}}$ defined by the two point function (1.91) is Hadamard. In particular, for $m > 0$, it holds[3]

$$\omega_{\mathbb{M}2}(x,y) = \frac{1}{4\pi^2}\frac{1}{\sigma_{0^+}(x,y)} + \frac{m^2}{2(2\pi)^2}\frac{I_1(m\sqrt{\sigma})}{m\sqrt{\sigma(x,y)}} \ln\left(m^2\sigma_{0^+}(x,y)\right) + w(x,y)$$

where w is smooth. The result holds also for $m = 0$ and in that case, only the first term in the right-hand side does not vanish in the expansion above. Similarly, quasifree states *invariant under the symmetries generated by a timelike Killing vector field* ζ as the states considered in Sect. 1.5.2 (with all the hypotheses specified therein) are Hadamard [28, 79] if the spacetime admits spacelike Cauchy surfaces normal to ζ, that is if the spacetime is *static*. This last condition is essential because there are spacetimes admitting lightlike Killing vectors but not spacelike Cauchy surfaces normal to them which do not admit *invariant Hadamard* quasifree states, like Kerr spacetime and Schwartzschild-de Sitter spacetime [48].

(4) Referring to the literature before the cornerstone results [69, 70] (we consider in Sec. 2.2.2), Definition 2.2 properly refers to *locally* Hadamard states. This is because there also exists a notion of *global Hadamard state* (Definition 3.4 in [69]), discussed in [48] in a completely rigorous way for the first time. This apparently more restrictive global condition essentially requires (see [48, 69] for the numerous technical details), for a certain open neighborhood $\mathcal{N}$

[3]The function $z \mapsto I_1(\sqrt{z})/\sqrt{z}$, initially defined for $Re(z) > 0$, admits a unique analytic extension on the whole space $\mathbb{C}$ and the formula actually refers to this extension.

of a Cauchy surface of $\boldsymbol{M}$ such that $\sigma(x, y)$ is always well defined if $(x, y) \in \mathcal{N} \times \mathcal{N}$ (and this neighbourhood can always be constructed independently from the Hadamard requirement), that (2.21) is valid producing the known singularity for causally related arguments, and there are no further singularities for arbitrarily far, spacelike separated, arguments $(x, y) \in \mathcal{N} \times \mathcal{N}$. In this regard a technically important result, proved in the appendix B of [48], is that, analogous to Proposition 1.76 in the case of Minkowski space,

$$M \ni x \mapsto \omega(\phi(f)\phi(x)) = \overline{\omega(\phi(x)\phi(f))} \in C^\infty(M) \tag{2.22}$$

if $f \in C_c^\infty(M)$ and ω is a quasifree *globally* Hadamard state on $\mathcal{A}(\boldsymbol{M})$. We shall prove this fact later using the microlocal approach. This fact has an important consequence we shall prove later using the microlocal approach: if ω and ω' are (locally) Hadamard states, then $M \times M \ni (x, y) \mapsto \omega_2(x, y) - \omega'_2(x, y)$ is smooth. This fact is far from obvious, since Definition 2.2 guarantees only that the difference is smooth when x and y belong to the same sufficiently small neighborhood.
An important feature of the global Hadamard condition for a quasifree Hadamard state is that it *propagates* [26, 79]: If it holds in a neighborhood of a Cauchy surface it holds in a neighborhood of any other Cauchy surface. We shall come back later to this property making use of the local notion only. This fact, together with the last comment in (3) proves that quasifree Hadamard states for massive fields (and $\xi = 0$) exist in globally hyperbolic spacetimes by means of a deformation argument similar to the one exploited in Sect. 1.5.2.
We shall not insist on the distinction between the *global* and the *local* Hadamard property because, in [70], it was established that a local Hadamard state on $\mathcal{A}(\boldsymbol{M})$ is also a global one (the converse is automatic). It was done exploiting the *microlocal approach*, which we shall discuss shortly.

(5) It is possible to prove that [79] if a globally hyperbolic spacetime has one (and thus all) compact Cauchy surface, all quasifree Hadamard states for the massive KG field (with $\xi = 0$) are unitarily equivalent. There is however a more general result [78] (actually stated in terms of Weyl algebras). Consider an open region O which defines a globally hyperbolic spacetime $\boldsymbol{O}$ in its own right, in a globally hyperbolic spacetime $\boldsymbol{M}$, such that $\overline{O}$ is compact, and a pair of quasifree Hadamard states ω_1, ω_2 for the massive KG field ($\xi = 0$) on $\mathcal{A}(\boldsymbol{M})$. It is possible to prove that the restriction to $\mathcal{A}(\boldsymbol{O}) \subset \mathcal{A}(\boldsymbol{M})$ of any density matrix state associated to the GNS construction of ω_1 coincides with the restriction to $\mathcal{A}(\boldsymbol{O})$ of some density matrix state associated to the GNS construction of ω_2.

(6) The author of these lecture notes discovered and closed in [63] a subtle technical gap in the original definition of Hadamard states [48]. The definition has to be slightly changed in order to agree with the microlocal analysis definition we shall se in the next section. ■

It is now possible to recast all the content of Sect. 2.1.1 in a generic globally hyperbolic spacetime $\boldsymbol{M}$ enlarging the algebra of observables $\mathcal{A}(\boldsymbol{M})$, at the level of quadratic forms, defining the expectation values of Wick monomials $:\phi^n:(f)$ with respect to Hadamard states ω or vector states $\Psi \in \mathcal{D}_\omega$ with ω Hadamard. Remarkably, all of that can be done simultaneously for all states in the said class without picking out any reference state. This is the first step for a completely *local* and *covariant* definition. First, define for smooth functions f_k supported in a convex normal neighborhood C

$$:\phi(f_1)\cdots\phi(f_n):_H := \int_{M^n} :\phi(x_1)\cdots\phi(x_n):_H \; f_1(x_1)\ldots f_n(x_n)\,\mathrm{dvol}_{\boldsymbol{M}^n}(x_1,\ldots,x_n)\,, \tag{2.23}$$

where we have defined the *completely symmetrized* formal kernels,

$$:\phi(x_1)\cdots\phi(x_n):_H := \frac{1}{i^n}\frac{\delta^n}{\delta f(x_1)\cdots\delta f(x_n)}\bigg|_{f=0} e^{i\phi(f)+\frac{1}{2}H_{0+}(f,f)}\,. \tag{2.24}$$

Notice that H_{0+} can be replaced with its symmetric part H^S_{0+} and that, in (2.23), only the symmetric part of the product $f_1(x_1)\ldots f_n(x_n)$ produces a contribution to the left-hand side. Equivalently, these monomials regularized with respect to the Hadamard parametrix can be define recursively as

$$\begin{aligned}
:\phi(f_1):_H \;&:=\; \phi(f_1)\\
:\phi(f_1)\cdots\phi(f_{n+1}):_H \;&:=\, :\phi(f_1)\cdots\phi(f_n):_H \;\phi(f_{n+1})\\
&\qquad -\sum_{l=1}^{n} :\phi(f_1)\cdots\widetilde{\phi(f_l)}\cdots\phi(f_n):_H \;\; \tilde{H}(f_l,f_{n+1})\,,
\end{aligned} \tag{2.25}$$
$$\text{where } \tilde{H} = H^S_{0+} + \frac{i}{2}E,$$

in analogy with the relation between Equations (2.11) and (2.14). Now consider a quasifree Hadamard state ω and indicate by ω_Ψ the generic state indexed by the normalized vector $\Psi \in \mathfrak{D}_\omega$ (so that $\omega = \omega_\Psi$ when Ψ is the Fock vacuum). By induction, it is possible to prove that, for $n \geq 2$, there is a *jointly smooth kernel*

$$\omega_\Psi(:\phi(x_1)\cdots\phi(x_n):_H)$$

which produces $\omega_\Psi(:\phi(f_1)\cdots\phi(f_n):_H)$ by integration when the supports of the functions f_k belong to C.

Exactly as for the Minkowski vacuum representation, this result arises from (2.23) as a consequence of the following list of facts:

(a) ω is quasifree so that Definition 1.57 can be used to compute the said kernels,

(b) $\Psi \in \mathfrak{D}_\omega$ so that the expansion (2.7) can be used,

(c) the functions in (2.22) are smooth (see (4) in Remark 2.3 and section 2.2.2),

(d) the local singularity of two-point functions of quasifree Hadamard states is the same as the one of H_{0+}.

Consider a normalized $\Psi \in \mathfrak{D}_\omega$, given without loss of generality by

$$\Psi = \sum_{n\geq 0, i_1,\ldots,i_n\geq 1} C^{(n)}_{i_1\ldots i_n}\hat{\Phi}_\omega(\psi^{(n)}_{i_1})\cdots\hat{\Phi}_\omega(\psi^{(n)}_{i_n})\Psi_\omega\,, \tag{2.26}$$

where only a finite number of coefficients $C^{(n)}_{i_1\ldots i_n} \in \mathbb{C}$ is non-vanishing, which defines the algebraic state $\omega_\Psi(\cdot) = \langle \Psi | (\cdot)\Psi\rangle$. Then, for instance, with the same argument used to achieve (2.10) we have

$$\omega_\Psi(:\!\phi(x_1)\phi(x_2)\!:_H) - \omega(\phi(x_1)\phi(x_2)) + \tilde{H}(x_1, x_2) \in C^\infty(M \times M)\,, \tag{2.27}$$

where the smoothness is assured because the resulting expression consists of a linear combination of products like $\omega(\phi(x_1)\phi(g))\omega(\phi(f)\phi(x_2))$, with some test functions f and g. Note that the combination of the second and third terms in (2.27) can be rewritten as

$$\begin{aligned}\omega(\phi(x_1)\phi(x_2)) - \tilde{H}(x_1, x_2) &= \omega(\phi(x_1)\phi(x_2)) - H^S_{0^+}(x_1, x_2) - \frac{i}{2}E(x_1, x_2)\\ &= \frac{1}{2}\omega(\phi(x_1)\phi(x_2)) - H_{0^+}(x_1, x_2)\\ &\quad + \frac{1}{2}\omega(\phi(x_2)\phi(x_1)) - H_{0^+}(x_2, x_1),\end{aligned}$$

which is obviously smooth by the very definition of the Hadamard property of ω. Hence $\omega_\Psi(:\!\phi(x_1)\phi(x_2)\!:_H)$ is also smooth. We are in a position to define the expectation values of the Wick monomials for $f \in C^\infty_c(M)$ such that its support is included in C,

$$\omega_\Psi(:\!\phi^n\!:_H(f)) = \int_{M^n} \omega_\Psi(:\!\phi(x_1)\cdots\phi(x_n)\!:_H) f(x_1)\delta(x_1, \ldots, x_n)\mathrm{dvol}_{\boldsymbol{M}^n} \tag{2.28}$$

Exactly as before, polarization extends the definition to a quadratic form on $\mathcal{D}_\omega \times \mathcal{D}_\omega$. There is no guarantee that operators fitting these quadratic forms really exist. The question of their existence as operators will be addressed later, in Section 2.2.3.

Remark 2.4.

(1) The restriction on the support of f is not very severe. The restriction can be removed making use of a partition of unity (see for example [59, 42] referring to more generally differentiated Wick polynomials).

(2) The given definition of $\omega(:\!\phi^n\!:_H(f))$ is affected by several ambiguities due to the effective construction of H_ϵ. A complete classification of these ambiguities, promoting Wick polynomials to properly defined elements of a $*$-algebra, can be presented from a very general viewpoint, adopting a *locally covariant framework* [40, 51], we shall not consider in this introductory review [14, 34]. We only say that these ambiguities are completely described by a class of scalar polynomials in the mass and Riemann curvature tensor and their covariant derivatives. The finite order of these polynomials is fixed by scaling properties of Wick polynomials. The coefficients of the polynomials are smooth functions of the parameter ξ. We stress that this classification is the first step of the ultraviolet renormalization program which, in curved spacetime and differently from flat spacetime where all curvature vanish, starts with classifying the finite renormalization counterterms of Wick polynomials instead of only dealing with time-ordered Wick polynomials.

(3) Easily extending the said definition, using the fact that $\omega_\Psi(:\!\phi(x_1)\phi(x_2)\!:_H)$ is smooth and thus can be differentiated, one can define a notion of *differentiated Wick polynomials* which include, in particular, the *stress energy tensor* as a Hermitian quadratic form evaluated on Hadamard states or vector states in the dense subspace $\mathcal{D}_\omega$ in the GNS Hilbert space of a Hadamard state ω. This would be enough to implement the computation of the back reaction of the quantum matter in a given state to the geometry of the spacetime through (2.3) especially in cosmological scenario (see [34]). This program has actually been initiated much earlier than the algebraic approach was adopted in QFT in curved spacetime [9] and the notion of Hadamard state was invented, through several steps, in this context. The requirements a physically sensible object $\omega(:T_{ab}:_H(x))$ should satisfy was clearly discussed by several authors, Wald in particular (see [79] for an complete account and [35] for more recent survey). The most puzzling issue in this context perhaps concerns the interplay of the conservation requirement $\nabla_a\omega(:T^{ab}:_H(x)) = 0$ and the appearance of the *trace anomaly*. We shall come back to these issues later, at the end of Section 2.2.3. ■

2.2 Micrololocal analysis characterization

2.2.1 The notion of wavefront set and its elementary properties

Microlocal analysis permits us to completely reformulate the theory of Hadamard states into a much more powerful formulation where, in particular, the Wick polynomials can be defined as proper operators and not only Hermitian quadratic forms.

Following [34, 77], let us start be introducing the notion of wave front set. To motivate it, let us recall that a smooth function on $\mathbb{R}^m$ with compact support has a rapidly decreasing Fourier transform. If we take an distribution u in $\mathcal{D}'(\mathbb{R}^m)$ and multiply it by an $f \in \mathcal{D}(\mathbb{R}^m)$ with $f(x_0) \neq 0$, then uf is an element of $\mathcal{E}'(\mathbb{R}^m)$, *i.e.*, a distribution with compact support. If fu were smooth, then its Fourier transform $\widehat{fu}$ would be smooth and rapidly decreasing (with all its derivatives). The failure of fu to be smooth in a neighbourhood of x_0 can therefore be quantitatively described by the set of directions in Fourier space where $\widehat{fu}$ is not rapidly decreasing. Of course it could happen that we choose f badly and therefore 'cut' some of the singularities of u at x_0. To see the full singularity structure of u at x_0, we therefore need to consider all test functions which are non-vanishing at x_0. With this in mind, one first defines the wave front set of distributions on (open subsets of) $\mathbb{R}^m$ and then extends it to curved manifolds in a second step.

In the rest of the chapter $\mathcal{D}(M) := C_c^\infty(M, \mathbb{C})$ for every smooth manifold M. An open neighbourhood G of $k_0 \in \mathbb{R}^m$ is called **conic** if $k \in G$ implies $\lambda k \in G$ for all $\lambda > 0$.

Definition 2.5. [Wavefront set] Let $u \in \mathcal{D}'(U)$, with open $U \subset \mathbb{R}^m$. A point $(x_0, k_0) \in U \times (\mathbb{R}^m \setminus \{0\})$ is called a **regular directed** point of u if there is $f \in \mathcal{D}(U)$ with $f(x_0) \neq 0$ such that, for every $n \in \mathbb{N}$, there is a constant $C_n \geq 0$ fulfilling

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

for all k in an open conic neighbourhood of k_0. The **wave front set** $WF(u)$, of $u \in \mathcal{D}'(U)$ is the complement in $U \times (\mathbb{R}^m \setminus \{0\})$ of the set of all regular directed points of u. ∎

Remark 2.6. Obviously, if $u, v \in \mathcal{D}'(U)$ the wavefront set is not additive and, in general, one simply has $WF(u+v) \subset WF(u) \cup WF(v)$.

As, an elementary example, let us consider the wavefront set of the distribution $\delta_y(x) = \delta(x-y)$ on $\mathbb{R}^n$ [77, p.103]:

$$WF(\delta_y) = \{(y, k_y) \in T^*\mathbb{R}^n \mid k_y \neq 0\}. \tag{2.29}$$

If $U \subset \mathbb{R}^m$ is an open and non-empty subset, T^*U is naturally identified with $U \times \mathbb{R}^m$. In the rest of the chapter $T^*U \setminus 0 := \{(x,p) \in T^*U \mid p \neq 0\}$.
If $U \subset \mathbb{R}^m$ is an open non-empty set, $\Gamma \subset T^*U \setminus 0$ is a **cone** when $(x, \lambda k) \in \Gamma$ if $(x,k) \in \Gamma$ and $\lambda > 0$. If the mentioned cone Γ is closed *in the topology of* $T^*U \setminus 0$, we define

$$\mathcal{D}'_\Gamma := \{u \in \mathcal{D}'(U) \mid WF(u) \subset \Gamma\}\,.$$

∎

Remark 2.7. All these definitions can be restated for the case of U replaced with a general smooth manifold and we shall exploit this opportunity shortly. ∎
We are in a position to define a relevant notion of convergence [44].

Definition 2.8. [Convergence in Hörmander pseudotopology] If $u_j \in \mathcal{D}'_\Gamma(U)$ is a sequence and $u \in \mathcal{D}'_\Gamma(U)$, we write $u_j \to u$ in $\mathcal{D}'_\Gamma(U)$ if both the conditions below hold.

(i) $u_j \to u$ weakly in $\mathcal{D}'(U)$ as $j \to +\infty$,

(ii) $\sup_j \sup_V |\xi|^N |\widehat{\phi u_j}(p)| < \infty$, $N = 1, 2, \ldots$, if $\phi \in \mathcal{D}(U)$ and $V \subset T^*U$ is any closed cone, whose projection on U is $\mathrm{supp}\,(\phi)$, such that $\Gamma \cap V = \varnothing$.
In this case, we say that u_j converges to u in the **Hörmander pseudotopology**. ∎

It turns out that test functions (whose wavefront set is always empty as said below) are dense even with respect to that notion of convergence [44].

Proposition 2.9. *If $u \in \mathcal{D}'_\Gamma(U)$, there is a sequence of smooth functions $u_j \in \mathcal{D}(U)$ such that $u_j \to u$ in $\mathcal{D}'_\Gamma(U)$.*
Let us immediately state a few elementary properties of wave front sets [43, 44, 77, 25]. We remind the reader that $x \in U$ is a **regular point** of a distribution $u \in \mathcal{D}'(U)$ if there is an open neighborhood $O \subset U$ of x such that $\langle u, f\rangle = \langle h_u, f\rangle$ for some $h_u \in \mathcal{D}(U)$ and every $f \in \mathcal{D}(U)$ supported in O. The closure of the complement of the set of regular points is the **singular support** of u by definition.

Theorem 2.10. [Elementary properties of WF] *Let $u \in \mathcal{D}'(U)$, $U \subset \mathbb{R}^m$ open and non-empty.*

(a) *u is smooth if and only if $WF(u)$ is empty. More precisely, the* singular support *of u is the projection of $WF(u)$ on $\mathbb{R}^m$.*

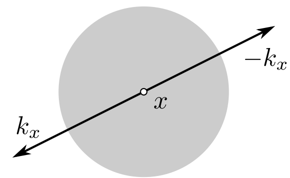

Figure 2.1: Wavefront set of $\delta(x,y)$ on $M \times M$, defined in (2.30), consists of points of the form $(x,x,k_x,-k_x)$, $(x,k_x) \in T^*M \setminus 0$.

(b) *If P is a partial differential operator on U with smooth coefficients:*

$$WF(Pu) \subset WF(u)\,.$$

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

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

where $\chi^* k$ denotes the pull-back of χ in the sense of cotangent vectors.

(d) *Let $V \subset \mathbb{R}^n$ be an open set and $v \in \mathcal{D}'(V)$, then $WF(u \otimes v)$ is included in*

$$(WF(u) \times WF(v)) \cup ((supp\, u \times \{0\}) \times WF(v)) \cup (WF(u) \times (supp\, v \times \{0\}))\,.$$

(e) *Let $V \subset \mathbb{R}^n$, $K \in \mathcal{D}'(U \times V)$ and $f \in \mathcal{D}(V)$, then*

$$WF(\mathcal{K}f) \subset \{(x,p) \in TU \setminus 0 \mid (x,y,p,0) \in WF(K) \text{ for some } y \in supp\,(f)\}\,,$$

where $\mathcal{K} : \mathcal{D}(V) \mapsto \mathcal{D}'(U)$ is the continuous linear map associated to K in view of Schwartz kernel theorem.

The result (e), with a suitably improved statement, can be extended to to the case of f replaced by a distribution [44].
From (c) we conclude that the wave front set transforms covariantly under diffeomorphisms as a subset of T^*U, with U an open subset of $\mathbb{R}^m$. Therefore we can immediately extend the definition of WF to distributions on a manifold M simply by patching together wave front sets in different coordinate patches of M with the help of a partition of unity. As a result, for $u \in \mathcal{D}'(M)$, $WF(u) \subset T^*M \setminus 0$. Also the notion of convergence in the Hörmander pseudotopology easily extends to manifolds. All the statements of theorem 2.10 extend to the case where U and V are smooth manifolds.

Following up on (2.29), an elementary example of a distribution on a manifold is $\delta(x,y)$ defined on $M \times M$. Its wavefront set is (Figure 2.1)

$$WF(\delta) = \{(x,x,k_x,-k_x) \in T^*M^2 \setminus 0 \mid (x,k_x) \in T^*M \setminus 0\}\,. \tag{2.30}$$

The necessity of the sign reversal in the covector $-k_x$ corresponding to the second copy of M can be seen from the formula $\delta(x, y) = \delta(x - y)$ on $\mathbb{R}^n$.

To conclude this very short survey, we wish to stress some remarkable results of wavefront set technology respectively concerning (a) the theorem of *propagation of singularities*, (b) the *product of distributions*, (c) *composition of kernels.*

Let us start with an elementary version of the celebrated *theorem of propagation of singularities* formulated as in [77].

Remark 2.11.

(1) Let us remind the reader that if, in local coordinates, $P = \sum_{|\alpha|\leq m} a_\alpha(x)\partial^\alpha$ is a differential operator of order $m \geq 1$ (it is assumed that $a_\alpha \neq 0$ for some α with $|\alpha| = m$) on a manifold M, where a is a *multi-index* [44], and a_α are smooth coefficients, then the polynomial $\sigma_P(x,p) = \sum_{|\alpha|=m} a_\alpha(x)(ip)^\alpha$ is called the **principal symbol** of P. It is possible to prove that $(x, \xi) \mapsto \sigma_P(x,p)$ determines a well defined function on T^*M which, in general is complex valued. The **characteristic set** of P, indicated by $char(P) \subset T^*M \setminus 0$, denotes the set of zeros of σ_P made of *non-vanishing* covectors. The principal symbol σ_P can be used as a *Hamiltonian function* on T^*M and the maximal solutions of Hamilton equations define the **local flow** of σ_P on T^*M.

(2) The principal symbol of the Klein-Gordon operator is $-g^{ab}(x)p_ap_b$. It is an easy exercise [77] to prove that if $\boldsymbol{M}$ is a Lorentzian manifold and P is a **normally hyperbolic operator**, i.e., the principal symbol is the same as the one of Klein-Gordon operator, then the integral curves of the local flow of σ_P are nothing but the lift to T^*M of the *geodesics* of the metric g parametrized by an *affine parameter*. Finally, $char(P) = \{(x,p) \in T^*M \setminus 0 \mid g^{ab}(x)p_ap_b = 0\}$ ■

Theorem 2.12. [Microlocal regularity and propagation of singularities] *Let P be a differential operator on a manifold M whose principal symbol is real valued, if $u, f \in \mathcal{D}'(M)$ are such that $Pu = f$ then the following facts hold.*

(a) *$WF(u) \subset char(P) \cup WF(f)$,*

(b) *$WF(u) \setminus Wf(f)$ is invariant under the local flow of σ_P on $T^*M \setminus WF(f)$.* Let us conclude with the famous Hörmander definition of *product of distributions* [43, 44]. We need a preliminary definition. If $\Gamma_1, \Gamma_2 \subset T^*M \setminus 0$ are closed cones,

$$\Gamma_1 + \Gamma_2 := \{(x, k_1 + k_2) \subset T^*M \mid (x, k_1) \in \Gamma_1,\ (x, k_2) \in \Gamma_2 \text{ for some } x \in M\}.$$

Theorem 2.13. [Product of distributions] *Consider a pair of closed cones $\Gamma_1, \Gamma_2 \subset T^*M \setminus 0$. If*

$$\Gamma_1 + \Gamma_2 \not\ni (x, 0) \quad \textit{for all } x \in M,$$

then there is a unique bilinear map, the **product** *of u_1 and u_2,*

$$\mathcal{D}'_{\Gamma_1} \times \mathcal{D}'_{\Gamma_2} \ni (u_1, u_2) \mapsto u_1u_2 \in \mathcal{D}'(M),$$

such that

(i) it reduces to the standard pointwise product if $u_1, u_2 \in \mathcal{D}(M)$,

(ii) it is jointly sequentially continuous in the Hörmander pseudotopology: If $u_j^{(n)} \to u_j$ in $D_{\Gamma_j}(M)$ for $j = 1, 2$ then $u_1^{(n)} u_2^{(n)} \to u_1 u_2$ in $\mathcal{D}_\Gamma(M)$, where Γ is a closed cone in $T^*M \setminus 0$ defined as $\Gamma := \Gamma_1 \cup \Gamma_2 \cup (\Gamma_1 \oplus \Gamma_2)$.
In particular the following bound always holds if the above product is defined:

$$WF(u_1 u_2) \subset \Gamma_1 \cup \Gamma_2 \cup (\Gamma_1 + \Gamma_2)\ . \tag{2.31}$$

From the examples (2.29) and (2.30) and the simple observation that

$$\mathbb{R}^n \setminus \{0\} + \mathbb{R}^n \setminus \{0\} = \mathbb{R}^n \ni 0, \tag{2.32}$$

it is clear that the multiplication of two δ-functions with overlapping supports, as is to be expected, does not satisfy the above conditions.

Let us come to the last theorem concerning the composition of distributional kernels. Let X, Y be smooth manifolds. If $K \in \mathcal{D}'(X \times Y)$, the continuous map associated to K by the Schwartz kernel theorem will be denoted by $\mathcal{K} : \mathcal{D}(Y) \to \mathcal{D}'(X)$. We shall also adopt the following standard notations:

$$\begin{aligned}
WF(K)_X &:= \{(x,p) \mid (x,y,p,0) \in WF(K) \quad \text{for some } y \in Y\}\ ,\\
WF(K)_Y &:= \{(y,q) \mid (x,y,0,q) \in WF(K) \quad \text{for some } x \in X\}\ ,\\
WF'(K) &:= \{(x,y,p,q) \mid (x,y,p,-q) \in WF(K)\}\ ,\\
WF'(K)_Y &:= \{(y,q) \mid (x,y,0,-q) \in WF(K) \quad \text{for some } x \in X\}\ .
\end{aligned}$$

Theorem 2.14. [Composition of kernels] *Consider three smooth manifolds X, Y, Z and $K_1 \in \mathcal{D}'(X \times Y)$, $K_2 \in \mathcal{D}'(Y \times Z)$. If $WF'(K_1)_Y \cap WF(K_2)_Y = \varnothing$ and the projection*

$$supp\, K_2 \ni (y,z) \mapsto z \in Z$$

is proper (that is, the inverse of a compact set is compact), then the composition $\mathcal{K}_1 \circ \mathcal{K}_2$ is well defined, giving rise to $K \in \mathcal{D}'(X, Z)$, and reduces to the standard one when the kernel are smooth. It finally holds (the symbol $\circ$ denoting the composition of relations)

$$\begin{aligned}
WF'(K) \subset WF'(K_1) \circ WF'(K_2) \cup (WF(K_1)_X \times Z \times \{0\})\\
\cup\, (X \times \{0\} \times WF'(K_2)_Z)\ .
\end{aligned} \tag{2.33}$$

Comparing with (2.30), note that $WF'(\delta)$ is the diagonal subset $\Delta \subset T^*M \times T^*$. In the composition of relations, Δ acts as an identity, which is consistent with the above theorem and the fact that $\delta(x,y)$ acts as an identity for the composition of distributional kernels.

2.2.2 Microlocal reformulation

Let us focus again on the two-point function of Minkowski quasifree vacuum state. Form (1.91) we see that the singular support of $\omega_{\mathbb{M}2}(x,y)$ is the set of couples $(x,y) \in \mathbb{M} \times \mathbb{M}$ such that $x-y$ is *light like*. From (a) in theorem 2.10, we conclude that $WF(\omega_{\mathbb{M}2})$ must project onto this set. On the other hand (1.92) can be re-written as

$$\omega_{\mathbb{M}2}(x,y) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^4} e^{-i(px+qy)} \theta(p^0) \delta(p^2+m^2) \delta(p+q) d^4q d^4p \,, \tag{2.34}$$

where translational invariance is responsible for the appearance of $\delta(p+q)$ in (2.34). From this couple of facts, also noticing the presence of $\theta(p^0)$ in the integrand, one guesses that the wave front set of the Minkowski two-point function must be

$$WF(\omega_{\mathbb{M}2}) = \left\{(x,y,p,-p) \in T^*M^2 \mid p^2 = 0,\ p \,||\, (x-y),\ p^0 > 0\right\} \,. \tag{2.35}$$

Identity (2.35) is, in fact, correct and holds true also for $m = 0$ [71]. The condition $p^0 > 0$ encodes the *energy positivity* of the Minkowski vacuum state. Notice that the couples $(x,y) \in \mathbb{M} \times \mathbb{M}$ giving contribution to the wavefront set are always connected by a *light-like geodesic* cotangent to p. For $x = y$ there are infinitely many such geodesics, if we allow ourselves to consider zero length curves (consisting of a single point) with a given tangent vector.

The structure (2.35) of the wavefront set of the two-point function of Minkowski vacuum is a particular case of the general notion of a Hadamard state. We re-adapt here the content of the cornerstone papers [69, 70] to our formulation. We note that we do not make use of the global Hadamard condition (see (4) in Remark 2.3). The following theorem collects various results of [69, 70].

Theorem 2.15. ["Radzikowski theorem"] *For a 4-dimensional globally hyperbolic (time oriented) spacetime $\boldsymbol{M}$ and referring to the unital $*$-algebra of Klein-Gordon quantum field $\mathcal{A}(\boldsymbol{M})$ with $m^2, \xi \in \mathbb{R}$ arbitrarily fixed, let ω be a state on $\mathcal{A}(\boldsymbol{M})$, not necessarily quasifree.*
(a) *The following statements are equivalent,*

(i) ω is Hadamard in the sense of Def. 2.2,

(ii) the wavefront set of the two-point function ω_2 has the **Hadamard form** *on $\boldsymbol{M}$ or equivalently, it satisfies the* **microlocal spectrum condition** *on $\boldsymbol{M}$:*

$$WF(\omega_2) = \left\{(x,y,k_x,-k_y) \in T^*M^2 \setminus 0 \mid (x,k_x) \sim (y,k_y),\ k_x \triangleright 0\right\} \stackrel{def}{=} \mathcal{H}. \tag{2.36}$$

Here, $(x,k_x) \sim (y,k_y)$ means that there exists a null geodesic γ connecting x to y such that k_x is coparallel and cotangent to γ at x and k_y is the parallel transport of k_x from x to y along γ, Figure 2.2. $k_x \triangleright 0$ means that k_x does not vanish and is future-directed ($k_x(v) \geq 0$ for all future-directed $v \in T_xM$), Figure 2.3.
(b) *If ω' is another Hadamard state on $\mathcal{A}(\boldsymbol{M})$, then $\omega_2 - \omega_2' \in C^\infty(M \times M, \mathbb{C})$.*

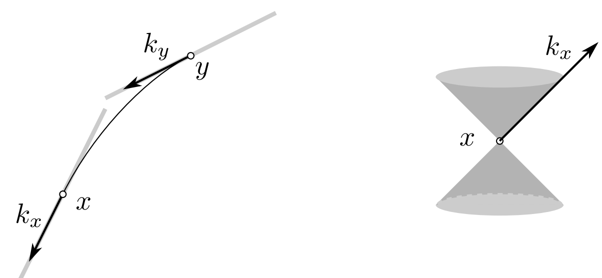

Figure 2.2: The null geodesic relation $(x, k_x) \sim (x, k_y)$ defined in Theorem 2.15. The points x and y must be linked by a null geodesic, the covectors k_x and k_y must be parallel transported images of each other and both covectors must be coparallel, all with respect to the same null geodesic. Any causal ordering between x and y is admissible. Also, k_x, $-k_x$ and λk_x ($\lambda \neq 0$) are all considered coparallel to the same geodesic. In the coincident case, $x = y$, we agree that there are infinitely many (zero-length) null geodesics joining x to itself, corresponding to different non-vanishing null covectors $k_x \in T^*_x M$.

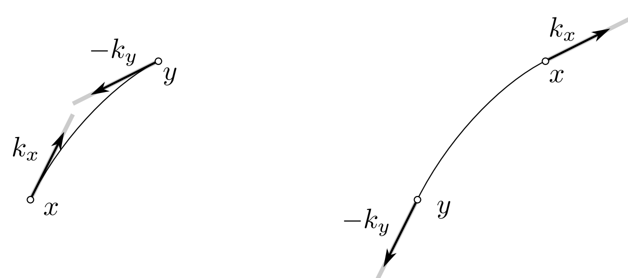

Figure 2.3: The Hadamard form $\mathcal{H}$ of a wavefront set, as defined in Theorem 2.15. It consists of a subset of points $(x, y, k_x, -k_y) \in T^*M^2$, where $(x, k_x) \sim (y, k_y)$ are linked but the null geodesic relation (Figure 2.2). The restriction is that $k_x \triangleright 0$, meaning that $k_x(v) \geq 0$ for any future-directed $v \in T_x M$. We illustrate the two possible causal orderings $x \in J^-(y)$ and $x \in J^+(y)$.

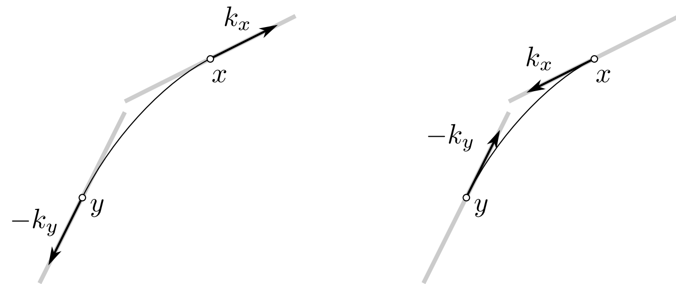

Figure 2.4: The wavefront sets of the retarded fundamental solution E^+ of the Klein-Gordon operator, as defined in Proposition 2.16, consist of the union of $WF(\delta)$ (Figure 2.1) and of the points $(x, k_x, y, -k_y) \in T^*M^2$, where $(x, k_x) \sim (y, k_y)$ are linked by the geodesic relation (Figure 2.2), with the causal precedence condition $x \in J^+(y)$. We illustrate the two cases when k_x is coparallel and anti-coparallel to the future-directed geodesic from y to x. The wavefront set of the advanced fundamental solution E^- is defined in the same way, with the exception that we require the causal precedence condition $x \in J^-(y)$ instead.

Proof. (a) Suppose that ω satisfies (i), then it is globally Hadamard in the sense[4] of [69] due to Theorem 9.2 in [70]. Theorem 5.1 in [69] implies that (ii) holds. Conversely, if (ii) is valid, Theorem 5.1 in [69] entails that ω is globally and thus locally Hadamard so that (i) holds true. (b) immediately arises from Theorem 4.3 in [70]. $\square$

It is also helpful to have a characterization of the wavefront set of the retarded and advanced fundamental solutions [69, 77].

Proposition 2.16. *The retarded and advanced fundamental solutions of the Klein-Gordon operator $P = \Box_{\boldsymbol{M}} + m^2 + \xi R$ on $\boldsymbol{M}$, $E^+, E^- \in \mathcal{D}'(M \times M)$ respectively, have the following wavefront sets (Figure 2.4):*

$$\begin{aligned} WF(E^\pm) &= WF(\delta) \\ &\quad \cup \big\{(x, y, k_x, -k_y) \in T^*M^2 \setminus 0 \mid (x, k_x) \sim (y, k_y), x \in J^\pm(y)\big\} \stackrel{def}{=} \mathcal{F}_\pm, \end{aligned} \tag{2.37}$$

where $\sim$ denotes the same relation as in Theorem 2.15.

With this result and the microlocal technology previously introduced we can prove some remarkable properties of Hadamard states, especially in relation with what was already discussed in (4) in Remark 2.3. The second statement, for $n = 4$, implies that the singularity structure of Hadamard states propagates through the spacetime.

[4]Results in [69, 70] are stated for $\xi = 0$ in KG operator, however they are generally valid for m^2 replaced by a given smooth function, as specified at the beginning of p. 533 in [69].

Proposition 2.17. *Consider a state ω on $\mathcal{A}(\boldsymbol{M})$, with $\omega_2 \in \mathcal{D}'(M \times M)$, where $\boldsymbol{M}$ is a (time oriented) globally hyperbolic spacetime with dimension $n \geq 2$. The following facts hold.*

(a) *If $WF(\omega_2)$ has the Hadamard form, then $M \ni x \mapsto \omega_2(x, f)$ is smooth for every $f \in C_c^\infty(M)$.*

(b) *If $WF(\omega_2 \restriction_{O\times O})$ has the Hadamard form on O, where O is an open neighborhood of a smooth spacelike Cauchy surface Σ of $\boldsymbol{M}$, then $WF(\omega_2)$ has the Hadamard form on $\boldsymbol{M}$.*

Proof. (a) From (e) in Theorem 2.10 and the Hadamard form of $WF(\omega_2)$ we conclude that $WF(\omega_2(\cdot, f)) = \varnothing$. Next, (a) in Theorem 2.10 implies the thesis.

(b) The 2-point function $\omega_2(x, y)$ is a bisolution of the Klein-Gordon operator $P = \Box_{\boldsymbol{M}} + m^2 + \xi R$, as in (1.49). So the value of $\omega_2(f, g)$, for $f, g \in C_0^\infty(M)$, depends on the arguments only up to the addition of any term from $P[C_0^\infty(M)]$. In fact, we can choose $h, k \in C^\infty$ such that $\operatorname{supp}(f + P[h])$ and $\operatorname{supp}(g + P[k])$ are both contained in O. More precisely, we can define an $S \in \mathcal{D}'(O \times M)$ such that the corresponding operator maps $\mathcal{S}\colon C_0^\infty(M) \to C_0^\infty(O)$ and we have the identity $\omega_2 = \mathcal{S}^t \circ \omega_2 \circ \mathcal{S}$. Then, using the result of Theorem 2.14 on the composition of kernels and the fact that ω_2 has the Hadamard form on O, we can show that ω_2 has the Hadamard form on all of M.

Consider a smooth partition of unity $\chi_+ + \chi_- = 1$ adapted to the Cauchy surface Σ. That is, there exist two other Cauchy surfaces, Σ_+ in the future of Σ and Σ_- in the past of Σ, such that $\operatorname{supp} \chi_+ \subset J^+(\Sigma_-)$ and $\operatorname{supp} \chi_- \subset J^-(\Sigma_+)$. Such an adapted partition of unity always exists if O is globally hyperbolic in its own right and, if not, since $\boldsymbol{M}$ is globally hyperbolic, any open neighborhood of Σ will contain a possibly smaller neighborhood of Σ that is also globally hyperbolic [8, 6].

Let $\mathcal{S}f = f - P[\chi_+ E^- f + \chi_- E^+ f]$, with the corresponding integral kernel

$$S(x, y) = \delta(x, y) - P_x[\chi_+(x) E^-(x, y) + \chi_-(x) E^+(x, y)], \tag{2.38}$$

where the subscript on P_x means that it is acting only on the x variable. A straight forward calculation shows that S has the desired properties. Multiplication by a smooth function and the application of a differential operator does not increase the wavefront set, hence

$$WF(S) \subset WF(\delta) \cup WF(E^-) \cup WF(E^+) \tag{2.39}$$

as a subset of $T^*(O \times M)$. The δ-function has the wavefront set

$$WF(\delta) = \{(x, x, k_x, -k_x) \in T^*M^2 \setminus 0 \mid (x, k_x) \in T^*M \setminus 0\}\,. \tag{2.40}$$

The wavefront sets $\mathcal{F}_\pm = WF(E^\pm)$ of the retarded and advanced fundamental solutions was given in Proposition 2.16. The Hadamard form $\mathcal{H}$ of the wavefront set was defined in Theorem 2.15. We can now appeal to Theorem 2.14 on the wavefront set of the composition of kernels to how that $WF(\omega_2) = WF(\mathcal{S}^t \circ \omega_2 \circ \mathcal{S}) \subset \mathcal{H}$. The first thing to check is that $WF(S)_{M_i}$, $WF(\omega_2)_{M_i}$, $i = 1, 2$ denoting respectively the first and the second factor in $M \times M$, are all empty, because they contain no element of the form $(x, y, k_x, 0)$ or $(x, y, 0, k_y)$. Second, due to the hypothesis $WF'(\omega_2)|_O \subset \mathcal{H}'_O$, the symmetry of the composition and the fact that composition with $\delta(x,y)$ leaves any wavefront set invariant, it is sufficient to check that the compositions of wavefront sets as relations satisfy $\mathcal{H}'_O \circ \mathcal{F}'_\pm \subset \mathcal{H}'_M$.

Consider any $(x,y,k_x,k_y) \in \mathcal{H}'_O$ and $(y,z,k_y,k_z) \in \mathcal{F}'_\pm$, so that $(x,z,k_x,k_z) \in \mathcal{H}'_O \circ \mathcal{F}'_\pm$. Then $(x,k_x) \sim (y,k_y)$ and $(y,k_y) \sim (z,k_z)$ in M according to the relation $\sim$ defined in Theorem 2.15, so that $(x,k_x) \sim (z,k_z)$ by transitivity of that relation in M. The only question is about the allowed orientations of k_x and k_y. By the Hadamard condition on O, we have $k_x \triangleright 0$ and $k_y \triangleright 0$. On the other hand, the condition of being a point in $\mathcal{F}_\pm$ induces the condition that either both $k_y \triangleright 0$ and $k_z \triangleright 0$ or both $k_y \triangleleft 0$ and $k_z \triangleleft 0$. Combining the two conditions we find that $k_z \triangleright 0$, and hence that $(x,z,k_x,k_z) \in \mathcal{H}'_M$. This concludes the proof. $\square$

Remark 2.18. With an elementary re-adaptation, statement (b) holds true weakening the hypotheses, only requiring that $\omega_2 \in \mathcal{D}'(M \times M)$ and that it satisfies KG equation in both arguments up to smooth functions $r, l \in C^\infty(M \times M, \mathbb{C})$, i.e. $P_x\omega_2(x,y) = l(x,y)$, $P_y\omega_2(x,y) = r(x,y)$. In this form, it closes a gap[5] present in the proof of the main result of [69], Theorem 5.1 (the fact that **1** implies **3**), and proves the statement on p. 548 of [69] immediately after the proof of the mentioned theorem. $\blacksquare$

The microlocal formulation gave rise to noticeable results also closing some long standing problems. In particular it was proved that the so called Unruh state describing black hole radiation is Hadamard [17] and that the analogous state, describing thermal radiation in equilibrium with a black hole, the so called Hartle-Hawking state is similarly Hadamard [73]. These results are physically important because they permit one to compute the back reaction of the quantum radiation on the geometry, since the averaged, renormalized stress-energy tensor $\omega(:T_{ab}:)$ can be defined in these states as previously discussed ((3) in Remark 2.4). Other recent applications concerned the definition of relevant Hadamard states in asymptotically flat spacetimes at null infinity [60, 31], and spacelike infinity [30]. Natural Hadamard states for cosmological models have been discussed [16] also in relation with the problem of the Dark Energy [15]. An improved semiclassical formulation where Einstein equations and the equation of evolution of the Hadamard quantum state and observables are solved simultaneously has been proposed in [68]. See [34, 5] for recent reviews also regarding fields with spin or helicity, in particular [18] for the vector potential field.

2.2.3 Algebra of Wick products

Let us come to the proof of existence of Wick monomials $:\phi^n:(f)$ as algebraic objects, since we only have defined the expectation values $\omega_\Psi(:\phi^n:(f))$ in (2.28). We first introduce normal Wick products *defined with respect to a reference quasifree Hadamard state* ω [13, 12, 40]. Referring to the GNS triple for ω, $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ Define the elements, symmetric under interchange of

[5]The gap is the content of the three lines immediately before th proof **(ii) 3 $\Rightarrow$ 2** on p. 547 of [69]: The reasoning presented there cannot exclude elements of the form either $(x_1, x_2, 0, p_2)$ or $(x_1, x_2, p_1, 0)$ from $WF(\omega_2)$ outside $\mathcal{N}$. The idea of our proof was suggested by N. Pinamonti to the authors.

$f_1, \ldots, f_n \in \mathcal{D}(M)$,

$$\hat{W}_{\omega,0} := \mathbb{1}\,, \quad \hat{W}_{\omega,n}(f_1,\ldots,f_n) :=:\hat{\Phi}_\omega(\psi_1)\cdots\hat{\Phi}_\omega(\psi_n):_\omega \quad \in \mathcal{A}(\boldsymbol{M})$$

for $n = 1, 2, \ldots$, where as before,

$$:\hat{\phi}_\omega(x_1)\cdots\hat{\phi}_\omega(x_n):_\omega := \frac{1}{i^n}\frac{\delta^n}{\delta f(x_1)\cdots\delta f(x_n)}\bigg|_{f=0} e^{i\hat{\phi}(f)+\frac{1}{2}\omega_2(f,f)} \tag{2.41}$$

The operators $\hat{W}_{\omega,n}(f_1,\ldots,f_n)$ can be extended to (or directly defined on) [12, 40] an invariant subspace of $\mathcal{H}_\omega$, the **microlocal domain of smoothness** [12, 40], $D_\omega \supset \mathcal{D}_\omega$, which is dense, invariant under the action of $\pi_\omega(\mathcal{A}(\boldsymbol{M}))$ and the associated unitary Weyl operators, and contains Ψ_ω and all of unit vectors of $\mathcal{H}_\omega$ which induce Hadamard quasifree states on $\mathcal{A}(\boldsymbol{M})$. The map

$$f_1 \otimes \cdots \otimes f_n \mapsto \hat{W}_{\omega,n}(f_1,\ldots,f_n)$$

uniquely extends by complexification and linearity to a map defined on

$$\mathcal{D}(M) \otimes \cdots \otimes \mathcal{D}(M)\,.$$

Finally, if $\Psi \in D_\omega$, the map $\mathcal{D}(M) \otimes \cdots \otimes \mathcal{D}(M) \ni h \mapsto \hat{W}_{\omega,n}(h)\Psi$ turns out to be continuous with respect to the relevant topologies: The one of $\mathcal{H}_\omega$ in the image and the one of $\mathcal{D}(M^n)$ in the domain. A *vector-valued distribution* $\mathcal{D}(M^n) \ni h \mapsto \hat{W}_{\omega,n}(h)$, uniquely arises this way. Actually, since $:\hat{\Phi}_\omega(\psi_1)\cdots\hat{\Phi}_\omega(\psi_n):_\omega$ is symmetric by construction, the above mentioned distribution is similarly symmetric and can be defined on the subspace $\mathcal{D}_n(M) \subset \mathcal{D}(M^n)$ of the symmetric test functions:

$$\mathcal{D}(M^n) \ni h \mapsto \hat{W}_{\omega,n}(h)\,.$$

By Lemma 2.2 in [12], if $\Psi \in D_\omega$ the wave front set $WF\left(\hat{W}_{\omega,n}(\cdot)\Psi\right)$ of the vector-valued distributions $t \mapsto \hat{W}_{\omega,n}(t)\Psi$, is contained in the set

$$\mathbf{F}_n(\boldsymbol{M}) := \{(x_1,k_1,\ldots,x_n,k_n) \in (T^*M)^n \setminus \{0\} | k_i \in V^-_{x_i}, i = 1,\ldots,n\}\,, \tag{2.42}$$

with $V_x^{+/-}$ denoting the set of all nonzero time-like and light-like covectors at x which are future/past directed. Theorem 2.13, which can be proved to hold in this case too, implies that we are allowed to define the product between a distribution t and a vector-valued distribution $\hat{W}_{\omega,n}(\cdot)\Psi$ provided $WF(t) + \mathbf{F}_n(M,\mathbf{g}) \not\ni \{(x,0)\,|\,x \in M^n\}$. To this end, with $\mathcal{D}'_n(M) \subset \mathcal{D}'(M^n)$ denoting the subspace of symmetric distributions, define

$$\mathcal{E}'_n(M) := \left\{t \in \mathcal{D}'_n(M)\,|\,\mathrm{supp}\,t \text{ is compact, } WF(t) \subset \mathbf{G}_n(M)\ \right\}$$

where

$$\mathbf{G}_n(M) := T^*M^n \setminus \left(\bigcup_{x\in M}(V_x^+)^n \cup \bigcup_{x\in M}(V_x^-)^n\right)\,.$$

It holds $WF(t) + \mathbf{F}_n(M) \not\ni \{(x,0) \,|\, x \in M^n\}$ for $t \in \mathcal{E}'_n(M)$. By consequence, the product

$$t \odot \hat{W}_{\omega,n}(\cdot)\Psi$$

of the distributions t and $\hat{W}_{\omega,n}(\cdot)\Psi$ can be defined for every $\Psi \in D_\omega$ and it turns out to be a well-defined vector-valued symmetric distribution, $\mathcal{D}_n(M) \ni f \mapsto t \odot \hat{W}_{\omega,n}(f)\Psi$, with values in D_ω. Thus, we have also defined an operator valued symmetric distribution, $\mathcal{D}_n(M) \ni f \mapsto t \odot \hat{W}_{\omega,n}(f)$, defined on and leaving invariant the domain D_ω, acting as $\Psi \mapsto t \odot \hat{W}_{\omega,n}(f)\Psi$. This fact permits us to smear $\hat{W}_{\omega,n}$ with $t \in \mathcal{E}'_n(M)$, just defining

$$\hat{W}_{\omega,n}(t) := \left(t \odot \hat{W}_{\omega,n}\right)(f) \,,$$

where $f \in \mathcal{D}_n(M)$ is equal to 1 on $\operatorname{supp} t$. It is simple to prove that the definition does not depend on f and the new smearing operation reduces to the usual one for $t \in \mathcal{D}_n(M) \subset \mathcal{E}'_n(M, \mathbf{g})$. Finally, since $f\delta_n \in \mathcal{E}'_n(M)$ for $f \in \mathcal{D}(M)$, where δ_n is the Dirac delta supported on the diagonal of $M^n = M \times \cdots \times M$ (n times), the following operator-valued distribution is well-defined on D_ω which, is then an invariant subspace,

$$f \mapsto :\hat{\phi}^n:_\omega (f) := \hat{W}_{\omega,n}(f\delta_n) \,,$$

Definition 2.19. $:\hat{\phi}^n:_\omega (f)$ is the **normal ordered product of n field operators with respect to ω**. $\mathcal{W}_\omega(\boldsymbol{M})$ is the $*$-algebra generated by $\mathbb{1}$ and the operators $\hat{W}_{\omega,n}(t)$ for all $n \in \mathbb{N}$ and $t \in \mathcal{E}'_n(M, \mathbf{g})$ with involution given by $\hat{W}_{\omega,n}(t)^* := \hat{W}_{\omega,n}(t)^\dagger\restriction_{D_\omega}$ $(= \hat{W}_{\omega,n}(\bar{t}))$. ■

Remark 2.20.

(1) As proved in [40], each product $\hat{W}_{\omega,n}(t)\hat{W}_{\omega,n'}(t')$ can be decomposed as a finite linear combination of terms $\hat{W}_{\omega,m}(s)$ extending the Wick theorem, and other natural identities, in particular related with commutation relations, hold.

(2) $\pi_\omega(\mathcal{A}(\boldsymbol{M}))$ turns out to be a sub $*$-algebra of $\mathcal{W}_\omega(\boldsymbol{M})$ since $\hat{\Phi}_\omega(\psi) = :\hat{\phi}:_\omega (f)$ for $f \in \mathcal{D}(M)$. ■

If ω, ω' are two quasifree Hadamard states, $\mathcal{W}_\omega(\boldsymbol{M})$ and $\mathcal{W}_{\omega'}(\boldsymbol{M})$ are isomorphic (not unitarily in general) under a canonical $*$-isomorphism

$$\alpha_{\omega'\omega} : \mathcal{W}_\omega(\boldsymbol{M}) \to \mathcal{W}_{\omega'}(\boldsymbol{M}) \,,$$

as shown in Lemma 2.1 in [40]. Explicitly, $\alpha_{\omega'\omega}$ is induced by linearity from the requirements

$$\alpha_{\omega'\omega}(\mathbb{1}) = \mathbb{1} \,, \quad \alpha_{\omega'\omega}(W_{n,\omega}(t)) = \sum_k W_{n-2k,\omega'}(\langle d^{\otimes k}, t\rangle) \,, \tag{2.43}$$

where $d(x_1,x_2) := \omega(x_1,x_2) - \omega'(x_1,x_2)$ (only the symmetric part matters here) and

$$\begin{aligned}\langle d^{\otimes k}, t\rangle(x_1,\ldots,x_{n-2k}) := \frac{n!}{(2k)!(n-2k)!} \int_{M^{2k}} & t(y_1,\ldots,y_{2k},x_1,\ldots,x_{n-2k}) \\ & \times \prod_{i=1}^{k} d(y_{2i-1},y_{2i}) \mathrm{dvol}_{\boldsymbol{M}}(y_{2i-1}) \mathrm{dvol}_{\boldsymbol{M}}(y_{2i})\end{aligned} \tag{2.44}$$

for $2k \leq n$ and $\langle d^{\otimes k}, t\rangle = 0$ if $2k > n$.
These $*$-isomorphisms also satisfy

$$\alpha_{\omega''\omega'} \circ \alpha_{\omega'\omega} = \alpha_{\omega''\omega}$$

and

$$\alpha_{\omega'\omega}(\hat{\phi}_\omega(t)) = \hat{\phi}_{\omega'}(t)\ .$$

The idea behind these isomorphisms is evident: Replace everywhere ω by ω'. For instance

$$\alpha_{\omega'\omega}(:\hat{\phi}^2:_\omega(f)) = :\hat{\phi}^2:_{\omega'}(f) + \int_M (\omega - \omega')(x,x) f(x) \mathrm{dvol}_{\boldsymbol{M}}\, \mathbb{1}$$

where $\omega - \omega'$ is smooth for (b) in Theorem 2.15.
One can eventually define an abstract unital $*$-algebra $\mathcal{W}(\boldsymbol{M})$, generated by elements $\mathbb{1}$ and $W_n(t)$ with $t \in \mathcal{E}'_n(M)$, isomorphic to each concrete unital $*$-algebra $\mathcal{W}_\omega(\boldsymbol{M})$ by $*$-isomorphisms $\alpha_\omega : \mathcal{W}(\boldsymbol{M}) \to \mathcal{W}_\omega(\boldsymbol{M})$ such that, if ω, ω' are quasifree Hadamard states, $\alpha_{\omega'} \circ \alpha_\omega^{-1} = \alpha_{\omega'\omega}$.
As above $\mathcal{A}(\boldsymbol{M})$ is isomorphic to the $*$-algebra of $\mathcal{W}(\boldsymbol{M})$ generated by $\mathbb{1}$ and $W_1(f) = :\hat{\phi}:(f) = \phi(f)$ for $f \in \mathcal{D}(M)$.

Remark 2.21. It is not evident how (Hadamard) states initially defined on $\mathcal{A}(\boldsymbol{M})$ (continuously) extend to states on $\mathcal{W}(\boldsymbol{M})$. This problem has been extensively discussed in [39] in terms of relevant topologies. ■

It is now possible to define a notion of local Wick monomial *which does not depend on a preferred Hadamard state*. If $t \in \mathcal{E}'_n(M)$ has support sufficiently concentrated around the diagonal of M^n, realizing $\mathcal{W}(\boldsymbol{M})$ as $\mathcal{W}_\omega(\boldsymbol{M})$ for some quasifree Hadamard state ω, we define a **local covariant Wick polynomial** as

$$W_n(t)_H := \alpha_\omega^{-1}\left(\alpha_{H\omega}(W_{n,\omega}(t))\right)$$

where $\alpha_{H\omega}$ is defined as in (2.44) replacing ω' by the Hadamard parametrix H_{0^+}. One easily proves that this definition does not depend on the choice of the Hadamard state ω. The fact that the support of t is supposed to be concentrated around of the diagonal of M^n it is due to the fact that $H_\epsilon(x,y)$ is defined only if x is sufficiently close to y. This definition is completely consistent with (2.28), where now the $:\phi(f_1)\cdots\phi(f_n):_H$ can be viewed as elements of $\mathcal{W}(\boldsymbol{M})$ and not only of $\mathcal{A}(\boldsymbol{M})$, and it makes sense to write in particular,

$$:\phi^2:_H(f) := W_2(f\delta_2)_H = \int_{M^2} :\phi(x)\phi(y):_H \delta(x,y) f(x) \mathrm{dvol}_{\boldsymbol{M}^2}(x,y)\ .$$

Analogous monomials $:\phi^n:_H(f)$ are defined similarly as elements of $\mathcal{W}(\boldsymbol{M})$. *With the said definition (2.28) holds true literally* and not only in the sense of quadratic forms.

Remark 2.22. The presented definition of locally covariant Wick monomials $:\phi^n:_H(f)$, though satisfying general requirement of locality and covariance [14, 34, 5] , remains however affected by several ambiguities. A full classification of them is the first step of ultraviolet renormalization program [40, 51]. The algebra $\mathcal{W}(\boldsymbol{M})$ also includes the so-called (locally covariant) time-ordered Wick polynomials, necessary to completely perform the renormalization procedure [41]. ■

The constructed formalism can be extended in order to encompass differentiated Wick polynomials in a generic globally hyperbolic spacetime with $P = \Box_{\boldsymbol{M}} + m^2 + \xi R$ and it has a great deal of effect concerning the definition of the stress energy tensor operator [59]. It is defined as an element of $\mathcal{W}(\boldsymbol{M})$ by subtracting the universal Hadamard singularity from the two-point function of ω, before computing the relevant derivatives.

$$:T_{ab}:_H(f) = \int_{M^2} D_{ab}(x,y)\, :\phi(x)\phi(y):_H\, \delta(x,y) f(x)\, \mathrm{dvol}_{\boldsymbol{M}^2}(x,y) \tag{2.45}$$

$D_{ab}(x,y)$ is a certain symmetrized second order partial differential operator obtained from (2.1) (cf. [59] Equation (10), and [34] where some minor misprints have been corrected and where the signature $(-{+}{+}{+})$ has been adopted differently from $(+{-}{-}{-})$ adopted in this work),

$$\begin{aligned}
D_{ab}(x,y) &:= D^{\mathrm{can}}_{ab}(x,y) - \frac{1}{3} g_{ab} P_x \\
D^{\mathrm{can}}_{ab}(x,y) &:= (1-2\xi) g_b^{b'} \nabla_a \nabla_{b'} - 2\xi \nabla_a \nabla_b - \xi G_{ab} \\
&\quad + g_{ab} \left\{ 2\xi \Box_x + \left(2\xi - \frac{1}{2}\right) g_c^{c'} \nabla^c \nabla_{c'} + \frac{1}{2} m^2 \right\} .
\end{aligned}$$

Here, covariant derivatives with primed indices indicate covariant derivatives w.r.t. y, $g_b^{b'}$ denotes the parallel transport of vectors along the unique geodesic connecting x and y, the metric g_{ab} and the Einstein tensor G_{ab} are considered to be evaluated at x. The form of the "canonical" piece D^{can}_{ab} follows from the definition of the classical stress-energy tensor, while the last term $-\frac{1}{3} g_{ab} P_x$, giving rise to a final contribution $-\frac{g_{ab}}{3} :\phi(x) P \phi(x):_H$ to the stress-energy operator, has been introduced in [59]. It gives no contribution classically, just in view of the very Klein-Gordon equation satisfied by the fields, however, in the quantum realm, its presence has a very important reason. Because the Hadamard parametrix satisfies the Klein-Gordon equation only up to smooth terms, the term with P_x is non vanishing. Moreover, without this additional term, the above definition of $:T_{ab}:_H$ would not yield a conserved stress-tensor expectation value (see [59] Theorem 2.1). On the other hand the added therm is responsible for the appearance of the famous *trace anomaly* [79]. An extended discussion on conservation laws in this framework appears in [42].

Chapter 3

Appendix: Notions of Lorentzian geometry and applications

This appendix presents, in a very quick way, some useful notions and results of differential geometry, especially Lorentzian geometry and some basic notions and results in the theory of spacetimes. We shall also introduce some elementary notions of tensor algebra and applications to tensor analysis on manifolds. For more extended discussions, the reader can consult [56] for the purely algebraic part and applications to special relativity and other examples, [57] for the differential geometry part and applications to general relativity and other examples, and references therein. Classic general references on the subject are [66, 4].

3.1 Smooth manifolds

3.1.1 Local charts, atlas, and all that

Definition 3.1. If M is topological space, a **local chart** (U, ψ) of **dimension** n on M, also called **local coordinate system**, is a map $\psi : U \to \mathbb{R}^n$ where $U \subset M$ is non-empty and open, such that

(i) $\psi(U)$ is open in $\mathbb{R}^n$,

(ii) ψ is a homeomorphism of U (equipped with the topology induced from M) onto $\psi(U)$.

U is said the **domain** of ψ and the n functions $x^k : U \to \mathbb{R}$, defined by the requirement $\psi(p) = (x^1(p), \ldots, x^n(p))$ for $p \in U$, are called **coordinates** of the local chart.

A local charts (U, ψ) on M is C^k**-compatible** $(k = 1, 2, \ldots + \infty)$ with another local chart (U', ψ') on M, if either $U \cap U' = \varnothing$ or the so-called **transition functions**

$$\psi \circ \psi'^{-1} : \psi'(U' \cap U) \to \psi(U' \cap U) \quad \text{and} \quad \psi' \circ \psi^{-1} : \psi(U \cap U') \to \psi(U \cap U')$$

are C^k functions $\mathbb{R}^n \to \mathbb{R}^n$. ■

Definition 3.2. A **smooth manifold** of **dimension** $\dim(M) = n = 1, 2, \ldots$, is a 2nd countable Hausdorff topological space M equipped with a *smooth structure* of dimension n.
A **smooth structure**[1] on M of **dimension** n is a family local charts $\mathcal{A} := \{(U_j, \psi_j)\}_{j\in J}$ such that

(i) $\bigcup_{j\in J} U_j = M$,

(ii) (U_i, ψ_i) and (U_j, ψ_j) are C^∞ compatible for every $i, j \in J$,

(iii) if (U, ψ) is a local chart on M which is C^∞ compatible with (U_j, ψ_j) for every $j \in J$, then $(U, \psi) \in \mathcal{A}$

A **smooth atlas** $\mathcal{A}$ on a smooth manifold M is a family of local charts such that (i) and (ii) above are valid. ■

Remark 3.3.

(1) It is easy to prove that an atlas can be completed in a unique way to a smooth structure on M, so that to assign a smooth structure is sufficient to assign a smooth atlas. This smooth structure is **generated** by the atlas per definition.

(2) A trivial example of smooth manifold is provided by an n-dimensional real affine space $\mathbb{A}$. Henceforth V denotes the space of translations of $\mathbb{A}$. The natural smooth structure of $\mathbb{A}$ is the one generated by the *Cartesian charts*. A **Cartesian (global) chart** $(\mathbb{A}, \psi)$ is defined by assigning an origin $o \in \mathbb{A}$ and a basis $\{e_1, \ldots e_n\} \in V$. Then, the map $\psi : \mathbb{A} \ni p \mapsto (x^1, \ldots, x^n) \in \mathbb{R}^n$ such that $\vec{op} = \sum_{k=1}^n x^k e_k$ is a bijection. Notice that every Cartesian coordinate chart endows $\mathbb{A}$ with the topology induced by $\mathbb{R}^n$ that is Hausdorff and second countable. If $(\mathbb{A}, \psi)$ with coordinates $x^1, \ldots, x^n$ and $(\mathbb{A}, \psi')$ with coordinates $x'^1, \ldots, x'^n$ are Cartesian (global) charts, the corresponding transformation of coordinates reads

$$x'^a = c^a + \sum_{b=1}^n A^a{}_b x^b, \quad a = 1, \ldots, n\,, \tag{3.1}$$

where c^a, $A^a{}_b$ are real constants and $\det[A^a{}_b]_{a,b=1,\ldots,n} \neq 0$. It is obvious that a transformation as above is an homeomorphism from $\mathbb{R}^n$ to $\mathbb{R}^n$ and therefore each Cartesian chart induces the same Hausdorff second-countable topology on $\mathbb{A}$. In turn, every cartesian chart $\psi : \mathbb{A} \to \mathbb{R}^n$ is a homeomorphism. This is not the whole story, since two such charts are also C^∞ compatible in view of (3.1) and thus they define a natural common smooth structure on $\mathbb{A}$. The case $\mathbb{A} = \mathbb{R}^n$ equipped with its natural affine space structure, where $V = \mathbb{R}^n$, is an even simpler example of smooth manifold.

(3) In view of (1) and (2) every open set $M \subset \mathbb{R}^n$ is a smooth n-dimensional manifold when equipped with the smooth structure generated by the identity map $\imath : M \ni x \mapsto x \in \mathbb{R}^n$. Open subsets of affine spaces analogously define smooth manifolds. Here the smooth structure

[1] Also called *differentiable smooth structure*.

is induced by every Cartesian coordinate systems restricted to the set. Every pair of Cartesian charts are trivially C^∞-compatible.

(4) The most interesting cases of smooth manifolds are not affines spaces or portions of them. An example is provided by the notion of embedded submanifold discussed in Def. 3.6 below, when viewing these types of submanifolds as smooth manifolds in their own right. A concrete example is presented in (5) Remark 3.23 where we consider a cylinder (surface) embedded in $\mathbb{R}^3$ ■

Definition 3.4. If M and N are smooth manifolds the following definitions are valid.

(a) A map $f : M \to N$ is said to be **smooth** if the map $\psi \circ f \circ \phi^{-1}$ is C^∞, where defined, for every choice of local charts (U, ψ) of N and (U, ϕ) of M. Furthermore

(i) $C^\infty(M; N)$ is the set of smooth functions $f : M \to N$,

(ii) $C^\infty(M) := C^\infty(M, \mathbb{R})$;

(iii) if $h \in C^\infty(M)$ its **support** is $supp(h) := \overline{\{p \in M \mid h(p) \neq 0\}}$ and

$$C^\infty_c(M) := \{f \in C^\infty(M) \mid supp(f) \text{ is compact}\} .$$

(b) A (smooth) **diffeomorphism** between M and N is a smooth map $f : M \to N$ that is bijective and its inverse is smooth as well. In this case, M and N are said to be **diffeomorphic** (through f).

(c) Let $I \subset \mathbb{R}$ be an *open* interval. A **(smooth) curve** $\gamma : I \to M$ is a smooth map when endowing I with its natural smooth structure according to (2) Remark 3.3 above.

(d) In case the interval $J \subset \mathbb{R}$ includes one or both (finite) endpoints, a map $\beta : J \to M$ is a **(smooth) curve** if there is an open interval $I \supset J$ and a smooth curve $\gamma : I \to M$ according to (c) such that $\beta = \gamma\restriction_J$. ■

Remark 3.5.

(1) Due to (1) Remark 3.3, to check if $f : M \to N$ is smooth it is sufficient to check the definition just referring to charts of atlases compatible with the smooth structures. The same fact is true concerning smooth curves.

(2) It should be obvious that a diffeomorphism is also a homeomorphism and that two diffeomorphic manifolds must have the same dimension.

(3) It is possible to prove that if $\dim(M) \geq 4$ for a smooth manifold, then it admits some inequivalent (non-diffeomorphic) smooth structures compatible with the topology of M.

(4) Hausdorff property is in particular useful in proving the existence [57] of a special family of technically useful functions. If M is a smooth manifold and $p \in M$, for every open neighborhood of p, U_p, there is a open neighborhood of p, V_p and a function $h \in C^\infty_0(M)$ such that:

(1) $\overline{V_p} \subset U_p$,

(2) $0 \leq h(q) \leq 1$ for all $q \in M$,

(3) $h(q) = 1$ if $q \in \overline{V_p}$,

(4) $\operatorname{supp} h \subset U_p$ is compact (in particular h vanishes outside U_p).

The function h is called **hat function** or **bump function** centered on p supported in U_p.
We shall use these functions in the rest of the chapter without specific comments. ■

We move on to introduce the notion of *embedded submanifold*. There are different equivalent definitions of this geometric notion. We adopt the most useful one from an applicative perspective. As a matter of fact an embedded submanifold N of M, in local coordinates of M, appears as a canonical n-plane embedded in $\mathbb{R}^m$, where $n := \dim(N)$ and $m := \dim(M)$.

Definition 3.6. Let M be a smooth manifold with $\dim(M) = m \geq 2$. An **embedded submanifold** N of M **of dimension** $n < m$ is a subset $N \subset M$, equipped with the induced topology, such that the following is satisfied. If $p \in N$, there is a local chart (U, ψ) of the smooth structure of M,

$$U \ni q \mapsto \psi(q) = (x^1(q), \ldots, x^m(q)) \in \psi(U) \subset \mathbb{R}^m$$

which is **adapted** to N around p according to the following requests

(i) $U \ni p$,

(ii) $\psi(U \cap N) = \{(x^1, \ldots, x^m) \in \psi(U) \mid x^{n+1} = \cdots = x^m = c\}$ for some constant $c \in \mathbb{R}$.

Each $\psi_N : U_N := U \cap N \ni q \mapsto (x^1(q), \ldots, x^n(a)) \in \mathbb{R}^n$ therefore defines a local chart on N and these local charts are C^∞ compatible. The smooth structure generated by the atlas of those local charts on N is said to be the smooth structure **induced** on N by M.
Saying that N has dimension n is equivalent to declaring that N has **codimension** $m - n$. ■

The choice of the *first* n coordinates of a local chart on M to describe N is not necessary in defining adapted coordinates. What matters is that $U \cap N$ in coordinates is described by assigning a constant value to $m - n$ coordinates. The remain coordinates range in an open set of $\mathbb{R}^n$ and define a local chart on the submanifold N.

3.1.2 Tangent and cotangent spaces

Let us introduce the notion of *tangent* and *cotangent* space to a point. To this end we should start by focusing on the space of smooth functions on M. If M is a smooth manifold, $C^\infty(M)$ acquires the structure of commutative ring (with unity) when the operations are the pointwise ones:

$$(f + g)(p) := f(p) + g(p) , \quad (f \cdot g)(p) := f(p)g(p) , \quad \forall p \in M ,$$

where $f, g \in C^\infty(M)$. This space is also a $\mathbb{R}$-vector space if we analogously define the pointwise product with real numbers

$$(af)(p) := \; af(p)\,, \quad \forall p \in M\,,$$

where $a \in \mathbb{R}$ and $f \in C^\infty(M)$. In the mathematical physics literature $f \in C^\infty(M)$ is called **(smooth) scalar field**.

Sticking to the vector space structure of $C^\infty(M)$, we can introduce the notion of tangent space. If $p \in M$, where M is a smooth manifold with dimension m, take a local chart (U, ψ) of M with $U \ni p$. Suppose that $\psi(q) =: (x^1, \ldots, x^m)$. We can then define the differential operator

$$\left.\frac{\partial}{\partial x^k}\right|_p : C^\infty(M) \to \mathbb{R}$$

evaluated at p and associated to the k-th coordinate

$$\left.\frac{\partial}{\partial x^k}\right|_p f := \left.\frac{\partial f \circ \psi^{-1}}{\partial x^x}\right|_{\psi(p)}\,, \quad \forall f \in C^\infty(M)\,. \tag{3.2}$$

This operator is a linear map from $C^\infty(M)$ to $\mathbb{R}$, referring to the vector space structure of $C^\infty(M)$, so it makes sense to consider linear combination of similar operators,

$$X_p := \sum_{k=1}^m t^k \left.\frac{\partial}{\partial x^k}\right|_p$$

with pointwise action on functions $f \in C^\infty(M)$:

$$X_p(af + bg) := aX_p(f) + bX_p(g)\,, \quad \forall f, g \in C^\infty(M)\,, \forall a, b \in \mathbb{R}\,, \tag{3.3}$$

As a matter of fact we end up with a certain linear space of linear (differential) operators.

Definition 3.7. If M is a smooth manifold with dimension m and $p \in M$, the **tangent space** at p is the real linear space of differential operators on $C^\infty(M)$ spanned by the m operators (3.2):

$$T_pM := \left\{ \sum_{k=1}^m t^k \left.\frac{\partial}{\partial x^k}\right|_p \;\middle|\; (t^1, \ldots, t^m) \in \mathbb{R}^m \right\} \tag{3.4}$$

where we adopted a local coordinate system (U, ψ) with coordinates $\psi(q) =: (x^1, \ldots, x^m)$ around p. The elements of T_pM are called **contravariant vectors** at p.

The special m elements $\left.\frac{\partial}{\partial x^k}\right|_p$ form the **canonical basis** of T_pM **associated** to (U, ψ). ■

We have to show that the above definition is well posed.

Proposition 3.8. *The definition of T_pM is well posed: its does not depend on the choice of the local chart (U, ψ) around $p \in M$. Furthermore* $\dim(T_pM) = \dim(M)$.

Proof. Let us start from the second assertion. It is obvious that $\dim(T_pM) \leq \dim(M)$. To prove that the dimensions are actually equal it is sufficient to prove that the m differential operators $\frac{\partial}{\partial x^k}\Big|_p$ are linearly independent. Suppose that, for some reals $c^1, \cdots, c^m$,

$$\sum_{k=1}^{m} c^k \left.\frac{\partial}{\partial x^k}\right|_p = 0$$

in the sense that the left-hand side is just the *zero differential operator*. We want to prove that $c^k = 0$ for every k. If $k_0 \in \{1, \ldots, m\}$, we can define an element of $f_{k_0} \in C^\infty(M)$ which coincides with the coordinate map $U \ni q \mapsto x^{k_0}(q)$ in a neighborhood of p, just by smoothing to 0 this function before reaching the boundary of U: $f_{k_0}(q) := 0$ if $q \notin U$ or $f_{k_0}(q) := x^{k_0}(q)\chi(q)$, where $\chi \in C^\infty(M)$ is such that $\chi(q) = 1$ in a neighborhood of p and $supp(\chi) \subset U$ (see [57] for details). If we expand

$$\sum_{k=1}^{m} c^k \left.\frac{\partial}{\partial x^k}\right|_p f_{k_0} = 0$$

in local coordinates $x^1, \ldots, x^n$, the identity can be re-phrased to

$$0 = \sum_{k=1}^{m} c^k \left.\frac{\partial x^{k_0}}{\partial x^k}\right|_p = \sum_{k=1}^{m} c^k \delta_k^{k_0} ,$$

namely $c^{k_0} = 0$ for every $k_0 \in \{1, \ldots, m\}$. We proved that the m operators $\frac{\partial}{\partial x^k}\Big|_p$ are linearly independent and thus $\dim(T_pM) = \dim(M)$.

Let us pass to the first assertion in the thesis. If we adopt a different local coordinate system (V, ϕ) around p with coordinates $y^1, \ldots, y^m$, a straightforward computation proves that

$$\sum_{k=1}^{m} t^k \left.\frac{\partial}{\partial x^k}\right|_p = \sum_{k=1}^{m} t^k \sum_{j=1}^{m} \left.\frac{\partial y^j}{\partial x^k}\right|_{\psi(p)} \left.\frac{\partial}{\partial y^j}\right|_p .$$

Above $\frac{\partial y^j}{\partial x^k}$ are the elements of the Jacobian matrix of $\phi \circ \psi^{-1} : \psi(U \cap V) \to \phi(U \cap V)$. Since this map is invertible, differentiable with differentiable inverse, its Jacobian matrix must be bijective (the inverse exists and is made of the derivatives $\frac{\partial x^k}{\partial y^i}$). The conclusion is that

$$\sum_{k=1}^{m} t^k \left.\frac{\partial}{\partial x^k}\right|_p = \sum_{j=1}^{m} t'^j \left.\frac{\partial}{\partial y^j}\right|_p$$

where the two types of components are one-to-one connected by the bijective linear map $\mathbb{R}^m \to \mathbb{R}^m$

$$t'^j = \sum_{j=1}^{m} \left.\frac{\partial y^j}{\partial x^k}\right|_{\psi(p)} t^k , \quad j = 1, \ldots, m .$$

We have proved that the definition of T_pM does not depend on the chosen local chart around p adopted in the right-hand side of (3.4). □

If we include the ring structure of $C^\infty(M)$ in this discussion, it is worth observing that the operators $X_p \in T_pM$, in addition to linearity (3.3), also satisfy the *Leibniz rule*:

$$X_p(f \cdot g) = f(p)X_p(g) + g(p)X_p(g)\,, \quad \forall f, g \in C^\infty(M)\,, \tag{3.5}$$

the proof is immediate just from the definition of T_pM in coordinates. It is a known remarkable result (see e.g. [57]) that every map $L_p : C^\infty(M) \to \mathbb{R}$ which satisfy linearity and the Leibniz rule (as written above) belongs to T_pM.

Remark 3.9.

(1) We remind the reader that if V is a vector space on the field $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$, the **dual space** V^* is the linear space of linear functionals $V^* := \{f : V \to \mathbb{K} \mid f \text{ linear }\}$. The adopted vector space structure on V^* is again the pointwise one one: if $f, g \in V^*$ and $a, b \in \mathbb{K}$,

$$(af + bg)(v) := af(v) + bg(v) \quad \forall v \in V\,.$$

If $n := \dim(V) < +\infty$ and $\{e_1, \ldots, e_n\} \subset V$ is a basis, then the associated **dual basis** in V is $\{e^{*1}, \ldots, e^{*n}\} \subset V^*$ defined by

$$e^{*k}(e_j) = \delta^k_j\,, \quad k, j \in \{1, \ldots, n\}\,. \tag{3.6}$$

Notice that the requirements above are sufficient to define e^{*k} in view of the fact that e^{*k} is linear and that every element of V can be finitely and uniquely decomposed along the basis of the e_j.

(2) It is easy to see that the functionals e^{*j} generate V^*. Indeed, for $f \in V^*$, taking advantage of linearity several times,

$$f(v) = f(\sum_j v^j e_j) = \sum_j v^j f(e_j) = \sum_k \sum_j \delta^k_j f(e_k) v^j = \sum_k \sum_j e^{*k}(e_j) f(e_k) v^j$$

$$= \left(\sum_k f(e_k) e^{*k}\right) (\sum_j v^j e_j)\,.$$

Arbitrariness of $v \in V$ yields

$$f = \sum_{k=1}^n f(e_k) e^{*k}\,.$$

Therefore the n elements e^{*k} generate V^* as asserted. More strongly they form a basis of V^*, since thay are also linearly independent. In fact, let suppose that

$$\sum_{k=1}^n c_k e^{*k} = 0\,.$$

This assumption implies in particular that, for every chosen $k_0 = 1, 2, \dots n$,

$$0 = \left(\sum_{k=1}^{n} c_k e^{*k}\right)(e_{k_0}) = \sum_{k=1}^{n} c_k e^{*k}(e_{k_0}) = \sum_{k=1}^{n} c_k \delta^k_{k_0} = c_{k_0} \ .$$

(3) Notice that we established in particular that $\dim(V) = \dim(V^*)$ if the former is finite.

(4) If $\dim(V) < +\infty$, another important elementary fact occurs: $(V^*)^*$ is naturally isomorphic to V, through the vector space injective homomorphism (which is in fact also surjective if $\dim(V) < +\infty$):

$$F : V \ni v \mapsto F_v \in (V^*)^* \quad \text{defined as } F_v(f) := f(v) \text{ for every } f \in V^*.$$

The proof that F is an injective homomorphism is immediate from the given definitions. Since $\dim((V^*)^*) = \dim(V^*) = \dim(V) < +\infty$ according to the proof above, the injective homomorphism F must be surjective.

(5) Due to (4), if $v \in V$ and $f \in V^*$, the action of f on v, i.e. $f(v)$, can be indifferently interpreted as $F_v(f)$. For this reason a bilinar map called **pairing** is defined $\langle \cdot, \cdot \rangle : V \times V^* \to \mathbb{K}$ as

$$\langle v, f \rangle := f(v) = F_v(f) \quad \forall v \in V \ , \forall f \in V^* \ .$$

We henceforth use these elementary algebraic notions and properties.

(6) Consider again the case of a finite dimensional vector space V and pick out a basis $\{e_j\}_{j \in J}$. If $V \ni v = \sum_{j \in J} v^j e_j$, we also have

$$\langle v, e^{*k} \rangle = \left\langle \sum_{j \in J} v^j e_j, e^{*k} \right\rangle = \sum_{j \in J} v^j \left\langle e_j, e^{*k} \right\rangle = \sum_{j \in J} v^j \delta^k_j = v^k \ .$$

In summary, even if there is no scalar product in V and the basis of the e_j is not orthonormal, we can write down the initial decomposition $v = \sum_{j \in J} v^j e_j$ in a way that resembles the standard orthogonal decomposition (but it is not!):

$$v = \sum_{k \in J} \langle v, e^{*k} \rangle e_k \ , \tag{3.7}$$

just by taking advantage of the nature of the dual basis. ■

Definition 3.10. If M is a smooth manifold with dimension m and $p \in M$, the **cotangent space** $T^*_p M$ at $p \in M$ is the dual space of $T_p M$. The elements of $T^*_p M$ are called **covariant vectors** at p or also **1-forms** at p.

If $\left\{ \left.\frac{\partial}{\partial x^k}\right|_p \right\}_{k=1,\dots,m}$ is the canonical basis of $T_p M$ associated to a local chart (U, ψ) around p with coordinates $U \ni q \mapsto \psi(q) = (x^1(q), \dots, x^m(q)$, the **dual canonical basis** in $T^*_p M$ is

$\left\{dx^k|_p\right\}_{k=1,\ldots,m} \subset T^*M$ as usual defined by

$$\left\langle \left.\frac{\partial}{\partial x^j}\right|_p, dx^k_p \right\rangle = \delta^j_k\,, \quad k,j = 1,\ldots,m\,. \tag{3.8}$$

■

Remark 3.11.

(1) If $N \subset M$ is an embedded submanifold of M, an obvious inclusion occurs $T_pN \subset T_pM$ according to Definition 3.6. If $p \in N$ and (U,ψ) is a local chart in M around p that satisfies the conditions (i) and (ii), the first $n = \dim(N)$ coordinates are also local coordinates on N around p. Therefore the first n elements $\frac{\partial}{\partial x^k}|_p \subset T_pM$ for $k = 1,2,\ldots,n$ defines a basis of T_pN as well. Therehence an injective linear map exists

$$j_N : T_pN \ni \sum_{k=1}^n t^k \left.\frac{\partial}{\partial x^k}\right|_p \mapsto \sum_{k=1}^n t^k \left.\frac{\partial}{\partial x^k}\right|_p \in T_pM\,.$$

We leave to the reader the proof of the fact that j_N does not depend on the used local chart (U,ψ) around $p \in N$ *provided it is adapted* to N.

(2) Focus on an n-dimensional real affine space $\mathbb{A}$, with space of translations V, viewed as smooth manifold according to (3) Remark 3.3. If $p \in \mathbb{A}$, there is a natural isomorphism $T_p : V \to T_p\mathbb{A}$ defined as follows. Consider a Cartesian global chart with origin $o \in \mathbb{A}$ and basis $e_1,\ldots,e_n \in V$. Let us indicate by $x^1,\ldots,x^n$ the coordinates of this global chart. The said isomorphism is just the unique linear extension of $T_p : V \mapsto T_p\mathbb{A}$ such that

$$T_p : e_k \mapsto \left.\frac{\partial}{\partial x^k}\right|_p \quad \text{for } k = 1,\ldots,n. \tag{3.9}$$

The written map is evidently an isomorphism of vector spaces by construction since it injectively sends a basis of a vector space to a basis of another vector space of the same (finite) dimension. The crucial point is that, if we change the origin to o' and the basis to $e'_1,\ldots,e'_n \in V$, obtaining the Cartesian coordinates $x'^1,\ldots,x^n$, and we define $T'_p : V \mapsto T_p\mathbb{A}$ as the unique linear extension of

$$T'_p : e'_j \mapsto \left.\frac{\partial}{\partial x'^j}\right|_p \quad \text{for } j = 1,\ldots,n.$$

it turns out that $T_p = T'_p$. Indeed (3.1) implies that

$$e_k = \sum_{j=1}^n A^j{}_k e'_j\,, \quad \left.\frac{\partial}{\partial x^k}\right|_p = \sum_{j=1}^n A^j{}_k \left.\frac{\partial}{\partial x'^j}\right|_p$$

Using these identities in both sides of the identity above and taking linearity of T'_p into accounts, yields

$$T'_p : e_k \mapsto \left.\frac{\partial}{\partial x^k}\right|_p \quad \text{for } k = 1,\ldots,n.$$

Comparing with (3.9), we conclude that $T_p = T'_p$. ■

3.1.3 Vector and covector fields on a smooth manifold

We are in a position that we can state a fundamental definition.

Definition 3.12. Let M be a smooth manifold with $\dim(M) = n$.

A **(smooth) contravariant vector field** X is an assignment

$$M \ni p \mapsto X_p \in T_pM$$

such that in every local chart (U, ψ) around every $p \in M$, decomposing X with respect to the canonical basis

$$X_p = \sum_{k=1}^{n} X_p^k \left.\frac{\partial}{\partial x^k}\right|_p$$

the maps $\psi(U) \ni (x^1, \ldots, x^n) \mapsto X^k_{\psi^{-1}(x^1,\ldots,x^n)}$ are C^∞. These maps are the **(local) components** of X in the considered local chart.

The set of all smooth contravariant vector fields on M is denoted by $\mathfrak{X}(M)$.

A **(smooth) covariant vector field**, also called 1**-form**, ω is an assignment

$$M \ni p \mapsto \omega_p \in T_p^*M$$

such that in every local chart (U, ψ) around every $p \in M$, decomposing ω with respect to the dual canonical basis

$$\omega_p = \sum_{k=1}^{n} \omega_{pk} \left. dx^k\right|_p$$

the maps $\psi(U) \ni (x^1, \ldots, x^n) \mapsto \omega_{\psi^{-1}(x^1,\ldots,x^n)k}$ are C^∞. These maps are the **(local) components** of ω in the considered local chart.

The set of all smooth covariant vector fields on M is denoted by $\Omega_1(M)$. ■

Remark 3.13.

(1) It should be clear that the smoothness condition of the components of a vector field can be checked only for the charts of an atlas of M.

(2) If we consider two local charts (U, ψ) with coordinates $x^1, \ldots, x^n$ and (U', ψ') with coordinates $x'^1, \ldots, x'^n$, the respective components of a given contravariant vector field X at $p \in U \cap U'$ are related by the following rule, whose proof is trivial matter of computation:

$$X_p'^k = \sum_{j=1}^{n} \left.\frac{\partial x'^k}{\partial x^j}\right|_{\psi(p)} X_p^j\,, \quad k = 1, \ldots, n. \tag{3.10}$$

To be compared with the transformation rule of the canonical bases

$$\left.\frac{\partial}{\partial x^j}\right|_p = \sum_{k=1}^{n} \left.\frac{\partial x'^k}{\partial x^j}\right|_{\psi(p)} \left.\frac{\partial}{\partial x'^k}\right|_p\,, \quad j = 1, \ldots, n. \tag{3.11}$$

Vice versa, if we assign smooth components on an atlas of M such that, varying the local chart, these components satisfy (3.10), we define a smooth contravariant vector field on M as it is easy to prove.

(3) If, as before, we consider two local charts (U, ψ) with coordinates $x^1, \ldots, x^n$ and (U', ψ') with coordinates $x'^1, \ldots, x'^n$, the respective components of a given covariant vector field ω at $p \in U \cap U'$ are related by the following rule, whose proof is trivial matter of computation:

$$\omega'_{pk} = \sum_{j=1}^{n} \left.\frac{\partial x^j}{\partial x'^k}\right|_{\psi'(p)} \omega_{pj} , \quad k = 1, \ldots, n. \tag{3.12}$$

To be compared with the transformation rule of the dual canonical bases

$$dx^j|_p = \sum_{k=1}^{n} \left.\frac{\partial x^j}{\partial x'^k}\right|_{\psi'(p)} dx'^k|_p , \quad j = 1, \ldots, n . \tag{3.13}$$

Vice versa, if we assign smooth components on an atlas of M such that, varying the local chart, these components satisfy (3.12) we define a smooth covariant vector field on M as it is easy to prove.

(4) $\mathfrak{X}(M)$ is also an $\mathbb{R}$-vector space of differential operators $X : C^\infty(M) \to C^\infty(M)$. In fact the action of $X \in \mathfrak{X}(M)$ on $f \in C^\infty(M)$ is well defined. In local coordinates

$$(X(f))(p) := \sum_{k=1}^{n} X^k_p \left.\frac{\partial f}{\partial x^k}\right|_p .$$

At this juncture, taking advantage of (2), it is easy to prove that $M \ni p \mapsto (X(f))(p)$ is well defined (it does not depends on the local chart around p) and C^∞.

(5) Since $f \cdot X \in \mathfrak{X}(M)$ if $f \in C^\infty(M)$ and $X \in \mathfrak{X}(M)$ where, obviously

$$(f \cdot X)(g) := f \cdot X(g)$$

we can also assert that $\mathfrak{X}(M)$ has also the structure of **module** on the commutative unital ring $C^\infty(M)$. As the latter is not a division ring (if $f \neq 0$ (the zero function), in general $M \ni x \mapsto \frac{1}{f(x)}$ is not well-defined), we cannot extend that module structure to a $C^\infty(M)$-vector space structure.
In any cases both $\mathfrak{X}(M)$ and $\Omega_1(M)$ are $\mathbb{R}$-vector spaces.

(6) If $f \in C^\infty(M)$, its **differential** $df \in \Omega_1(M)$ is defined as

$$df(p) = \sum_{k=1}^{n} \left.\frac{\partial f \circ \psi^{-1}}{\partial x^k}\right|_{\psi(p)} dx^k|_p ; \quad \forall p \in U$$

where we are referring to a local chart (U, ψ) with coordinates $x^1, \ldots, x^n$. Taking advantage of (3), it is easy to prove that this definition does not depend on the used local chart

(7) If $X \in \mathfrak{X}(M)$ and $\omega \in \Omega_1(M)$ we can define the **contraction of them**: a scalar field, namely an element $\langle X, \omega\rangle \in C^\infty(M)$. It is defined as follows

$$\langle X, \omega\rangle(p) := \langle X_p, \omega_p\rangle = \sum_{k=1}^{n} X_p^k \omega_{kp} \quad \forall p \in U\,.$$

A trivial computation which uses bilinearity of the pairing, the decomposition in components of X and ω and (3.8), proves that

$$\langle X_p, \omega_p\rangle = \sum_{k=1}^{n} X_p^k \omega_{kp}$$

in every local chart (U, ψ), in particular showing that $\langle X, \omega\rangle$ is smooth as declared because it is a linear combination of products of smooth functions.

(8) If $\gamma : I \ni s \mapsto \gamma(s) \ni M$ is a smooth curve (where I is an interval of $\mathbb{R}$), the **tangent vector** $\gamma'(s) \in T_{\gamma(s)}M$ at $\gamma(s)$ is defined as

$$\gamma'(s) = \sum_{k=1}^{n} \left.\frac{d\gamma^k}{ds}\right|_s \left.\frac{\partial}{\partial x^k}\right|_{\gamma(s)}$$

where we are referring to a local chart (U, ψ) with coordinates $x^1, \ldots, x^n$ and $\gamma^k(s) := x^k(\gamma(s))$. Once again, taking advantage of (2), it is easy to prove that this definition does not depend on the used local chart.

(9) As an exercise, prove that

$$\frac{d}{ds} f(\gamma(s)) = \langle \gamma'(t), df(\gamma(t))\rangle\,,$$

where $f \in C^\infty(M)$ and $\gamma : I \to M$ is a smooth curve.

(10) If $X, Y \in \mathfrak{X}(M)$, we can consider them as linear differential operators $C^\infty(M) \to \mathbb{R}$ and define a composed differential operator, indicated by $[X, Y]$ as follows

$$[X, Y](f) := X(Y(f)) - Y(X(f))\,. \tag{3.14}$$

Notably $[X, Y]$ is still a contravariant vector field. The shortest way to prove it is just observing that, in local coordinates,

$$[X, Y]_p(f) = \sum_k [X, Y]_p^k \frac{\partial f}{\partial x^k}|_{\psi(p)}$$

where

$$[X, Y]_p^i = \sum_{j=1}^{n} X_p^i \frac{\partial Y^j}{\partial x^i}|_{\psi(p)} - \sum_{j=1}^{n} Y_p^i \frac{\partial X^j}{\partial x^i}|_{\psi(p)}\,, \tag{3.15}$$

and finally checking that the rule (3.10) is satisfied when replacing X^k for $[X, Y]^k$ therein. The map $[\cdot, \cdot] : \mathfrak{X}(M) \times \mathfrak{X}(M) \to \mathfrak{X}(M)$ is called **Lie bracket**. It is bilinear, antisymmetric (namely $[X, Y] = -[Y, X]$) and satisfies the **Jacobi rule**:

$$[X, [Y, Z]] + [Z, [X, Y]] + [Y, [Z, X]] = 0\,, \quad X, Y, Z \in \mathfrak{X}(M)\,.$$

These three properties make the real vector space $\mathfrak{X}(M)$ endowed with the map $[\cdot,\cdot]$ a real **Lie algebra**. ■

3.1.4 Tangent and cotangent bundle

If M is a smooth manifold and with dimension n, consider the set

$$TM := \{(p,v) \mid p \in M\ ,\ v \in T_pM\}\ .$$

It is possible to endow TM with a structure of a smooth manifold with dimension $2n$. That structure is naturally induced by the analogous structure of M.
First of all let us define a suitable second-countable Hausdorff topology on TM. If $\mathcal{M}$, is the differentiable structure of M, consider the class $\mathcal{B}$ of all open sets $U \subset M$ such that there is a local chart $(U,\phi) \in \mathcal{M}$. It is straightforwardly proved that $\mathcal{B}$ is a basis of the topology of M. Then consider the class $T\mathcal{B}$ of all subsets V of TM defined as follows.

(a) take $(U,\phi) \in \mathcal{M}$ with $\phi : p \mapsto (x^1(p),\ldots,x^n(p))$;

(b) take an open nonempty set $B \subset \mathbb{R}^n$;

(b) define
$$V_{U,\phi,B} := \{(p,v) \in TM \mid p \in U\ ,\ v \in \hat{\phi}_p B\}\ ,$$
where $\hat{\phi}_p : \mathbb{R}^n \to T_pM$ is the linear isomorphism associated to ϕ:
$$\hat{\phi}_p : (v_p^1,\ldots,v_p^n) \mapsto \sum_{i=1}^n v_p^i \frac{\partial}{\partial x^i}|_p \tag{3.16}$$

Let $\mathcal{T}_{T\mathcal{B}}$ finally denote the family that includes $\varnothing$ and all the sets in TM which are unions of the above sets $V_{U,\phi,B}$. Notice that $TM \in \mathcal{T}_{T\mathcal{B}}$.
It is easy to prove that $\mathcal{T}_{T\mathcal{B}}$ is a topology and, trivially, the sets $V_{U,\phi,B}$ (varying U,ϕ,B) form a basis of that topology. $\mathcal{T}_{T\mathcal{B}}$ is also second-countable and Hausdorff. Finally, it turns out that TM, equipped with the topology $\mathcal{T}_{T\mathcal{B}}$, is locally homeomorphic to $\mathbb{R}^n \times \mathbb{R}^n$. Indeed, if (U,ϕ) is a local chart of M with $\phi : U \ni p \mapsto (x^1(p),\ldots,x^n(p)) \in \mathbb{R}^n$, we may define a local chart of TM, (TU,Φ), where
$$TU := \{(p,v) \mid p \in U\ \ ,\ v \in T_pM\}$$
by defining
$$T\phi : (p,v) \mapsto (x^1(p),\ldots,x^n(p),v_p^1,\ldots,v_p^n) \in \mathbb{R}^{2n}\ ,$$
where $v = \sum_i v_p^i \frac{\partial}{\partial x^i}|_p$. Notice that $T\phi$ is injective and $T\phi(TU) = \phi(U) \times \mathbb{R}^n \subset \mathbb{R}^{2n}$. As a consequence of the definition of the topology $\mathcal{T}_{T\mathcal{B}}$ on TM, every $T\phi$ defines a local homeomorphism from TM to $\mathbb{R}^{2n}$. As the union of domains of every $T\phi$ is TM itself
$$\bigcup TU = TM\ ,$$

TM is locally homeomorphic to $\mathbb{R}^{2n}$.

Remark 3.14. An equivalent but more implicit way to define the topology of TM is to declare that $A \subset TM$ is open if $T\phi(A \cap \Pi^{-1}(U))$ is open in $\mathbb{R}^{2n}$ for every local chart (U, ϕ) on M and where $\Pi : TM \ni (p, v) \mapsto p \in M$ is the canonical projection of TM onto M. ■

The next step consists of defining a smooth differentiable structure on TM. Consider two local charts on TM, $(TU, T\phi)$ and $(TU', T\phi')$ respectively induced by two local charts (U, ϕ) and (U', ϕ') of the differentiable structure of M. As a consequence of the given definitions, $(TU, T\phi)$ and $(TU', T\phi')$ are trivially compatible. Moreover, the class of charts $(TU, T\phi)$ induced from all the charts (U, ϕ) of the differentiable structure of M defines an atlas $\mathcal{A}(TM)$ on TM (in particular because, as said above, $\bigcup TU = TM$). The differentiable structure $\mathcal{M}_{\mathcal{A}(TM)}$ induced by $\mathcal{A}(TM)$ makes TM a smooth manifold with dimension $2n$.

An analogous procedure gives rise to a natural smooth differentiable structure for

$$T^*M := \{(p, \omega) \mid p \in M \ , \ \omega_p \in T_p^*M\} .$$

Definition 3.15. [Tangent and Cotangent Bundles or Spaces] Let M be a smooth manifold with dimension n and differentiable structure $\mathcal{M}$. If (U, ϕ) is any local chart of $\mathcal{M}$ with $\phi : p \mapsto (x^1(p), \ldots, x^n(p))$ define

$$TU := \{(p, v) \mid p \in U \ , \ v \in T_pM\} \ , \quad T^*U := \{(p, \omega) \mid p \in U \ , \ \omega \in T_p^*M\}$$

and

$$V_{U,\phi,B} := \{(p, v) \mid p \in U \ , \ v \in \hat{\phi}_p B\} \ , \quad {}^*V_{U,\phi,B} := \{(p, \omega) \mid p \in U \ , \ \omega \in^* \hat{\phi}_p B\} \ ,$$

where $B \subset \mathbb{R}^n$ are open nonempty sets and $\hat{\phi}_p : \mathbb{R}^n \to T_pM$ and ${}^*\hat{\phi}_p : \mathbb{R}^n \to T_p^*M$ are the linear isomorphisms naturally induced by ϕ as in (3.16) for $\hat{\phi}_p$ and

$$ {}^*\hat{\phi}_p : (\omega_{p1}, \ldots, \omega_{pn}) \mapsto \sum_{i=1}^{n} \omega_{pi} dx^i|_p \ . \tag{3.17}$$

Finally define $T\phi : TU \to \phi(U) \times \mathbb{R}^n \subset \mathbb{R}^{2n}$ and $T^*\phi : T^*U \to \phi(U) \times \mathbb{R}^n \subset \mathbb{R}^{2n}$ such that

$$T\phi : (p, v) \mapsto (x^1(p), \ldots, x^n(p), v_p^1, \ldots, v_p^n) \ ,$$

where $v = \sum_i v_p^i \frac{\partial}{\partial x^i}|_p$ and

$$T^*\phi : (p, v) \mapsto (x^1(p), \ldots, x^n(p), \omega_{1p}, \ldots, \omega_{p_n}) \ ,$$

where $\omega = \sum_i \omega_{ip} dx^i|_p$.

(a) The **tangent bundle** associated with M is the smooth manifold obtained by equipping

$$TM := \{(p, v) \mid p \in M \ , \ v \in T_pM\}$$

with:
(1) the topology generated by the sets $V_{U,\phi,B}$ above varying $(U, \phi) \in \mathcal{M}$ and B in the class of open non-empty sets of $\mathbb{R}^n$,
(2) the differentiable structure induced by the atlas

$$\mathcal{A}(TM) := \{(U, T\phi) \mid (U, \phi) \in \mathcal{M}\} .$$

The local charts $(TU, T\phi)$ of $\mathcal{A}(TM)$ are said **natural local charts** on TM or also local chart adapted to the fiber-bundle structure of TM.

(b) The **cotangent bundle** associated with M is the manifold obtained by equipping

$$T^*M := \{(p, \omega) \mid p \in M \ , \ \omega \in T_p^*M\}$$

with:
(1) the topology generated by the sets ${}^*V_{U,\phi,B}$ above varying $(U, \phi) \in \mathcal{M}$ and B in the class of open non-empty sets of $\mathbb{R}^n$,
(2) the differentiable structure induced by the atlas

$${}^*\mathcal{A}(TM) := \{(U, T^*\phi) \mid (U, \phi) \in \mathcal{M}\} .$$

The local charts $(TU, T^*\phi)$ of ${}^*\mathcal{A}(TM)$ are said **natural local charts** on T^*M or also local chart adapted to the fiber-bundle structure of T^*M.

■

3.1.5 Normal covector to a codimension-1 submanifold and product manifolds

Let M be a smooth manifold of dimension m and $N \subset M$ an embedded smooth submanifold of codimension 1 (i.e. the dimension of N is $m-1$). Locally, i.e. in the neighborhood U of $p \in N$, the submanifold is made of the points $q \in M$ such that $f(q) = 0$, where $f \in C^\infty$ and $df \neq 0$ in $U \cap N$. The function f is nothing but the coordinate x^m (smoothly extended to zero outside U) in a local coordinate system (U, ψ) which is adapted to N and with coordinates $x^1, \ldots, x^m$. Locally $df(q) = dx^m|_q \neq 0$. The reasoning can be reversed according to the following result that is an immediate consequence of the *theorem of regular values* [57].

Proposition 3.16. *Let M be a smooth manifold. If $f \in C^\infty(M)$ and $N := \{q \in M \mid f(q) = 0\}$, then N is an embedded smooth submanifold of M of codimension 1, provided $df|_N \neq 0$.*

Proposition 3.17. *Let $N \subset M$ be an embedded smooth submanifold of codimension 1 and suppose that $f \in C^\infty(M)$ vanishes in $U \cap N$, where $U \subset M$ is open, with $df|_{U\cap N} \neq 0$. It turns out that $df|_{U\cap N}$ is fixed up to a nonvanishing smooth factor which depends on $q \in U \cap M$. Furthermore*

$$\langle X_q, df(q)\rangle = 0 \quad \textit{if } X \in T_qN .$$

Proof. Consider a local coordinate system $x^1, \ldots, x^m$ on U adapted to N, so that $x^m = 0$ on $U \cap N$ and the remaining coordinates are local coordinates on N. It holds $0 \neq df(q) = \sum_k \frac{\partial f}{\partial x^k}|_{\psi(q)} dx^k|_q$ where the first n derivatives vanish because f is constant on N. In summary, $df(q) = \frac{\partial f}{\partial x^m}|_{\psi(q)} dx^m|_q$. Another similar function differs from the previous one just for smooth nn vanishing factor $\frac{\partial f}{\partial x^m}|_{\psi(q)}$. The final identity is obvious per direct inspection by observing that T_qN is spanned by the $m-1$ vectors $\left.\frac{\partial}{\partial x^k}\right|_q$ with $k \neq m$. □

Definition 3.18. Let $N \subset M$ be an embedded smooth submanifold of codimension 1 and suppose that $f \in C^\infty(M)$ vanishes in $U \cap N$, where $U \subset M$ is open, with $df|_{U\cap N} \neq 0$. The covector $n_N := df|_{U\cup N}$ – defined up to a smooth non vanishing factor – is called the **conormal** vector to N. ■

Let us now move on to another useful technical notion.

If M and N are smooth manifolds, it is possible to define a smooth structure on $M \times N$ of dimension $\dim(M) + \dim(N)$ as follows. Obviously the topology we put on $M \times N$ is the *product topology*, that is Hausorff and second-countable since the two topologies are. If (U, ψ) and (V, ϕ) are two local charts on M and N respectively, with respective coordinate functions $\psi : U \ni p \mapsto (x^1, \ldots, x^m) \in \mathbb{R}^m$ and $\psi : V \ni q \mapsto (y^1, \ldots, y^n) \in \mathbb{R}^n$, then $(U \times V, \psi \times \phi)$ is a local chart on on the topological space $M \times N$ where

$$\psi \times \phi : U \times V \ni (p, q) \mapsto (x^1, \ldots, x^m, y^1, \ldots, y^n) \in \mathbb{R}^{m+n} . \tag{3.18}$$

Couples of local charts $(U' \times V', \psi' \times \phi')$ are automatically C^∞ compatible. Since this family of charts form an atlas on $M \times N$, we can define a smooth structure on $M \times N$ as the one induced by the atlas.

Definition 3.19. If M and N are smooth manifolds of dimension m and n respectively, the **(smooth) product manifold** of them is the smooth manifold of dimension $m + n$ on $M \times N$ defined as follows.

(i) The topology on $M \times N$ is the product topology.

(ii) The smooth structure is the one which includes all the local chart of the form (3.18), when (M, ψ) and (N, ϕ) are local charts of the smooth structure of M and N respectively.

The local charts (3.18) are said **adapted** to (the product structure of) $M \times N$. ■

Remark 3.20. If $(p,q) \in M \times N$, we have the direct decomposition $T_{(p,q)}M \times N = T_pM \oplus T_qN$ where T_pM and T_qN are viewed as subspaces of $T_{(p,q)}M \times N$ respectively given by

$$\text{span}\left\{ \left.\frac{\partial}{\partial x^k}\right|_{(p,q)} \right\}_{k=1,\ldots,m} \quad \text{and} \quad \text{span}\left\{ \left.\frac{\partial}{\partial y^j}\right|_{(p,q)} \right\}_{j=1,\ldots,n}$$

referring to an adapted local chart (3.18). It is easy to prove that these subspaces of $T_{(p,q)}M \times N$ do not depend on the choice of the local charts (U, ψ) and (V, ϕ) around p and q respectively. ■

3.1.6 (Pseudo)Riemannian manifolds

We move on to introduce the notion of *(pseudo)Riemannian* manifold, that is nothing but a smooth manifold equipped with a smooth assignment of a (non-degenerate) *inner product* at each tangent space. Before giving the definition a recap on some elementary notions of linear algebra is in order.

Remark 3.21.

(1) If V is a vector space on $\mathbb{R}$ an **inner product** is a map $g : V \times V \to \mathbb{R}$ that is

(i) **symmetric**: $g(u,v) = g(v,u)$ if $u, v \in V$;

(ii) **bi-linear**: $g(au + bv, w) = ag(u,w) + bg(v,w)$ and the same swapping the arguments, if $a, b \in \mathbb{R}$ and $u, v, w \in V$;

(iii) **non-degenerate**: $g(u,v) = 0$ for every $u \in V$ implies $v = 0$.

g, defined as above, is a **scalar product** if it is also **positive**: $g(u,u) \geq 0$ for every $u \in V$, and $g(u,u) = 0$ imposes $u = 0$. If g is not positive (but is non-degenerate) is a **pseudo-scalar product**.

(2) If $g : V \times V \to \mathbb{R}$ satisfies (i) and (ii) for a finite dimensional vector space V and $\{e_j\}_{j\in J}$ is a basis, consider the matrix $G := [g(e_i, e_j)]_{i,j\in J}$. The following two facts are true.

(a) If g is a inner product then $\det G \neq 0$. (Indeed, if $\det G = 0$ then there is $v \in V \setminus \{0\}$ such that $Gv = 0$ and thus, contrarily to the non-degenerateness hypothesis, $g(u,v) = U^tGV = 0$ for every $u \in V$, where $U = (u^1, \ldots, u^n)^t$ and $V := (v^1, \ldots, v^n)^t$ are the $\mathbb{R}^n$-vectors of the components of u and v respectively according to the given basis.)

(b) If $\det G \neq 0$, then g is an inner product. (Indeed, with the same notation as above, if g is degenerate there is $V \in \mathbb{R}^n \setminus \{0\}$ with $U^tGV = 0$ for every $U \in \mathbb{R}^n$. Choosing $U := GV$, it must be $(GV)^tGV = 0$ and thus $GV = 0$, which implies $\det G = 0$ since $V \neq 0$.)

(3) Let us suppose that $\dim(V) = n < +\infty$. As an immediate consequence of the *Sylvester therem*, an inner product $g : V \times V \to \mathbb{R}$ admits **(pseudo)orthonormal basis**. That is a basis $\{e_1, \ldots e_n\}$ of V such that

$$g(e_i, e_j) = 0 \quad \text{if } i \neq j,$$

$$g(e_1,e_1) = \cdots = g(e_p,e_p) = 1\ , \quad g(e_{p+1},e_{p+1}) = \cdots = g(e_n,e_n) = -1\ ,$$

where p *only* depends on g and not on the used basis. The **signature** of g is $sign(g) := (p, n-p)$.

(4) If $p = n$, evidently g is a scalar product, namely is positive. The same happens for $-g$ if $p = 0$.

The inner product is said a **Lorentzian scalar product** if $p = 1$, so that the signature is $(1, n-1)$[2].

(5) Consider a pair of (pseudo)orthonormal bases $(e_1, \ldots, e_n)$ and $(e'_1, \ldots, e'_n)$ so that $e'_k = \sum_{j=1}^n A^j{}_k e_j$. In both bases the matrix of the metric has identical diagonal form:

$$\eta^{(g)} := \mathrm{diag}(1, \cdots, 1, -1, \cdots, -1), \tag{3.19}$$

where the diagonal is defined by the signature of g. Therefore,

$$\eta^{(g)}_{hk} = g(e'_h, e'_k) = \sum_{i,j=1}^{n} A^i{}_h A^j{}_k g(e_i, e_j) = \sum_{i,j=1^n} A^i{}_h A^j{}_k \eta^{(g)}_{ij}\ .$$

In matricial form,

$$A^t \eta^{(g)} A = \eta^{(g)}\ . \tag{3.20}$$

The set

$$O(sign(g)) := \{A \in M(n,\mathbb{R}) \mid A^t \eta^{(g)} A = \eta^{(g)}\} \tag{3.21}$$

is the **stability group** of the (pseudo)scalar product g.

(5) It is easy to prove that, indeed, $O(sign(g))$ is a group, subgroup of $GL(n,\mathbb{R})$, that is closed with respect to the transposition operation: $A \in O(sign(g))$ implies $A^t \in O(sign(g))$.

$O(1, n-1) = O(n-1, 1)$ is called **Lorentz group** of dimension n. $O(n,0) = O(0,n) := O(n)$ is nothing but the standard orthogonal group of dimension n.

(6) If g is a inner product according to the definition in (1), since it is non-degenerate, the map

$$\flat : V \ni v \mapsto v^\flat := g(v, \cdot) \in V^*$$

is injective. Since the space have the same dimension, it is also surjective and thus define a (natural) isomorphism between V and V^*. In components, using a basis and its dual basis and where $g_{ab} := g(e_a, e_b)$, the isomorphism above reads

$$\flat : \sum_{a=1}^{n} v^a e_a = v \mapsto v^\flat = \sum_{b=1}^{n} v_b e^{*b} \quad \text{where } v_b := \textstyle\sum_{a=1}^n v^a g_{ab}\ . \tag{3.22}$$

That is because, with the said definition and taking (6) Remark 3.9 into account,

$$\sum_{b=1}^{n} v_b e^{*b}(u) = \sum_{b=1}^{n} v_b u^b = \sum_{a,b=1}^{n} v^a g_{ab} u^b = g(v,u) = g(v,\cdot)(u)\ , \quad \forall u \in V\ .$$

[2] Another convention as in [56, 57] defines Lorentzian scalar products the inner products with $p = n-1$, i.e., signature $(n-1, 1)$.

From this perspective there are no contravariant and covariant vectors, but just vectors, which admit both contravariant and covariant representations. The numbers v_a in (3.22) are said the **covariant components** of the contravariant vector v with respect to the considered basis.
The inverse isomorphism of $\flat$ is $\sharp : V^* \to V$

$$\sharp : \sum_{a=1}^{n} \omega_a e^{*a} = \omega \mapsto \omega^\sharp = \sum_{b=1}^{n} \omega^b e_b \quad \text{where } \omega^b := \textstyle\sum_{a=1}^{n} \omega_a g^{ab} . \tag{3.23}$$

Above g^{ab} are the coefficients of $[g_{ab}]^{-1}_{a,b=1,\ldots,n}$ which exists for (2). ■

Definition 3.22. A **(pseudo)Riemannian** manifold is a smooth manifold M equipped with an assignment $M \ni p \mapsto g_p : T_pM \times T_pM \to \mathbb{R}$, of inner products, called the **metric** of M, such that

(i) the assignment is smooth: in each local chart (U, ψ) of M[3] with coordinates $U \ni p \mapsto (x^1, \ldots, x^n) \in \psi(U)$ the map $\psi(U) \ni (x^1, \ldots, x^n) \mapsto g_{hk}(p) := g_p\left(\frac{\partial}{\partial x^h}\Big|_p , \frac{\partial}{\partial x^k}\Big|_p \right)$ is C^∞;

(ii) $sign(g_p) = sign(g_q)$ for every $p, q \in M$.

Furthermore

(a) The functions $U \ni p \mapsto g_{hk}(p)$ are said **metric coefficients** in the considered local chart.

(b) If every g_p is a scalar product, thus positive, then the manifold is said **Riemannian** and the metric is said to be **Euclidean** or, equivalently, **Riemannian**.

(c) If every g_p is Lorentzian, the manifold and the metric are called **Lorentzian**.

(d) If every g_p is not positive, the manifold and the metric are called **pseudo Riemannian**.

(e) A (pseudo)Riemannian manifold (M, g) is said to be **locally flat**, if there is an atlas such that each coefficient $U \ni p \mapsto g_{hk}(p)$ is a constant function in every local chart (U, ψ) of the atlas and for every choice of $h, k = 1, \ldots, \dim(M)$. It is said **globally flat** if the said atlas contains a chart with domain M ■

Remark 3.23.

(1) According to the given definition, if $Y, Y \in \mathfrak{X}(M)$, we can for instance define a scalar field $g(X, Y) \in C^\infty(M)$, where locally, i.e., in every local chart

$$g(X, Y)(p) = g_p(X_p, Y_p) = \sum_{a,b=1}^{n} g_{ab}(p) X_p^a Y_p^b .$$

(2) Let (M, g) be locally flat and let (U, ψ) be a local chart where the coefficients g_{hk} are constant. The Sylvester theorem immediately implies that with a linear transformation of these

[3] As usual it is sufficient that this condition is valid on an atlas of M.

coordinates (thus defining another local chart with the same domain) we can diagonalize the matrix of these coefficients and obtain new coefficients in canonical form (3.19):

$$[g_{hk}(p)]_{h,k=1,\ldots,n} = \eta^{(g)}$$

according to the signature of g. In this new local chart the canonical basis $\left.\frac{\partial}{\partial x^k}\right|_p$ is (pseudo) orthonormal at each point $p \in U$.

(3) $(\mathbb{R}^n, g_n)$ is globally flat with respect to the standard Euclidean metric g_n that is, by definition, represented by the metric coefficients δ_{ij} in each tangent space $T_p\mathbb{R}^n$, using the canonical basis associated to the standard coordinates of $\mathbb{R}^n$.

(4) The most elementary example of a locally flat Riemannian manifold which is not globally flat is a cylinder $C := \{(x, y, z) \in \mathbb{R}^3 | x, y, z \in \mathbb{R}, x^2+y^2 = 1\}$ viewed as an embedded submanifold of $\mathbb{R}^3$ endowed with the metric naturally indiced by $\mathbb{R}^3$ as follows. If $u, v \in T_pC$ we can view them as elements of $T_p\mathbb{R}^3$, so that we can define a metric $g_C(u, v) := g_3(u, v)$, where g_3 is the standard Euclidean metric on $\mathbb{R}^3$. Using cylindrical coordinates r, θ, z in $\mathbb{R}^3$, and redefining $r* := r - 1$, the local chart (r^*, θ, ϕ) is adapted to C. When taking $r^* = 0$, the surviving coordinates on C, $\theta \in (-\pi, \pi)$, $z \in \mathbb{R}$ define a local chart with domain $C \setminus \{(x, y, z) \in \mathbb{R}^3 \mid x = -1\}$. Changing the origin of θ we have a different chart. All these charts are C^∞ compatible and their domains cover C. In summary C turns out to be a 2-dimensional embedded submanifold of $\mathbb{R}^2$ and the atlas generated by the said family of charts defines the smooth structure of C. We leave to the reader the easy proof of the fact that, in each local chart of this type, the coefficients of the metric are $(g_C)_{ij}(\theta, z) = \delta_{ij}$. Nevertheless none of the considered charts covers C completely and it is possible to prove that no global chart of this sort exists on C referring to the said metric. (The reason is the following one. The considered metric admits complete geodesic given by closed (thus non injective) maps $\mathbb{R} \ni s \mapsto \gamma(s)$ locally described by $\theta(s) = \theta$, $z(s) = z_0$, in particular $\gamma(0) = \gamma(2\pi)$. If (C, g_C) where globally flat, there would exist a global chart (C, ψ). ψ whould diffeomorphically map C to a portion of the $\mathbb{R}^2$ plane, also identifying the metric g_C with the flat metric of the plane. The map $\mathbb{R} \ni s \mapsto \psi(\gamma(s)) \in \psi(C)$ would be a geodesic in $\mathbb{R}^2$. The geodesics of $(\mathbb{R}^2, \delta_2)$ are straight lines, thus injective with respect to their parametrization. *Vice versa* $\psi(\gamma(0)) = \psi(\gamma(2\pi))$. We conclude that (C, ψ) as requested does not exist.)

(5) An important example of globally flat (pseudo)Riemannian manifold is provided by an n-dimensional real affine space $\mathbb{A}$ equipped with an inner product g in the vector space of translations V. The metric is defined taking advantage of the natural isomorphism $T_p : V \to T_pM$ defined in (3.9) just by defining $g_p(t_p, t'_p) := g(T_p^{-1}t_p, T_p^{-1}t'_p)$ for every $p \in \mathbb{A}$ and $t_p, t'_p \in T_p\mathbb{A}$. In every Cartesian coordinate system the coefficients describing the metric are constant by construction. Since these charts are global $(\mathbb{A}, g)$ is globally flat. Every open set of $\mathbb{A}$ equipped with the natural structures induced by $(\mathbb{A}, g)$, turns out another example of locally flat (pseudo)Rieannian manifold. ■

3.2 Covariant derivative and Levi-Civita connection

3.2.1 Affine connection and covariant derivative

Consider a smooth manifold M and a pair of contravariant vector fields $X, Y \in \mathfrak{X}(M)$, our intention is to define a suitable notion of *derivative of* X *with respect to* Y, indicated by $\nabla_Y X$. We stress that we are assuming that $\nabla_Y X$ is a vector field as well: $\nabla_Y X \in \mathfrak{X}(M)$.

We could naively expect that in any given local chart (U, ψ) with coordinates $x^1, \ldots, x^n$,

$$(\nabla_Y X)^a_p = \sum_{b=1}^n Y^b_p \left.\frac{\partial X^a}{\partial x^b}\right|_{\psi(p)} . \tag{3.24}$$

Let us show that, unfortunately, the expression above cannot be valid in all coordinate systems when assuming that $\nabla_Y X \in \mathfrak{X}(M)$. To show it, referring to another local chart (U', ψ') with coordinates $x^1, \ldots, x^n$, let us define

$$(\nabla'_Y X)^e_p := \sum_{d=1}^n Y'^d_p \left.\frac{\partial X'^e}{\partial x'^d}\right|_{\psi'(p)} . \tag{3.25}$$

We want to check if $(\nabla_Y X)_p = (\nabla'_Y X)_p$ for $p \in U \cap U'$.

$$(\nabla_Y X)^a_p = \sum_{b=1}^n Y^b \frac{\partial X^a}{\partial x^b} = \sum_{b,c,d=1}^n \frac{\partial x^b}{\partial x'^c} \frac{\partial x'^d}{\partial x^b} Y'^c \frac{\partial X^a}{\partial x'^d} = \sum_{d=1}^n Y'^d \frac{\partial X^a}{\partial x'^d} = \sum_{d,e=1}^n Y'^d \frac{\partial}{\partial x'^d} \frac{\partial x^a}{\partial x'^e} X'^e$$

$$= \sum_{d,e=1}^n Y'^d \frac{\partial x^a}{\partial x'^e} \frac{\partial X'^e}{\partial x'^d} + (\cdots) = \sum_{e=1}^n \frac{\partial x^a}{\partial x'^e} \left(\sum_{d=1}^n Y'^d \frac{\partial X'^e}{\partial x'^d} \right) + (\cdots) = \sum_{e=1}^n \frac{\partial x^a}{\partial x'^e} (\nabla'_Y X)^e + (\cdots) .$$

The dots vanish only if the coordinate transformation $x^a = x^a(x'^1, \ldots, x'^n)$, $a = 1, \ldots, n$, is affine: $x^a = c^a + \sum_{j=1}^n A^a{}_j x'^j$ (where $[A^a{}_j]_{a,j=1,\ldots,n}$ is non singular because it is nothing but the Jacobian matrix of the coordinate transformation). The terms $(\cdots)$ are made of second derivatives of functions $x^a = x^a(x'^1, \ldots, x'^n)$ and of the inverse transformation, thus they vanish as asserted if the coordinate transformation is of the said type. In summary, we obtained that $(\nabla_Y X)_p \neq (\nabla'_Y X)_p$ in general.

At this juncture, what we can do is just listing the properties we want to be satisfied by a suitable map, if any, $\nabla : \mathfrak{X}(M) \times \mathfrak{X}(M) \ni (X, Y) \mapsto \nabla_X Y \in \mathfrak{X}(M)$. If a map with the wanted properties exists, we cannot expect that $\nabla_Y X$ has the expression (3.24) in every coordinate system. A reasonable set of conditions is listed in the following definition. We already know these properties are valid for special case $M = \mathbb{R}^n$ with $\nabla_Y X$ is defined in the usual way (3.24) in standard coordinates.

Definition 3.24. Let M be a smooth manifold. An **affine connection** or **covariant derivative operator** ∇ is a map

$$\nabla : \mathfrak{X}(M) \times \mathfrak{X}(M) \ni (Y, X) \mapsto \nabla_Y X \in \mathfrak{X}(M) ,$$

which obeys the following requirements for every point $p \in M$:

(1) $(\nabla_{fY+gZ}X)_p = f(p)(\nabla_Y X)_p + g(p)(\nabla_Z X)_p$, for all $f, g \in C^\infty(M)$ and $X, Y, Z \in \mathfrak{X}(M)$;

(2) $(\nabla_Y fX)_p = Y_p(f)X_p + f(p)(\nabla_Y X)_p$ for all $X, Y \in \mathfrak{X}(M)$ and $f \in C^\infty(M)$;

(3) $(\nabla_X(aY + bZ))_p = a(\nabla_X Y)_p + b(\nabla_X Z)_p$ for all $a, b \in \mathbb{R}$ and $X, Y, Z \in \mathfrak{X}(M)$.

The contravariant vector field $\nabla_Y X$ is called the **covariant derivative vector of X with respect to Y** (and the affine connection ∇). ■

Remark 3.25.

(1) If M is an *affine space* of dimension n, we can define $\nabla_Y X$ using (3.24) in a given global system of Cartesian coordinates that globally identifies M with $\mathbb{R}^n$. Since the system is global, $\nabla_Y X$ turns out to be globally defined and it also satisfies the requirements in the above definition, because we are using nothing but the standard definition in $\mathbb{R}^n$. If we use a different *Cartesian* coordinate system, the vector field $\nabla_Y X$ takes the form (3.24) as well because the transformation law between Cartesian coordinate systems is affine. As discussed above, this fact implies that the form (3.24) is preserved. Therefore in affine spaces (in particular $\mathbb{R}^n$) an affine connection can be defined. The issue of the existence of affine connections concerns manifolds which are not affine spaces and which do not admit a global coordinate system.

(2) An important consequence of $\mathbb{R}$-linearity in both arguments of ∇ and the requirements $(\nabla_{fY}X)_p = f(p)(\nabla_Y X)_p$ and $(\nabla_Y fX)_p = Y_p(f)X_p + f(p)(\nabla_Y X)_p$ is that $(\nabla_Y X)_p$ only depends of the values of X, Y in an arbitrarily small neighborhoods of p. Indeed, if $X = X'$ in a neighborhood U of p, then $X - X'$ vanishes in that neighborhood. Taking $f \in C^\infty(M)$ such that $f = 0$ in smaller neighborhood $V \subset U$ of p, but $f = 1$ outside it ($1 - f$ is a suitable *bump function*), we have $f \cdot (X - X') = X - X'$ and thus the difference $(\nabla_Y X)_p - (\nabla_Y X')_p$ can be computed as

$$(\nabla_Y(X - X')))_p = (\nabla_Y(f(X - X')))_p = Y_p(f)(X_p - X'_p) + f(p)(\nabla_Y(X - X'))_p = 0 + 0 = 0\,.$$

Similarly, if $Y = Y'$ in a neighborhood U of p, then $Y - Y'$ vanishes in that neighborhood. Taking again $f \in C^\infty(M)$ such that $f = 0$ in smaller neighborhood $V \subset U$ of p, but $f = 1$ outside it, we have $f \cdot (Y - Y') = Y - Y'$ and thus the difference $(\nabla_Y X)_p - (\nabla_{Y'} X)_p$ can be computed as

$$(\nabla_{Y-Y'}X))_p = (\nabla_{f(Y-Y')}X)_p = f(p)(\nabla_{Y-Y'}X)_p = 0\,.$$

As a further finer result we shall see shortly that, actually, the Y dependence is even more local: $(\nabla_Y X)_p$ only depends on the value of Y exactly at p (and on the values of X in a neughborhood of p). ■

Suppose that we are given such an affine connection ∇ on M. We can compute the covariant derivative $\nabla_Y X$ in components at the point $p \in U$ of a local chart (U, ψ) as follows. First expand $Y = \sum_a Y^a \frac{\partial}{\partial x^a}$ and $X = \sum_b X^b \frac{\partial}{\partial x^b}$, these expressions being valid in U. Next extend the vector fields $\frac{\partial}{\partial x^a}$ to the whole manifold, thus defining elements of $\mathfrak{X}(M)$, by smoothing to 0 them before reaching the boundary of U. Do the same for the functions X^k and Y^k which therefore become elements of $C^\infty(M)$. The details of these extensions are irrelevant since we are interested to what happens around p where these objects remain untouched as proved in the remark above. We keep the original names of all these extended vector fields and functions, but remembering that they are now everywhere defined and thus we can make use of the axioms above.

$$(\nabla_Y X)_p = \left(\nabla_{\sum_a Y^a \frac{\partial}{\partial x^a}} \sum_b X^b \frac{\partial}{\partial x^b}\right)_p = \sum_{a,b} Y^a(p) \left(\nabla_{\frac{\partial}{\partial x^a}} X^b \frac{\partial}{\partial x^b}\right)_p$$

$$= \sum_{a,b} Y^a(p) \left(\nabla_{\frac{\partial}{\partial x^a}} X^b\right)_p \frac{\partial}{\partial x^b} + \sum_{a,b} Y^a(p) X^b(p) \left(\nabla_{\frac{\partial}{\partial x^a}} \frac{\partial}{\partial x^b}\right)_p$$

$$= \sum_{a,b} Y^a(p) \frac{\partial X^b}{\partial x^a}|_{\psi(p)} \left.\frac{\partial}{\partial x^b}\right|_p + \sum_{a,b} Y^a(p) X^b(p) \left(\nabla_{\frac{\partial}{\partial x^a}} \frac{\partial}{\partial x^b}\right)_p$$

$$= \sum_{a,b} Y^a(p) \frac{\partial X^b}{\partial x^a}|_{\psi(p)} \left.\frac{\partial}{\partial x^b}\right|_p + \sum_{a,c} Y^a(p) X^c(p) \left(\nabla_{\frac{\partial}{\partial x^a}} \frac{\partial}{\partial x^c}\right)_p .$$

Finally, taking advantage of (3.7), we can rearrange the final term as follows

$$\left(\nabla_{\frac{\partial}{\partial x^a}} \frac{\partial}{\partial x^c}\right)_p = \sum_b \left\langle \left(\nabla_{\frac{\partial}{\partial x^a}} \frac{\partial}{\partial x^c}\right)_p , dx^b|_p \right\rangle \left.\frac{\partial}{\partial x^b}\right|_p = \sum_b \Gamma^b_{ac}(p) \left.\frac{\partial}{\partial x^b}\right|_p .$$

The final expression of $(\nabla_Y X)_p$ in coordinates is

$$(\nabla_Y X)_p = \sum_{a,b=1}^n Y^a(p) \left(\frac{\partial X^b}{\partial x^a}|_{\psi(p)} + \sum_{c=1}^n \Gamma^b_{ac}(p) X^c(p)\right) \left.\frac{\partial}{\partial x^b}\right|_p .$$

Per direct inspection (see e.g.,[57]), using the definition above of the functions Γ^b_{ac}, one easily sees that if $p \in U, U'$ for a couple of local charts (U, ψ) and (U', ψ') and referring to the corresponding families of functions, respectively denoted by Γ and Γ':

$$\Gamma^k_{ij}(p) = \sum_{h=1}^n \frac{\partial x^k}{\partial x'^h}|_p \frac{\partial^2 x'^h}{\partial x^i \partial x^j}|_p + \sum_{h,r,s=1}^n \frac{\partial x^k}{\partial x'^h}|_p \frac{\partial x'^r}{\partial x^i}|_p \frac{\partial x'^s}{\partial x^j}|_p {\Gamma'}^h_{rs}(p) ,$$

where we wrote $|_p$ in place of $|_{\psi(p)}$ or $|_{\psi'(p)}$ (the relevant case should be evident from the considered Jacobian matrix) to simplify the notation.
All the procedure can be reversed and one ends up with the following general result.

Proposition 3.26. *The assignment of an affine connection on a smooth manifold M of dimension n is completely equivalent to the assignment of functions $U \ni p \mapsto \Gamma^k_{ij}(p) \in \mathbb{R}$,*

$i,j,k = 1,\ldots,n$, for each local chart (U,ψ) with coordinates $x^1,\ldots,x^n$, which smoothly depend on the point p and transform as

$$\Gamma^k_{ij}(p) = \sum_{h=1}^{n} \frac{\partial x^k}{\partial x'^h}|_p \frac{\partial^2 x'^h}{\partial x^i \partial x^j}|_p + \sum_{h,r,s=1}^{n} \frac{\partial x^k}{\partial x'^h}|_p \frac{\partial x'^r}{\partial x^i}|_p \frac{\partial x'^s}{\partial x^j}|_p {\Gamma'}^h_{rs}(p)\,, \tag{3.26}$$

under change of local coordinates. More precisely,

(a) if an affine connection ∇ is given, coefficients Γ^i_{ij} associated with ∇ which satisfy (3.26) are defined by

$$\Gamma^k_{ij}(p) := \left\langle \nabla_{\frac{\partial}{\partial x^i}|_p} \frac{\partial}{\partial x^j}|_p\,, dx^k|_p \right\rangle \,,$$

(b) if coefficients $\Gamma^k_{ij}(p)$ are assigned for every point $p \in M$ and every coordinate system of an atlas of M, such that (3.26) hold, an affine connection associated with this assignment is given by

$$(\nabla_Y X)^i_p = \sum_{j=1}^{n} Y^j_p \left(\frac{\partial X^i}{\partial x^j}|_p + \sum_{k=1}^{n} \Gamma^i_{jk}(p) X^k_p \right) . \tag{3.27}$$

in every coordinate patch of the atlas, for all vector fields X, Y and every point $p \in M$;

(c) *if ∇ and ∇' are two affine connections on M such that the coefficients $\Gamma^k_{ij}(p)$ and ${\Gamma'}^k_{ij}(p)$ respectively associated to the connections as in (a) coincide for every point $p \in M$ and every coordinate system around p in a given atlas on M, then $\nabla = \nabla'$.* ■

3.2.2 Levi-Civita connection

Do affine connection exist on a smooth manifold? The answer is positive (see e.g. [57]). First of all, it is possible to prove that every smooth manifolds always admits a (positive) metric that makes it a Riemannian manifold. Next it is possible to prove that every (pseudo)Riemannian manifold always admit a special affine connection called the *Levi-Civita connection*. Finally it is possible to modify this affine connection to produce a different connections by adding some terms to its connection coefficients with a certain arbitrariness.

Theorem 3.27. *Let (M,g) be a (pseudo)Riemannian manifold of dimension n. For every local chart (U,ψ) with coordinates $x^1,\ldots,x^n$ define the functions, called* **Christoffel symbols**

$$\Gamma^a_{bc}(p) := \frac{1}{2}\sum_{d=1}^{n} g^{ad}(p) \left(\frac{\partial g_{cd}}{\partial x^b} + \frac{\partial g_{db}}{\partial x^c} - \frac{\partial g_{bc}}{\partial x^d} \right)\Bigg|_{\psi(p)} , \quad p \in U\,, \tag{3.28}$$

where $g_{ab}(p) := g_p\left(\frac{\partial}{\partial x^a}\Big|_p, \frac{\partial}{\partial x^b}\Big|_p \right)$ and $g^{ab}(p)$ is the generic element of $[g_{ab}(p)]^{-1}_{a,b=1,\ldots,n}$ (it exists in view of (2) Remark 3.21). The Christoffel symbols transform according to (3.26) and thus they define an affine connection ∇^g on M named the **Levi-Civita connection**.

Thel Levi-Civita connection is the unique affine connection $\nabla : \mathfrak{X}(M) \times \mathfrak{X}(M) \to \mathfrak{X}(M)$ such that is

(a) **metric***: $Z(g(X,Y)) = g(\nabla_Z X, Y) + g(X, \nabla_Z Y)$,   for $X, Y, Z \in \mathfrak{X}(M)$,*

(b) **symmetric** *(or* **torsion-free***): $\nabla_X Y - \nabla_Y X = [X, Y]$,   for $X, Y \in \mathfrak{X}(M)$.*

Remark 3.28. In $\mathbb{R}^n$ equipped with the standard metric g_n, the Christoffel symbol vanish in standard coordinates since the metric is there represented by constant coefficients δ_{ij}. In that case the Levi-Civita covariant derivative coincides with the standard derivative of vector fields respect to vector fields. ■

3.2.3 Geodesics

An affine connection ∇ on M defines a special family of smooth curves called *geodesics* of utmost relevance in General Relativity. We need some preliminary notion to introduce these curves. First of all we notice that, from (3.27), the Y-dependence in $(\nabla_Y X)_p$ only concerns the single vector $Y_p \in T_pM$ and not what happens to Y around p. (This property is false regarding the second argument X). If $Y \neq Y'$ but $Y_p = Y'_p$, then $(\nabla_Y X)_p = (\nabla_{Y'} X)_p$. On the other hand, every vector $y \in T_pM$ can be extended to a smooth vector field Y on M[4]. As a consequence, if $y_p \in T_pM$ and $X \in \mathfrak{X}(M)$, it is well defined

$$\nabla_{y_p} X := (\nabla_Y X)_p \,, \quad \text{where } Y \in \mathfrak{X}(M) \text{ satisfies } Y_p (:= Y(p)) = y_p \,. \tag{3.29}$$

In the rest of this section we shall take advantage of the above definition. To go on, we give the definition of a *smooth vector field assigned on a smooth curve.*

Definition 3.29. If M is a smooth manifold and $\gamma : (a,b) \to M$ a smooth curve, a **smooth vector field X on γ** is a map

$$(a,b) \ni t \mapsto X(t) \in T_{\gamma(t)}M \,,$$

whose components are smooth functions of t in every local chart of M around $\gamma(t)$ for every $t \in (a,b)$. $\mathfrak{X}(\gamma)$ denotes the space of smooth vector field X on γ. ■

Remark 3.30. Notice that we have not required γ is injective, so that we may have $\gamma(t_1) = \gamma(t_2)$ but $X(t_1) \neq X(t_2)$. ■

A special case is when (a) γ is injective and (b) $X(t) = Y|_{\gamma(t)}$ for some $Y \in \mathfrak{X}(M)$. In this case we can define the derivative of X respect to γ' at $t = t_0$ trivially as

$$\nabla_{\gamma'(t_0)} X := \nabla_{\gamma'(t_0)} Y \,,$$

[4]Consider a local chart (U, ψ) with $p \in U$, define a a smooth vector field Y' in U which has constantly the components of y in coordinates of ψ. Define Y as $Y_q := \chi(q) Y'_q$ if $q \in U$ and $Y_q := 0$ if $q \notin U$, where $\chi \in C^\infty(M)$ is a *bump function*, it takes the value 1 in a neighborhood of p and smoothly vanishes before reaching the boundary of U, that is the support of χ is completely included in U.

where the right-hand side is the covariant derivative of a vector field with respect to a vector at a point of M as defined in (3.29). In a local chart (U,ϕ) around $\gamma(t_0)$, where $\phi(\gamma(t)) = (x^1(t),\ldots,x^n(t)))$,

$$\begin{aligned}
\left(\nabla_{\gamma'(t_0)}X\right)^b &= \sum_a \frac{dx^a}{dt}|_{t_0}\frac{\partial Y^b}{\partial x^a}|_{\phi(\gamma(t_0))} + \sum_{a,c}\Gamma^b_{ac}(\gamma(t_0))\frac{dx^a}{dt}|_{t_0}Y^c(\gamma(t_0))\\
&= \frac{dY^b(\gamma(t))}{dt}|_{t=t_0} + \sum_{a,c}\Gamma^b_{ac}(\gamma(t_0))\frac{dx^a}{dt}|_{t_0}Y^c(\gamma(t_0))\\
&= \frac{dX^b(t)}{dt}|_{t=t_0} + \sum_{a,c}\Gamma^b_{ac}(\gamma(t_0))\frac{dx^a}{dt}|_{t_0}X^c(t_0)\,.
\end{aligned}$$

We see that, in the last line, *only* the restriction X of Y to γ is used. The formula is consistently written even if γ is not injective, since it depends on the map $(a,b) \ni t \mapsto X(t)$. The final result can be used to give the wanted definition of the covariant derivative of a smooth vector field on γ as in Definition 3.29.

Proposition 3.31. *Let M be a smooth manifold with dimension n equipped with an affine connection ∇, and consider a smooth curve $\gamma : (a,b) \to M$. There is a unique map associating a smooth field X on γ to another smooth field X' on γ such that, in any local chart (U,ϕ) around $\gamma(t)$ for any given $t \in (a,b)$ where $\phi(p) = (x^1(p),\ldots,x^n(p))$ if $p \in U$, satisfies*

$$X'(t) = \sum_{b=1}^n \left(\frac{dX^b(t)}{dt} + \sum_{a=1}^n \Gamma^b_{ac}(\gamma(t))\frac{dx^a}{dt}X^c(t)\right)\frac{\partial}{\partial x^b}|_{\gamma(t)} \quad \text{for every } X \in \mathfrak{X}(\gamma). \tag{3.30}$$

$X'(t)$ is called **(covariant) derivative of** X **on** γ **at** t *and it also enjoys the following properties.*

(a) $(aX + bY)'(t) := aX'(t) + bY'(t)$ *if* $a,b \in \mathbb{R}$, $X,Y \in \mathfrak{X}(\gamma)$, *and* $t \in (a,b)$;

(b) $(fX)'(t) := \frac{df}{dt}X(t) + f(t)X'(t)$ *if* $f \in C^\infty((a,b))$, $X \in \mathfrak{X}(\gamma)$, *and* $t \in (a,b)$;

(c) $X'(t) = \nabla_{\gamma(t)}Y$ *if* γ *is injective,* $X(t) = Y|_{\gamma(t)}$ *for some* $Y \in \mathfrak{X}(M)$, *and* $t \in (a,b)$.

$X'(t)$ is denoted by $\nabla_{\gamma'(t)}X$ also if γ is not injective and X is defined only on γ.

Proof. One easily sees from (3.26) that the definition (3.30) is independent from the used coordinate charts to cover γ and uniquely defines a smooth vector field along γ. The remaining properties arise directly from the the definition in coordinates. □

Definition 3.32. (**Parallel transport and geodesic curves**.) Let M be a smooth manifold equipped with an affine connection ∇ and consider a smooth curve $\gamma : (a,b) \ni u \mapsto \gamma(u) \in M$.

(a) A vector field $X \in \mathfrak{X}(\gamma)$ is said to be **parallely transported along** γ (according to ∇) if

$$\nabla_{\gamma'(u)} X = 0 \quad \text{for all } u \in (a,b) \, ,$$

(b) γ is an open **geodesic segment** if it transports its tangent vector parallely to itself:

$$\nabla_{\gamma'(u)} \gamma'(u) = 0 \quad \text{for all } t \in (a,b). \tag{3.31}$$

This equation is called **geodesic equation**. In coordinates of a local chart (U, ψ), if γ is represented by $I \ni u \mapsto \psi(\gamma(u)) =: (x^1(u), \ldots, x^n(u)) \in U$, the geodesic equation reads

$$\frac{d^2 x^a}{du^2} + \sum_{b,c=1}^{n} \Gamma^a_{bc}(\gamma(u)) \frac{dx^b}{du} \frac{dx^c}{du} = 0 \, , \quad a = 1, \ldots, n \, . \tag{3.32}$$

A geodesic segment is a **geodesic** if it is not the restriction of a geodesic segment defined on a larger (open) interval.
A geodesic is said to be **complete** if its domain is the whole $\mathbb{R}$. ■

In general, a local chart alone is not sufficient to cover the maximal solution of the geodesic equation (3.31).
The following important results is valid In view of the existence and uniqueness theorem for geodesics (see, e.g., [57]).

Theorem 3.33. *Consider a smooth manifold M is equipped with the affine connection ∇. If $(p,v) \in TM$, then there is a unique geodesic $\gamma : I \to M$, where $I \ni 0$, starting at $p \in M$ with initial vector $\gamma'(0) = v \in T_pM$. As a consequence, all geodesic segments are restrictions of geodesics.*

Notice that the theorem implies immediately that a geodesic is constant $\gamma(u) = p$ for every $u \in \mathbb{R}$ if and only if $\gamma'(0) = 0$. Since the system of equations is autonomomous, this implies that 0 can be replaced by any other point in the domain of the geodesic:

Proposition 3.34. *The tangent vector to a geodesic vanishes nowhere unless the geodesic is constant.*

Proposition 3.35. *In a smooth manifold M equipped with an affine connection ∇, the parameter u used to describe a* non constant *geodesic (3.31) can only be changed to $u' := au + b$, where $a \neq 0$ to preserve the form of (3.31).*

Proof. If we pass from u to $u = u(u')$, for some smooth function with non vanishing derivative and $\gamma(u) := \gamma_1(u'(u))$, then

$$\nabla_{\gamma_1'} \gamma_1'(u') = \nabla_{\frac{du}{du'}\gamma'} \frac{du}{du'} \gamma(u) = \frac{du}{du'} \nabla_{\gamma'} \frac{du}{du'} \gamma(u) = \frac{du}{du'} \left(\frac{du}{du'} \nabla_{\gamma'} \gamma(u) + \frac{d^2 u}{du'^2} \gamma'(u) \right) = \frac{du}{du'} \frac{d^2 u}{du'^2} \gamma'(u).$$

The right most side vanishes if and only if $\frac{d^2u}{du'^2} = 0$. $\square$

The parameters which preserve the form (3.31) of the geodesic equation for a non constant geodesic are said **affine parameters**.

3.3 Spacetimes, causal structures, Klein-Gordon equation

In this section we introduce the notion of spacetime presenting also some basic definitions and facts about *causality theory*.

3.3.1 Lorentzian structures and their physical intepretation

We start by listing the basic geometric notions with physical interpretation.

Definition 3.36. Let (M, g) a Lorentzian manifold of dimension n.

(1) If $p \in M$, a vector $v \in T_pM$ is called

   (a) **spacelike** if either $v = 0$ or $g_p(v, v) < 0$,

   (b) **timelike** if $g_p(v, v) > 0$,

   (c) **null** – or equivalently **lightlike** – if $g_p(v, v) = 0$ and $v \neq 0$,

   (d) **causal** if it is either timelike or null.

   A covector $\omega \in T_p^*M$ is classified similarly according to the associated $\omega^\sharp \in T_pM$ (see (6) Remark 3.21).

(2) $X \in \mathfrak{X}(M)$ and $\omega \in \Omega_1(M)$ are classified as in (1) if their type is constant: they are **spacelike**, **timelike**, **null**, **causal** if X_p, respectively ω_p, is such for every $p \in M$.

(3) Let $\gamma : I \ni u \to \gamma(u) \in M$ be a smooth curve, where I is an interval. γ is classified according to its tangent vector γ' provided it is of constant type along γ: it is **spacelike**, **timelike**, **null**, **causal** if $\gamma'(u)$ is respectively such for every $u \in I$.

(4) Let $N \subset M$ be an embedded submanifold of dimension $n-1$. It is said **spacelike** if every $v \in T_pN$, for $p \in N$, is spacelike when viewed as a vector of T_pM due to the canonical inclusion $T_pN \subset T_pM$. $\blacksquare$

The following definition is also valid for a Riemannian manifold.

Definition 3.37. Let (M, g) be a (pseudo)Riemannian manifold. If $\gamma : I \ni u \mapsto \gamma(u) \in M$ is a smooth curve, we can define the **arch parameter**

$$s(u) := \int_{u_0}^{u} \sqrt{|g(\gamma'(r), \gamma'(r))|}dr \tag{3.33}$$

where $u_0 \in I$ is a given point. ■

It is immediate from the given definition that s is *invariant under re-parametrization* of γ: if we pass from u to the new parameter $u' = f(u)$, where f is smooth with $\frac{df}{du} > 0$ on I, then the right-hand side above remains untouched. On the other hand, (3.33) implies that, if $g(\gamma'(u), \gamma'(u))$ vanishes nowhere, then also $s = s(u)$ is a smooth function with non-vanishing derivative $\frac{ds}{du} = \sqrt{|g(\gamma'(u), \gamma'(u))|} > 0$, and thus the inverse function $u = u(s)$ exists and is smooth as well. In this case s itself can be used as a new parameter $\gamma = \gamma(u(s))$.

Proposition 3.38. *If $\gamma : I \ni u \mapsto \gamma(u) \in M$ is a smooth curve, and $g(\gamma'(u), \gamma'(u)) \neq 0$ for every $u \in I$, then $s = s(u)$ can be used as parameter to describe γ.*

Notation 3.39. When using the arch parameter – and we simply write $\gamma = \gamma(s)$ – the tangent vector will be denoted by $\dot\gamma(s)$. ■

Since

$$s(s) := \int_{s_0}^{s} \sqrt{|g(\dot\gamma(r), \dot\gamma(r))|}dr$$

we conclude that, taking the s-derivative to both sides,

$$g(\dot\gamma(s), \dot\gamma(s)) = \pm 1 \tag{3.34}$$

where the sign is fixed by the one of $g(\dot\gamma(s_0), \dot\gamma(s_0))$ because the left-hand side is smooth, thus continuous, function of $s \in I$ which is connected it being an interval.

Definition 3.40. Let us consider a Lorentzian manifold (M, g) of dimension n. The arch parameter of a *timelike* smooth curve γ – so that $g(\dot\gamma(s), \dot\gamma(s)) = +1$ – is called **proper time** and it is denoted by τ, the tangent vector $\dot\gamma(\tau)$ is said n**-velocity**. ■

Proposition 3.41. *If (M, g) is a (pseudo)Riemannian manifold and γ a geodedesic with respect to the Levi-Civita connection, then $I \ni u \mapsto g(\gamma'(u), \gamma'(u)) \in \mathbb{R}$ is constant. As a consequence, the arch parameter is an affine parameter if $g(\gamma'(u^*), \gamma'(u^*)) \neq 0$ at some point $u^* \in I$ (and thus everywhere) and can be used to parametrize the geodesic according to Proposition 3.35.*

Proof. Since $\nabla_{\gamma'(u)}\gamma'(u) = 0$, and (a) in Theorem 3.27 are valid, it holds

$$\frac{d}{du} g\left(\gamma'(u), \gamma'(u)\right) = \nabla_{\gamma'(u)} g\left(\gamma'(u), \gamma'(u)\right) = g\left(\nabla_{\gamma'(u)}\gamma'(u), \gamma'(u)\right) + g\left(\gamma'(u), \nabla_{\gamma'(u)}\gamma'(u)\right) = 0\,.$$

As a consequence, for some constants $c, k \in \mathbb{R}$,

$$s(u) = \int_{u_0}^{u} \sqrt{|g\left(\gamma'(r), \gamma'(r)\right)|}dr = cu + k\,.$$

Above $k := -cu_0$ where $c := \sqrt{|g(\gamma'(u), \gamma'(u))|}$ that is constant. So $c \neq 0$ if $g(\gamma'(u^*), \gamma'(u^*)) \neq 0$ at some point (and thus everywhere). $\square$

Remark 3.42. Let us consider a Lorentzian manifold (M, g) with dimension $n \geq 2$. The physically interesting case is $n = 4$. We have the following physical interpretation of geometric objects arising form the notion of Lorentzian manifold.

(p1) The physical interpretation of (M, g) is a *spacetime*. The points of M are called *events* and represent the absolute minimal localizations, in space and in time, of facts defined in physics.

(p2) The *stories* of physical particles of matter are described in terms of causal smooth curves $\gamma = \gamma(u)$. Timelike curves describes the stories of particles with strictly positive mass, lightlike curves describe massless particles (like photons).

(p3) For timelike curves, $\gamma = \gamma(\tau)$ the proper time τ represents, up to the choice of the origin, the temporal coordinate measured with an *ideal clock* at rest with the particle. Notice that this interpretation is possible if a suitable unit to measure time has been fixed. In fact, we have tacitly assumed that $g(u, u)$ has the dimensions of $[L]^2$. This means that the physically correct definition of proper time is

$$\tau(u) := \frac{1}{c}\int_{u_0}^{u} \sqrt{|g(\gamma'(r), \gamma'(r))|}dr \tag{3.35}$$

where c is a physical constant with dimensions $[L][T]^{-1}$ *which should be provided directly by physics*. It is called the *light speed* and we shall comment later on this terminology. We are always free to change our units to put the value of this constant $c = 1$ as we shall do henceforth.

(p4) The *local rest space* with the particle around $\gamma(\tau)$ is described by the $n-1$ plane of $T_{\gamma(\tau)}M$ defined by $\Sigma^\gamma_\tau := \{v \in T_{\gamma(\tau)} \mid g(v, \dot\gamma(\tau)) = 0\}$. Notice that, in view of the signature of the metric, an de fact that $g(\dot\gamma(\tau), \dot\gamma(\tau)) = 1$, we can pick out $n-1$ vectors $v_2, \ldots, v_n \in \Sigma^\gamma_\tau$, such that $v_1 := \dot\gamma(\tau), v_2, \ldots, v_n$ is a pseudo orthonormal basis of g. In particular

$$e^\gamma_\tau := -g|_{\Sigma^\gamma_\tau \times \Sigma^\gamma_\tau} : \Sigma^\gamma_\tau \times \Sigma^\gamma_\tau \to \mathbb{R}$$

is a scalar product in proper sense: it is positive. Physically speaking, the scalar product e^γ_τ represents the physical instruments uses in the rest space of the particle to measure distances and angles. Due to the *proper time structure* and the *rest space structure*, stories of timelike type are interpreted as *observers*.

(p5) It is clear that, if γ is an observer,

$$T_{\gamma(\tau)} = \mathrm{span}(\dot\gamma(\tau)) \oplus_g \Sigma^\gamma_\tau \tag{3.36}$$

where the direct sum is orthogonal with respect to g. Observe that if two observers meet in $p = \gamma(\tau) = \gamma'(\tau')$ we have

$$T_p = \mathrm{span}(\dot\gamma(\tau)) \oplus_g \Sigma^\gamma_\tau = \mathrm{span}(\dot\gamma'(\tau')) \oplus_g \Sigma^{\gamma'}_{\tau'}$$

but in general $\dot\gamma(\tau) \neq \dot\gamma'(\tau')$ and $\Sigma^\gamma_\tau \neq \Sigma^{\gamma'}_{\tau'}$ contrarily to what happens in classical physics. In any cases, the metric g of the spacetime defines temporal end spatial metric structures for every observer.

(p6) Consider two stories γ, of timelike type, and $\beta = \beta(u)$ of causal type, thus also lightlike and without the possibility to define the proper time coordinate along it in general. At the instant τ for γ, we have a well defined decomposition of β' according to (3.36). For the occasion we restore the value of the light velocity:

$$\beta' = c\delta\tau\dot\gamma(\tau) + \vec{\delta x}\ , \quad \vec{\delta x} \in \Sigma^\gamma_\tau\ .$$

The natural interpretation of

$$\vec{v}|_\gamma(u) := \frac{\vec{\delta x}}{\delta\tau} \in \Sigma^\gamma_\tau$$

is the *velocity of β with respect to the observer γ* at the considered event (where they meet). We stress that this notion depends on the observer we use to define the velocity of a given history. The notion of n-velocity, in case that history is timelike, does not need an observer to be defined: it is absolute.

(p7) As a first consequence of the notion of velocity, we see that $\beta'(u)$ is lightlike if and only if (where $||\cdot||$ is the norm of e^γ_τ)

$$0 = g(\beta'(u), \beta'(u)) = c^2\delta\tau^2 - ||\vec{\delta x}||^2$$

namely

$$||\vec{v}|_\gamma(u)|| = c\ .$$

If instead β is timelike, using its proper time parametrization $u = \tau'$, we have

$$1 = g(\dot\beta(\tau'), \dot\beta(\tau')) = c^2\delta\tau^2 - ||\vec{\delta x}||^2$$

(where 1 in the left-hand side has physical dimensions $[L]^2$) and thus

$$0 \leq ||\vec{v}|_\gamma(u)|| = c\sqrt{1 - \frac{1}{c^2\delta\tau^2}} \leq c\ .$$

We conclude that (a) there is a *maximal speed*, $c = 1$ with our choice of unities, that is reached only by lightlike stories. (b) This fact is absolute: if a history has maximal velocity for an observer it happens for all observers.
The velocity c is physically identified with the speed of light in empty space, that is the greatest possible speed in physics.

(p8) According to *General Relativity* (see e.g., [57]), a causal geodesic is the physical description of the history of a particle subjected to a gravitational field only (in other words "free falling"). *The gravitational interaction is completely described by the Lorentzian metric of spacetime.* This viewpoint revealed to be physically more correct than the one of classical physics, where the gravitational interaction is described by a suitable vector field, the gravitational field in agreement with Newton's gravitational theory. For instance, the classical framework gives rise to false predictions for the orbits of the planets around the Sun, in particular Mercury. The orbit of Mercury is correctly predicted by General Relativity which explain the observed *precession of perihelion*. Finally classical Cosmology, based on Newton's gravitational theory, is physically inconsistent. Instead, General Relativity produced a modern cosmology which is in substantial agreement with experimental observations, though several issues exist (dark energy and dark matter problems).

3.3.2 Light cone, time orientation, and the notion of spacetime

If (M, g) is an n-dimensional Lorentzian manifold and $p \in M$ a natural structure arises of utmost relevance in Relativity.

Definition 3.43. Let (M, g) be a n-dimensional Lorntzian manifold and $p \in M$. The **(open) light cone** at p is

$$V_p := \{v \in T_pM \mid g(v, v) > 0\} . \tag{3.37}$$

■

Let $\{e_1, \ldots, e_n\} \subset T_pM$ be a pseudo orthonormal basis, so that $g_p(e_1, e_1) = 1$, $g_p(e_i, e_i) = -1$ for $i > 1$ and $g_p(e_i, e_j) = 0$ if $i \neq j$. The elements $v \in V$ are decomposed as $v = \sum_{j=1}^n v^j e_j$, so that $v^1 = g_p(v, e_1)$ and $v^j = -g_p(v, e_j)$ if $j > 1$ by direct use of the above pseudo orthonormality relations and linearity of g. If $v \in V_p$, it must be $v^1 := g_p(e_1, v) \neq 0$. Otherwise $0 < g_p(v, v) = (v^1)^2 - \sum_{j=2}^n (v^j)^2$ whould not be possible. As a consequence, V_p turns out to be the union of two disjoint cones $V_p := V_p^{(1)} \cup V_p^{(2)}$ where

$$V_p^{(1)} := \{v \in T_pM \,|\, g_p(v, v) > 0 \,, \, g_p(e_1, v) > 0\} \,, \quad V_p^{(2)} := \{v \in T_pM \,|\, g_p(v, v) > 0 \,, \, g_p(e_1, v) < 0\} . \tag{3.38}$$

In components referred to the used pseudo orthonormal basis of T_pM:

$$V_p^{(1)} \equiv \left\{ (v^1, \ldots, v^n) \in \mathbb{R}^n \;\middle|\; v^1 > 0 \,, \quad (v^1)^2 - \sum_{j=2}^n (v^j)^2 > 0 \right\} \,, \tag{3.39}$$

$$V_p^{(2)} \equiv \left\{ (v^1, \ldots, v^n) \in \mathbb{R}^n \;\middle|\; v^1 < 0 \,, \quad (v^1)^2 - \sum_{j=2}^n (v^j)^2 > 0 \right\} \,, \tag{3.40}$$

and we see that the coordinate representations of $V^{(1)}$ and $V^{(2)}$ are open connected sets of $\mathbb{R}^n$. This analysis permits to prove an important result.

Proposition 3.44. *If (M,g) is a Lorentzian manifold, the following holds.*

(i) The disjoint decomposition $V_p = V_p^{(1)} \cup V_p^{(2)}$ (3.38), (3.39), (3.40) does not depend on the used basis of T_pM: a different choice interchanges $V_p^{(1)}$ and $V_P^{(2)}$ at most.

(ii) $t, t' \in V_p$ stay in the same half $V_p^{(1)}$ or $V_p^{(2)}$ if and only if $g_p(t,t') > 0$.

Proof. Put on T_pM the topology induced by $\mathbb{R}^n$ through the choice of a basis as follows. Let $\phi : T_pM \to \mathbb{R}^n$ the linear map which associates $v \in T_pM$ with its components $(v^1, \ldots, v^n) \in \mathbb{R}^n$. According to the said topology, $A \subset T_pM$ is open if and only if $A = \phi^{-1}(\tilde{A})$ for $\tilde{A} \subset \mathbb{R}^n$ open. This topology on T_pM actually does not depend on the used basis as we are about proving. First of all, observe that changes of basis correspond to linear bijective maps between the components, thus homeomorphisms $\chi : \mathbb{R}^n \to \mathbb{R}^n$. As a consequence, an open set $A \subset T_pM$ defined by ϕ referred to a certain basis, turns out to be open also when using ϕ' referred to another basis (and *vice versa*), since

$$A = \phi'^{-1}(\chi \circ \phi(A))$$

where $\chi \circ \phi(A) = \chi(\tilde{A}) \subset \mathbb{R}^n$ is open by construction. Referring to this topology on T_pM, but looking at their expression in components, we see that $V_p^{(1)}$, $V_p^{(2)}$ are open connected and disjoint sets whose union is the open set V_p itself. Therefore they are the connected components of V_p. This fact is of purely topological nature and thus independent from the used basis. Changing basis we obtain the same connected components at most with exchanged order. At this juncture, since $g_p(t,t) > 0$ by hypothesis, define $e_1 = \frac{t}{\sqrt{g_p(t,t)}}$ and complete it to a pseudo orthonormal basis by adding spacelike elements $e_2, \ldots, e_n$. Decomposing the vectors of V_p with respect to this basis, the condition $t' \in V^{(1)}$ – namely t and t' stay in the same half of V_p – reads just $t'^1 = g_p(e_1, t') > 0$, that is $g_p(t,t') > 0$ since $1/\sqrt{g_p(t,t)} > 0$. □

The found characterization of the absolute decomposition of V_p gives rise to a crucial definition.

Definition 3.45. Consider a Lorentzian manifold (M,g).

(a) (M,g) is **time orientable** if there is $T \in \mathfrak{X}(M)$ such that T_p is timelike for every $p \in M$.

(b) If (M,g) is time orientable, two smooth timelike vector fields T, T' have the same **time orientation** if $g_p(T_p, T'_p) > 0$ (i.e. they stay in the same half of V_p) for every $p \in M$.

(c) If (M,g) is time orientable, an equivalence class of the defined equivalence relation on the set of smooth timelike vector fields is a **time orientation** $\mathfrak{o}$.
(M,g) itself is **time oriented** if is equipped with a time orientation $\mathfrak{o}$.

(d) If $(M, g, \mathfrak{o})$ is a time-oriented Lorentzian manifold and $T \in \mathfrak{o}$, the half of V_p which includes T_p for any $p \in M$ is said the **future (open) cone** at p and it is denoted by V_p^+.
Every causal vector $t \in \overline{V_p} \setminus \{0\}$ is said **future oriented** or, equivalently, **future directed**. The other half of V_p, indicated by V_p^- is said the **past (open) cone** and analogous definitions are stated for causal vectors.

(e) If $(M, g, \mathfrak{o})$ is a time-oriented Lorentzian manifold, a causal smooth curve $\gamma : I \to M$ is said to be **future directed** if $\gamma'(u)$ is future directed for every $u \in I$. **Past directed** causal curves are defined analogously. ■

We are in a position to state the definition of *spacetime*.

Definition 3.46. A triple $(M, g, \mathfrak{o})$, where M is a smooth manifold with dimension $n \geq 2$, is a **n-dimensional spacetime** if:

(i) M is connected,

(ii) (M, g) is a time orientable Lorentzian manifold,

(iii) $\mathfrak{o}$ is a temporal orientation.

Points of a spacetime are called **events**. ■

Proposition 3.47. *A spacetime admits only two time orientations.*

Proof. Let us fix a smooth timelike vector field $T \in \mathfrak{X}(M)$. Consider any other smooth timelike vector field $T' \in \mathfrak{X}(M)$. We want to prove that the time orientation of T' is either the one of T or the one of $-T$, which obviously have different time orientation it being $g(T, -T) < 0$ everywhere. The map $M \ni p \mapsto g_p(T_p, T'_p) \in \mathbb{R}$ is continuous and M is connected, hence it cannot change sign, otherwise we would have $g_{p_0}(T_{p_0}, T'_{p_0}) = 0$ for some $p_0 \in M$. (That is not possible because it would imply that the component t^1 of T'_{p_0} with respect to the pseudo orthonormal basis $e_1 := T_{p_0}/\sqrt{g(T_{p_0}, T_{p_0})}, e_2, \ldots, e_n$ would vanish contrarily to the hypothesis $g_{p_0}(T'_{p_0}, T'_{p_0}) > 0$.) In summary, given $p_0 \in M$, T' has the same time orientation of T if T'_{p_0} stays in the half of V_{p_0} determined by T_{p_0}, otherwise it has the time orientation of $-T$. □

Remark 3.48.

(1) The most elementary example of n-dimensional spacetime is the well-known n-dimensional **Minkowski spacetime** $(\mathbb{M}, \eta, \mathfrak{o})$ [56]. As a Lorentzian manifold it is a real affine n-dimensional space $\mathbb{M}$ (with the naturally associated smooth structure) equipped with a Lorentzian metric η obtained by a Lorentzian metric in the space of translations $V_{\mathbb{M}}$ of $\mathbb{M}$ according to (5) Remark 3.23. In every Cartesian global chart the metric assumes constant components as a consequence.

(2) A **Minkowski coordinate system** is the special case of global Cartesian coordinates where the metric assumes the constant form $\eta_{ij} = 0$ is $i \neq j$, $\eta_{11} = 1$ and $\eta_{kk} = -1$ for $k \geq 2$. These coordinate systems $(\mathbb{M}, \psi)$ with $\mathbb{M} \ni p \mapsto (x^1(p), \ldots, x^n(p)) \in \mathbb{R}^n$, are constructed out of pseudo orthonormal basis $e_1, \ldots, e_n$ in the space of translations $V_{\mathbb{M}}$ of $\mathbb{M}$ and any origin $o \in \mathbb{M}$ and, according to the general definition of Cartesian coordinates associated to a basis and an origin, are completely defined by the requirement

$$V_{\mathbb{M}} \ni \vec{op} = \sum_{j=1}^{n} (x^k(p) - x^k(o)) e_k \,.$$

(3) In view of the nature of η, it easily arises that the geodesics of $(\mathbb{M}, \eta)$ with respect to the Levi-Civita connection ∇^η are nothing but *straight lines* of the affine-space structure. In fact, in Minkowski coordinates $x^1, \ldots, x^n$ all connection coefficients (3.28) vanishes, since the metric has constant coefficients and thus the geodesic equation (3.32) boils down to

$$\frac{d^2 x^a}{du^2} = 0 \quad a = 1, \ldots, n \,.$$

Every geodesic is therefore complete and has the coordinate form $x^a(u) = v^a u + c^a$, for $a = 1, \ldots, n$ and real constants v^a, c^a. Since Minkowski coordinates are Cartesian, we conclude that a geodesic is an affine straight line and *vice versa*.

(4) Minkowski coordinate systems in Special Relativity are the ones at rest with *inertial reference frames* [56, 57]. The Lorentzian manifold $(\mathbb{M}, \eta)$ is evidently time orientable since every vector field $\frac{\partial}{\partial x^1}$ of every Minkowski coordinate system is timelike and smooth by definition. One of the two possible time orientations $\mathfrak{o}$ is just chosen by choosing one of these vectors as future directed. Further interesting facts of Minkowski coordinate systems are valid.

(i) The integral lines of every vector field $\frac{\partial}{\partial x^1}$ define parallel timelike smooth curves: *observers* according to Remark 3.42. The coordinate x^1 is a *common proper time* with all these observers.

(ii) The 3-planes Σ_{x^1} defined by $x^1 =$ constant are *common rest spaces* of all these observers. In other words, the clocks of these observers are *synchronized* to define a common family of rest spaces Σ_{x^1} labeled by the coordinate x^1. These rest spaces are embedded $n-1$ dimensional submanifolds and they are trivially equipped with a *flat Euclidean metric* induced by $g_{\mathbb{M}}$: it is just the $g_{\mathbb{M}}$-scalar vector, with the reversed sigh, of two vectors tangent to Σ_{x^1} and viewed as vectors in $\mathbb{M}$. The metric is Euclidean and flat because trivially $-\eta\left(\frac{\partial}{\partial x^k}, \frac{\partial}{\partial x^j}\right) = \delta_{kj}$ if $k, j = 2, 3, \ldots, n$ noticing that $x^2, \ldots, x^n$ are global coordinate on each Σ_{x^1}.

(iii) However, differently to what happens in classical physics, changing Minkowski coordinate system, the decomposition of $\mathbb{M}$ is space (the planes Σ_{x^1}) and time x^1 associated to the coordinate system results to change accordingly. There is no notion of *absolute space* and *absolute time*.

(5) If $(\mathbb{M}, \psi)$ with coordinates $x^1, \ldots, x^n$ and $(\mathbb{M}, \psi')$ with coordinates $x'^1, \ldots, x'^n$ are Minkowski global charts with $\frac{\partial}{\partial x^1}$ and $\frac{\partial}{\partial x'^1}$ future oriented, the coordinate transformation reads:

$$x^a = c^a + \sum_{b=1}^{n} \Lambda^a{}_b x'^b \,, \quad a = 1, \ldots, n \,. \tag{3.41}$$

Above, $c^a \in \mathbb{R}$ are constants and, if $\Lambda := [\Lambda^a{}_b]_{a,b=1,\ldots,n}$, it must be (see also (5) in Remark 3.21)

$$\Lambda \in O(1, n-1)_+ := \{\Lambda \in O(1, n-1) \mid \Lambda^1{}_1 > 0\} .$$

$O(1, n-1)_+$ is a subgroup of $O(1, n-1)$ called **orthochronous Lorentz group** of dimension n. Notice that the fact that the set of these matrices is closed with respect to composition and inverse operation is not evident, however it is true [56]. The restriction $\Lambda^1{}_1 > 0$ is equivalent to the requirement that $\frac{\partial}{\partial x^1}$ and $\frac{\partial}{\partial x'^1}$ have the same time orientation, i.e.

$$\eta\left(\frac{\partial}{\partial x'^1}, \frac{\partial}{\partial x^1}\right) > 0 .$$

In fact, since

$$\frac{\partial}{\partial x'^b} = \sum_{a=1}^{n} \Lambda^a{}_b \frac{\partial}{\partial x'^a} ,$$

we have

$$\eta\left(\frac{\partial}{\partial x'^1}, \frac{\partial}{\partial x^1}\right) = \Lambda^1{}_1 .$$

The full family of transformations $\mathbb{R}^n \to \mathbb{R}^n$ defined in (3.41) when varying $\Lambda \in O(1, n-1)_+$ and $(c^1, \ldots, c^n) \in \mathbb{R}^n$ forms a group as well [56] (with respect to the composition of bijective maps $\mathbb{R}^n \to \mathbb{R}^n$). This group is called **orthochronous Poincaré** group of dimension n. It is indicated by $IO(1, n-1)_+$ and enjoys the structure of a *semidirect* product of the abelian additive group $\mathbb{R}^n$ and $O(1, n-1)_+$ [56]. ■

3.3.3 Causal sets, Cauchy surfaces, globally hyperbolic spacetimes

Consider a pair of events $p, q \in M$, where M is a spacetime. According to the physical idea that physical information is transported by physical objects made of particles whose histories are causa and future directed, we can give the following definition.

Definition 3.49. Let $(M, g, \mathfrak{o})$ be a spacetime and consider two events $p, q \in M$.

(a) p and q are **causally related** if either $p = q$ or there is a causal future-directed smooth curve (according to (d) Def. 3.4) $\gamma : [a, b] \to M$, $a < b$, such that $\gamma(a) = p$ and $\gamma(b) = q$ or $\gamma(a) = q$ and $\gamma(b) = p$.

(b) p and q are are **causally separated** if they are not causally related. ■

It is possible to make more precise the above definitions by introducing the notion of *causal sets*.

Definition 3.50. Let $(M, g, \mathfrak{o})$ be a spacetime and $A \subset M$.

(a) The **chronological future** $I^+(A)$ **of** A is defined as follows

$$I^+(A) := \{q \in M \mid \text{a timelike future-directed smooth curve}$$
$$\gamma : [a,b] \to M,\ a < b, \text{ exists such that } \gamma(a) \in A,\ \gamma(b) = q\}\ .$$

We use the notation $I^+(p) := I^+(\{p\})$.

(b) The **causal future** $J^+(A)$ **of** A is defined as follows

$$I^+(A) := \{q \in M \mid \text{a causal future-directed smooth curve}$$
$$\gamma : [a,b] \to M,\ a < b, \text{ exists such that } \gamma(a) \in A,\ \gamma(b) = q\}\ .$$

We use the notation $J^+(p) := J^+(\{p\})$.

The **chronological past** $I^-(A)$ and the **causal past** $J^-(A)$ are defined similarly and we use the notations $I^-(p) := I^-(\{p\})$ and $J^+(p)\mathrm{def}J^+(\{p\})$. ■

Remark 3.51.

(1) The following facts are valid in Minkowski spacetime $\mathbb{M}$ [56] considering a pair of events $p, q \in \mathbb{M}$ with $p \neq q$.

(i) p and q are *causally related* if and only if there is a *causal segment* of the affine structure (that is the same as a causal geodesic segment) which connects them.

(ii) p and q are *causally separated* if and only if there is a *spacelike segment* which connect them (that is the same as a spacelike geodesic segment connecting them). For this reason, in Minkowski spacetime causally separated events are also called *spatially related* or also *spatially separated*.

(iii) p and q are connected by a *timelike* smooth curve if and only if there is a *timelike segment* of the affine structure (that is the same as a timelike geodesic segment) which connects them.

We stress that these facts are generally false (even replacing segments for geodesics) in generic spacetimes.

(2) [66] The chronological sets $I^{\pm}(A)$ enjoy the following general properties if $A \subset M$.

(a) $I^{\pm}(\overline{A}) = I^{\pm}(A)$,

(b) $I^{\pm}(I^{\pm}(A)) = I^{\pm}(A)$.

(3) [66] As general relations between causal and chronological sets we have that

(a) $J^{\pm}(A) \subset \overline{I^{\pm}(A)}$,

(b) $I^{\pm}(A) = Int(J^{\pm}(A))$ so that, in particular, $I^{\pm}(A)$ are *open sets*. ■

There exists a wide literature on the properties of the causal sets $I^{\pm}(S)$ and $J^{\pm}(S)$ and a corresponding classification of spacetimes, essentially started by R. Penrose [67, 66, 4] and see [55] for a recent review.

To go on we need a definition of general nature.

Definition 3.52. Let $(M, g, \mathfrak{o})$ be a spacetime and consider a causal (in particular timelike) future-directed curve $\gamma : (a, b) \to M$ where $-\infty \leq a < b \leq +\infty$.

(a) γ is said to be **future inextendible** if there is no $p \in M$ such that $\gamma(u) \to p$ when $u \to b^-$.

(b) γ is said to be **past inextendible** if there is no $p \in M$ such that $\gamma(u) \to p$ when $u \to a^+$.

γ is **inextendible** if it is both future and past inextendible. ■

We shall now focus attention on the so called *globally hyperbolic spacetimes*. This kind of spacetimes is of the utmost physical interest for many reasons, in particular because a wide family of, roughly speaking, hyperbolic PDEs of great physical relevance—as the *Einstein equations*, *Klein–Gordon equations*, *Dirac equations* — admit existence and uniqueness theorems. Cauchy data are given on special subsets called Cauchy surfaces. Very interestingly, the definition of globally hyperbolic spacetime and Cauchy surface is not related to PDEs, but only relies on the above geometric causal structures. *Smooth spacelike Cauchy surfaces* are also the natural representation of instantaneous rest spaces of globally extended observers.

Definition 3.53. A spacetime $(M, g, \mathfrak{o})$ is said to be **globally hyperbolic** if it admits a **Cauchy surface**. That is a set $S \subset M$ which intersects every inextendible timelike smooth curve exactly once. ■

Remark 3.54.

(1) Every Cauchy surface S is evidently **achronal**: if $p, q \in S$ then there is no smooth *timelike* curve which join them.

(2) It possible to prove that a Cauchy surface also meets by every causal inextendible curve, but not necessarily once [66].

(3) As it was established by R. Geroch, a Cauchy surface S is a closed (in M) embedded C^0-submanifold of codimension 1 of M. (The definition is exactly the same as of smooth embedded submanifold when using C^0-compatible charts adapted to S in place of C^∞-compatible charts). Finally, M results to be homeomorphic to $\mathbb{R} \times S$. All Cauchy surfaces are homeomorphic. [66] ■

An important issue is the existence of *smooth* Cauchy surfaces. If a Cauchy surface S is also a smooth embedded codimension 1 submanifold of M, then its tangent vectors at each point must be either spacelike or lightlike, since S does not contain timelike curves. Such a Cauchy surfaces, if any, is called **smooth Cauchy surface**. It is **spacelike** if its tangent vectors are spacelike.

The issue of the existence smooth Cauchy surfaces in a globally hyperbolic spacetime remained open until 2003 when Bernal and Sánchez published their proof[5] in [7] (see also [6, 8]). We state here a summary of various relevant results by these authors.

Theorem 3.55. [Bernal and Sánchez] *Let* $(M, g, \mathfrak{o})$ *be a globally hyperbolic spacetime of dimension* $n \geq 2$. *The following facts are valid.*

(a) *All smooth Cauchy surfaces in* M *are diffeomorphic. Spacelike smooth Cauchy surfaces exist for* M.

(b) *If* S *is a spacelike smooth Cauchy surface, then* $M \equiv \mathbb{R} \times S$ *through a diffeomorphism such that*

(i) $\tau : \mathbb{R} \times S \ni (t, p) \mapsto t \in \mathbb{R}$ *is a* **temporal function**, *i.e.,* $d\tau$ *is everywhere timelike and future directed*[6];

(ii) $S_t \equiv \{t\} \times S$ *is a spacelike Cauchy surface for every* $t \in \mathbb{R}$.

(c) *It is possible to choose the diffeomorphism in (b) in order that* $\frac{\partial}{\partial t}$ *and* $d\tau^\sharp$ *are parallel, so that, in particular, the curves* $\mathbb{R} \ni s \mapsto (t_0 + s, p) \in \mathbb{R} \times S$ *are timelike and future directed*[7].

With the choice in (c), in a local chart $(\mathbb{R} \times U, \tau \times \psi)$ *adapted to the product manifold* $\mathbb{R} \times S$ *(Def. 3.19), the metric* g *in* M *takes the form*

$$g_p\left(\left.\frac{\partial}{\partial t}\right|_p, \left.\frac{\partial}{\partial y^k}\right|_p\right) = 0, \quad g_p\left(\left.\frac{\partial}{\partial t}\right|_p, \left.\frac{\partial}{\partial t}\right|_p\right) = \beta(t, \vec{y}), \quad g_p\left(\left.\frac{\partial}{\partial y^h}\right|_p, \left.\frac{\partial}{\partial y^k}\right|_p\right) = -h(t, \vec{y}), \tag{3.42}$$

for $M \ni p \equiv (t, y^1, \ldots, y^n)$, *where* $\vec{y} := (y^1, \ldots, y^n)$ *are the coordinates of* ψ.
The functions $\beta > 0$ *and* h_{hk} *defined in* $\mathbb{R} \times U$, *for* $h, k = 1, \ldots, n$, *are smooth. In particular, the coefficients* $h_{hk}(t, \cdot)$, *when varying the local charts* $(\mathbb{R} \times U, \tau \times \psi)$, *define the metric induced by* g *on every slice* S_t, *this metric is Riemannian.*

Proof. See Theorem 1, Lemma 2 in [7] and Theorem 1.2 in [6] for (a),(b) and (c). The final statement on the form of the metric is an easy consequence of (c). In fact, using adapted coordinates to the product structure, the components of $\frac{\partial}{\partial t}$ are δ^a_1 and the components of $d\tau^\sharp$ are $\sum_b g^{ab}\delta_{1b} = g^{a1} = g^{1a}$. Therefore the parallelism condition yelds $g^{1b} = g^{b1} = 0$ if $b = 2, \ldots, n$. The inverse matrix $[g^{ab}]_{a,b=1,\ldots,n}$ of the metric g is therefore made of two blocks on the diagonal: g^{11} and a remaining $(n-1) \times (n-1)$ block. Taking the inverse this structure is preserved and g is describend by a $n \times n$ matrix with a block $\beta = g_{11}$and a further block $[-h_{ab}]_{a,b=2,\ldots,n}$, while $g_{1a} = g_{a1} = 0$ for $a = 2, \ldots, n$. By definition, these elments satisfy (3.42) so that $\beta > 0$ since $\frac{\partial}{\partial t}$ is timelike and h is positive since the vectors $\frac{\partial}{\partial y^k}$, $k = 2, \ldots, n$, are spacelike. Smoothness of all considered functions is automatic since they are components of a smooth metric. □

[5] This result was already stated before 2003, but the proofs were incomplete. The proof by Bernal and Sánchez is of different nature with respect to the previous attempts and it had many other implications.

[6] With the opposite choice of the signature of g as in [7, 8, 6] $d\tau$ is past directed.

[7] In principle these curves may be not even causal.

Remark 3.56.

(1) A spacelike smooth Cauchy surface S meets exactly once also every inextendible causal curve [7]. In particular, S is therefore **acausal**: if $p, q \in S$ then there is no smooth *causal* curve which join them. Referring to the decomposition of $\boldsymbol{M}$ as $\mathbb{R} \times S$ in (c) Theorem 3.55, it is immediate to prove that $I^+(\{t_0\} \times S)$ is the region with $t > t_0$ and $J^+(\{t_0\} \times S)$ is the region with $t \geq t_0$.

(2) An important physical consequence of the existence of Cauchy surfaces (and in particular spacelike smooth Cauchy surfaces and (1) above) is that a globally hyperbolic spacetime *cannot contains closed timelike (causal) curves.* Actually even stronger restrictions are valid [55] regarding non existence of "almost" timelike and closed causal curves. ■

To conclude, some technically important facts are stated in the following proposition.

Proposition 3.57. *$(M, g, \mathfrak{o})$ is a globally hyperbolic spacetime and $K \subset M$ is compact, then*

(a) *$J^\pm(K)$ are closed sets;*

(b) *$J^\pm(K) \cap S$ and $J^\pm(K) \cap J^\mp(S)$ are compact (in particular empty) as well if S is a Cauchy surface;*

(c) *$J^\pm(K) \cap J^\pm(K')$ is compact (in particular empty) for every other compact set $K' \subset M$.*

Proof. (a) follows from 22 Lemma, Chapter 14 [66] and Lemma A.5.1 in [3]. (b) is Corollary A.5.4 in [3]. (c) is Lemma 4.5.7 in [3]. □

3.3.4 The Cauchy problem for the Klein-Gordon equation in a globally hyperbolic spacetime

If $\boldsymbol{M} := (M, g)$ is a Lorentzian manifold we can define a differential operator

$$\Box_{\boldsymbol{M}} : C^\infty(M) \to C^\infty(M)$$

taking advantage of the Levi-Civita connection. First of all we define a differential operator called **covariant divergence**, $\mathrm{div}_{\boldsymbol{M}} : \mathfrak{X}(M) \to C^\infty(M)$, defined as follows in a local chart (U, ψ) with coordinates $x^1, \ldots, x^n$:

$$(\mathrm{div}_{\boldsymbol{M}} X)_p := \sum_{a=1}^{n} (\nabla_a^g X^a)_p \,, \quad \text{where} \quad \nabla_a^g := \nabla^g_{\frac{\partial}{\partial x^a}\big|_p} \tag{3.43}$$

as usual, the vector field $\left.\frac{\partial}{\partial x^a}\right|_p$ in the right-hand side is smoothed to 0 before reaching the boundary of $U \ni p$. By direct inspection, one immediately sees that the definition written above does not depend on the used local chart (U, ψ) around $p \in M$ and thus $\mathrm{div}_{\boldsymbol{M}} : \mathfrak{X}(M) \to C^\infty(M)$ is well defined.

At this juncture we can define the **d'Alembert operator** also known as the **d'Alembertian** (see (6) in Remark 3.21 for the notation):

$$\Box_{\boldsymbol{M}} : C^\infty(M) \ni \varphi \to \mathrm{div}_{\boldsymbol{M}}(d\varphi)^\sharp \in C^\infty(M) \,. \tag{3.44}$$

In local coordinates of (U, ψ) and with a simplified notation

$$\Box_{\boldsymbol{M}} f = \sum_{a,b=1}^{n} \frac{\partial}{\partial x^a}\left(g^{ab}\frac{\partial f}{\partial x^b}\right) + \sum_{a,b,c=1}^{n} \Gamma^c_{ca} g^{ab}\frac{\partial f}{\partial x^b} \tag{3.45}$$

where the smooth functions g^{ab}, as usual, denote the coefficients of the inverse matrix $[g_{ab}]^{-1}_{a,b=1,\ldots,n}$ of the matrix in coordinates $x^1, \ldots, x^n$ of the used local chart (U, ψ), and the smooth function Γ^a_{bc} are the coefficients of the Levi-Civita connection (the Christoffel coefficients) in the chart (U, ψ). As a very well known computational result (see e.g. [57]), the right hand side of (3.45) can be re-arranged to

$$\Box_{\boldsymbol{M}} f = \sum_{a,b=1}^{n} \frac{1}{\sqrt{|\det g|}}\frac{\partial}{\partial x^a}\sqrt{|\det g|}g^{ab}\frac{\partial f}{\partial x^b} \,, \tag{3.46}$$

where $\det g := \det[g_{ab}]_{a,b=1,\ldots,n}$.

Remark 3.58. It is worth stressing that the same definition can be given for the case where $\boldsymbol{M} := (M, g)$ is a Riemannian manifold. In this case the right-hand side of (3.44) is called the **Laplace-Beltrami operator** and is denoted by $\Delta_{\boldsymbol{M}}$. The above coordinate representations of this operator are valid also in the Riemannian case. ■

The d'Alembert operator $\Box_{\boldsymbol{M}}$ is of **normally hyperbolic type**, that is the higher order derivative term (the second order) is constructed out of the inverse metric g^{ab}:

$$\sum_{a,b=1}^{n} g^{ab}\frac{\partial^2}{\partial x^a \partial x^b}$$

i.e. the coefficients g^{ab} are the ones of the inverse matrix of the Lorentzian metric). In particular the matrix of the g^{ab} has the so called **hyperbolic signature**: with a suitable change of coordinates it can be written, *at a given point of* M, as $diag(1, -1, \ldots, -1)$ due to the Sylvester theorem. These types of 2nd order differential operators satisfy an existence and uniqueness theorem [3] for the *Cauchy problem* stated in a *globally hyperbolic spacetime.*

Theorem 3.59. *Let $\boldsymbol{M} := (M, g, \mathfrak{o})$ be a globally hyperbolic spacetime and $S \subset M$ a smooth spacelike Cauchy surface. Consider the Cauchy problem for the unknown $\varphi \in C^\infty(M)$, given by*

(i) the 2nd order, linear, generally non-homogeneous, differential equation called **Klein-Gordon equation**

$$\Box_{\boldsymbol{M}}\varphi + V\varphi = s \,, \tag{3.47}$$

where $V \in C^\infty(M)$ and the **source function** *$s \in C^\infty_c(M)$ are given;*

(ii) initial data

$$\varphi\restriction_S = f_0 \quad \textit{and} \quad \nabla_{\mathbf{n}_S}\varphi = f_1 \tag{3.48}$$

where $f_0, f_1 \in C_c^\infty(S)$ *are given,* $\mathbf{n}_S := \frac{n_S^\sharp}{\sqrt{g(n_S^\sharp, n_S^\sharp)}}$ *is the (timelike) unit vector normal to* S *and future directed and* $\nabla_{\mathbf{n}_S}\varphi := \langle \mathbf{n}_S, d\varphi\restriction_S\rangle$ *the derivative of* φ *normal to* S*.*

Then

(a) *there exists a unique solution* $\varphi \in C^\infty(M)$ *that satisfies (i) and (ii),*

(b) φ *has the following support property, if we define the compact set* $K := supp(g) \cup supp(f_0) \cup supp(f_1)$*,*

$$supp(\varphi) \subset J^+(K) \cup J^-(K)\,. \tag{3.49}$$

Remark 3.60.

(1) $\mathbf{n}_S$, in practice, is constructed as follows. Since S is an embedded $m-1$ dimensional submanifold of M with dimension m, we can consider a local coordinate system (U, ψ) around $p \in S$ which is adapted to S, namely $S \cap U$ is described by $x^1 = 0$ (we can equivalently choose another coordinate among the m coordinates $x^1, \ldots, x^m$). A covector normal to S at p is by definition $n_s := dx^1|_p$. All other possible choices of normal covectors are proportional to it as discussed in Section 3.1.5 where we used the coordinate x^m to locally describe S). Now we move to the tangent space with the natural isomorphism $T_pM \ni \omega \mapsto \omega^\sharp \in T^*M$ (3.23), passing from $n_s \in T_p^*M$ to $n_S^\sharp \in T_pM$. At this juncture, $\mathbf{n}_S$ is obtained by normalizing $n_S^\sharp$: $\mathbf{n}_S = \frac{n_S^\sharp}{\sqrt{g(n_S^\sharp, n_S^\sharp)}}$. In generic local coordinates $\nabla_{\mathbf{n}_S}\varphi = \langle \mathbf{n}_S, d\varphi\restriction_S\rangle = \sum_a n_s^a \frac{\partial \varphi}{\partial x^a}$, where n_S^a are the components of $\mathbf{n}_S$.

(2) If $\mathcal{D}(M) := C_c^\infty(M) \oplus iC_c^\infty(M)$ denotes the complex vector space of **complex test functions**, and $\mathcal{E}(M) := C^\infty(M) \oplus iC^\infty(M)$, we can extend $\Box_{\boldsymbol{M}} : \mathcal{E}(M) \to \mathcal{E}(M)$ in the obvious way:

$$\Box_{\boldsymbol{M}}(f + ih) := \Box_{\boldsymbol{M}} f + i\Box_{\boldsymbol{M}} h\,, \quad f, h \in C^\infty(M)\,. \tag{3.50}$$

Taking $V \in C^\infty(M)$, the theorem above still works when $s \in \mathcal{D}(M)$ and $f_0, f_1 \in \mathcal{D}(S)$, just by separately study the real and the imaginary parts of the solutions.

(3) The Klein-Gordon equation with $V = 0$ is known as (non-homogeneous if s is present) **wave equation** or also **d'Alembert equation**. ■

Corollary 3.61. *Assume the hypotheses of Theorem 3.59. If* $S' \subset M$ *is a Cauchy surface and* φ *is a solution as in Theorem 3.59, then* $supp(\varphi) \cap S'$ *is compact.*

Proof. $supp(\varphi) \cap S'$ is closed because S' is closed ((3) Remark 3.54). Since $supp(\varphi) \cap S' \subset J^+(K) \cup J^-(K)) \cap S'$ which is compact according to Proposition 3.57, $supp(\varphi) \cap S'$ must be compact as well. □

An important proposition for applications in QFT follows.

Proposition 3.62. *Let* $\boldsymbol{M} := (M, g, \mathfrak{o})$ *be a globally hyperbolic spacetime and define the* **Klein-Gordon operator**

$$P := \Box_{\boldsymbol{M}} + V : C^\infty(M) \to C^\infty(M)\,, \tag{3.51}$$

where $V \in C^\infty(M)$ *is given. Consider the differential equation in the unknown* $\varphi \in C^\infty(M)$

$$P\varphi = s\,, \tag{3.52}$$

where the $s \in C^\infty_c(M)$. *The following holds.*

(a) *There exist a unique solution* $\varphi_+ \in C^\infty(M)$ *that satisfies the condition*

$$supp(\varphi_+) \subset J^+(supp(s))\,. \tag{3.53}$$

Equivalently, φ_+ *is the unique solution with zero Cauchy data on a smooth spacelike Cauchy surface* S *with* $supp(s) \subset I^+(S)$.

(b) *There exist a unique solution* $\varphi_- \in C^\infty(M)$ *that satisfies the condition*

$$supp(\varphi_-) \subset J^-(supp(s))\,. \tag{3.54}$$

Equivalently, φ_- *is the unique solution with zero Cauchy data on a smooth spacelike Cauchy surface* S *iwith* $supp(s) \subset I^-(S)$.

(c) *The* **retarded propagator** *(also known as the* **retarded fundamental solution***)*

$$R : C^\infty_c(M) \ni s \mapsto \varphi_+ \in C^\infty(M)\,,$$

and the **advanced propagator** *(also known as the* **advanced fundamental solution***)*

$$A : C^\infty_c(M) \ni s \mapsto \varphi_- \in C^\infty(M)\,,$$

are well-defined linear maps satisfying

$$PR = PA = id_{C^\infty_c(M)}\,. \tag{3.55}$$

Sketch of proof. We provide a sketch of proof for the case φ_+, the other case is analogous. In view of (a)-(c) Theorem 3.55, we represent the spacetime $\boldsymbol{M}$ as the product $\mathbb{R} \times S$ and use the Cauchy surfaces $S_t := \{t\} \times S$. $M_{t_0} \subset M$ indicates the open subset defined by the events $(t, p) \in \mathbb{R} \times S$ with $t > t_0$ according to that representation M: in other words $M_{t_0} = I^+(S_{t_0})$. Since $supp(s)$ is compact, the smooth function $\tau : (t, p) \mapsto t$ takes bounded values on $supp(s)$, so that there is t_0, such that $supp(s) \subset M_{t_0}$. If $\epsilon > 0$, the manifold $M^{t_0-\epsilon} := (M \setminus J^+(supp(s))) \cap M_{t_0-\epsilon}$, equipped with the restriction of the metric g and the restriction of the time orientation, is a globally hyperbolic spacetime as the reader can prove (notice that in globally hyperbolic spacetimes $J^{\pm}(K)$ are closed sets if K is compact in view of Proposition 3.57) because S_{t_0} is a smooth spacelike Cauchy surfaces of this spacetime. At this juncture, φ_+ denotes the unique solution of $P\varphi = s$ in the whole spacetime $\boldsymbol{M}$ with vanishing Cauchy data on S_{t_0}. It exists and is unique due to Theorem 3.59. The restriction of this function to $M^{t_0-\epsilon}$ solves $P\varphi = 0$ with vanishing Cauchy data on S_{t_0} and thus is the zero function in $M^{t_0-\epsilon}$. Since t_0 can be taken arbitrarily close to $-\infty$, this means that φ_+ must vanish M outside $J^+(supp(s))$ as asserted. Two solutions of $P\varphi = s$, φ_+ and φ'_+ whose support is contained in $J^+(supp(s))$ must coincide according to Theorem 3.59 since the are the unique solution of the Cauchy problem in $\boldsymbol{M}$ with source s and zero Cauchy data on S_{t_0}. The map $R : s \mapsto \varphi_+$ is therefore well defined and $PR = id_{C_c^\infty(M)}$ is valid by construction. Let us prove that R is linear. Consider two solutions $\varphi_i = R(s_i)$ of $P\varphi_i = s_i$ with $supp(\varphi_i) \subset J^+(supp(s_i))$ for $i = 1, 2$ where s_i is smooth and compactly supported. We can always fix t_0 in the past of both $supp(s_i)$. Since P is linear, if $a, b \in \mathbb{R}$, $\varphi := a\varphi_1 + b\varphi_2$ is the unique solution of the Cauchy problem with zero Cauchy data on S_{t_0} and source $as_1 + bs_2$. In other words, $\varphi = R(as_1 + as_2)$. In summary, $\varphi = a\varphi_1 + b\varphi_2$ can be rephrased to $R(as_1 + bs_2) = aR(s_1) + bR(s_2)$. □

Remark 3.63. Taking (2) Remark 3.60 into account, one immediately sees that, if $V \in C^\infty(M)$ in the definition of P, then A, R extend to complex-valued functions. Defining for instance

$$A(f + ih) := Af + iAh\,, \quad f, g \in C_c^\infty(M) \tag{3.56}$$

Proposition 3.62 is still valid for complex valued smooth functions and the constructed pair of operators $A, R : \mathcal{D}(M) \to \mathcal{E}(M)$ satisfy (c) of that proposition:

$$PR = PA = id_{\mathcal{D}(M)} \tag{3.57}$$

This is the starting point for studying the Klein-Gordon equation from the perspective of the theory of distributions on manifolds [3]. ■

3.3.5 Integration on (pseudo)Riemannian manifolds

If (M, g) is a (pseudo)Riemannian manifold, there is a natural Borel measure induced by the metric g (see e.g., Section 5.3 of [57])

Theorem 3.64. *Let $\boldsymbol{M} := (M, g)$ be a (pseudo) Riemannian manfold. There exists a unique positive Borel measure $vol_{\boldsymbol{M}}$ on M such that, if (U, ψ) is a local chart with coordinates $x^1, \ldots, x^n$ and $A \subset U$ is Borel*

$$vol_{\boldsymbol{M}}(A) = \int_{\psi(U)} 1_{\psi(A)}(x^1, \ldots, x^n)\sqrt{|\det g_{(U,\psi)}|}dx^1 \cdots dx^n\,. \tag{3.58}$$

Above $g_{(U,\psi)} := [g_{ab}^{(U,\psi)}]_{a,b=1,\ldots,n}$ where $g_{ab}^{(U,\psi)}$ are the coefficients of the metric in the considered local chart, written as functions of the coordinates, and $dx^1 \cdots dx^n$ being the standard Lebesgue *measure in* $\mathbb{R}^n$*.* $1_E(x) := 1$ *if* $x \in E$ *and* $1_E(x) := 0$ *otherwise.*

Suppose that M is a smooth manifold. We recall the reader that, if $K \subset M$ is compact and $\{U_i\}_{i\in I}$ is a covering of K made of a *finite* number of *relatively-compact* open sets, it is possible to define a so-called **partition of the unity** for K **subordinated** to $\{U_i\}_{i\in I}$. It is a family $\{\chi_i\}_{i\in I}$ of maps $\chi_i \in C_c^\infty(M)$ such that

(i) $\chi_i(p) \geq 0$ if $p \in M$;

(ii) *supp*$(\chi_i) \subset U_i$ for $i \in M$;

(iii) $\sum_{i\in I} \chi_i(p) = 1$ if p belongs to an open neighborhood of K.

Actually the existence of a partition of the unity as above can be seen as an elementary consequence of a much more general result concerning *locally-finite coverings* which exist due to *paracompactness* property [57].

Proposition 3.65. *Let* $\boldsymbol{M} := (M, g)$ *be a (pseudo) Riemannian manifold and* $f \in C_c^\infty(M)$*. Let* $K \supset$ *supp*(f) *be a compact set (possibly the same supp*(f)*) and* $\{U_i\}_{i\in I}$ *a finite covering of* K *made of open domains of local charts* (U_i, ψ_i)*. If* $\{\chi_i\}_{i\in I}$ *is a partition of the unity for* K *subordinated to* $\{U_i\}_{i\in I}$*, it holds*

$$\int_M f \mathrm{dvol}_{\boldsymbol{M}} = \sum_{i\in I} \int_{\psi_i(U_i)} \chi_i \circ \psi_i^{-1} \cdot f \circ \psi_i^{-1} \sqrt{|\det g_{(U_i,\psi_i)}|} dx_i^1 \cdots dx_i^n \,. \tag{3.59}$$

Proof. Evidently, f is Borel measurable and $\mathrm{Vol}_{\boldsymbol{M}}$ integrable. From (3.58) and the standard construction of the integral in therms of limit of integrals of simple functions, we easily have that, if $f \in C_c^\infty(M)$ satisfies *supp*$(f) \subset U_j$ for some $j \in I$, then

$$\int_M f \mathrm{dvol}_{\boldsymbol{M}} = \int_{\psi_j(U_j)} f \circ \psi_j^{-1} \sqrt{|\det g_{(U_j,\psi_j)}|} dx_j^1 \cdots dx_j^n \,.$$

If f does not satisfy the said support property, it however holds $\mathrm{supp}\,(\chi_i \cdot f) \subset U_i$. At this juncture we observe that $f = \sum_{i\in I} \chi_i \cdot f$. On the other hand, linearity of the integral yields

$$\int_M f \mathrm{dvol}_{\boldsymbol{M}} = \sum_{i\in I} \int_{U_i} \chi_i \cdot f \mathrm{dvol}_{\boldsymbol{M}} = \sum_{i\in I} \int_{\psi_i(U_i)} \chi_i \circ \psi_i^{-1} \cdot f \circ \psi_i^{-1} \sqrt{|\det g_{(U_i,\psi_i)}|} dx_i^1 \cdots dx_i^n \,.$$

$\square$

A useful technical lemma is the following one.

Lemma 3.66. ["Fundamental lemma of variantional calculus"] *Let* $\boldsymbol{M} := (M, g)$ *be a (pseudo) Riemannian manifold and consider a continuous map* $f : M \to \mathbb{R}$*. It holds* $f(p) = 0$ *for every* $p \in M$ *if and only if*

$$\int_M h \cdot f \mathrm{dvol}_{\boldsymbol{M}} = 0 \quad \forall h \in C_c^\infty(M) \,.$$

Proof. We only prove the non-trivial implication. Suppose that $f(p) > 0$ for some $p \in M$. By continuity, there is an open neighborhood $U \ni p$ such that $f(q) > f(p) - \epsilon = L > 0$ if $q \in U$. We can assume that U is the domain of a local chart (U, ψ). Using also the fact that $\sqrt{|\det g|} > 0$ in U, and working in local coordinates in U we can construct $h \in C_c^\infty(M)$ supported in U such that $\int_{\psi(U)} h \circ \psi^{-1} \sqrt{|\det g|} dx^1 \cdots dx^n = 1$. We have the contradiction

$$\int_M h \cdot f \mathrm{dvol}_{\boldsymbol{M}} = \int_{\psi(U)} f \circ \psi^{-1} \cdot h \circ \psi^{-1} \sqrt{|\det g|} dx^1 \cdots dx^n$$

$$\geq L \int_{\psi(U)} h \circ \psi^{-1} \sqrt{|\det g|} dx^1 \cdots dx^n \geq L > 0 \,.$$

The case $f(p) < 0$ is analogous. □

3.3.6 More on Klein-Gordon operator and its propagators

We are in a position to state and prove an important property of the Klein-Gordon operator P defined in (3.51) with some remarkable consequences for its propagators A and R . Actually the result below is clearly also valid in Riemannian manifolds for the Laplace-Beltrami operator (Remark 3.58) since the proof disregards the signature of the metric.

Proposition 3.67. *Let* $\boldsymbol{M} := (M, g)$ *be a Lorentzian Manifold and* P *the Klein-Gordon operator defined in (3.51). Then* P *is* **formally selfadjoint***:*

$$\int_M f P h \, \mathrm{dvol}_{\boldsymbol{M}} = \int_M (P f) h \, \mathrm{dvol}_{\boldsymbol{M}} \quad \forall f, h \in C_c^\infty(M) \,. \tag{3.60}$$

This identity is more generally true if $f, h \in C^\infty(M)$ *and either* f *or* h *is compactly supported.*

Proof. Let $n := \dim(M)$. We shall make use of the representation (3.46) of $\Box_{\boldsymbol{M}}$ in local coordinates. It is evidently sufficient to prove the thesis for $V = 0$ so that $P = \Box_{\boldsymbol{M}}$. We observe that the closed set *supp*$(f) \cap$ *supp*(h) is compact (closed set in a compact set) and includes the support of fh and also the ones of fPh and $(Pf)h$. Taking advantage of a partition of the unity for the compact *supp*$(f) \cap$ *supp*(h), and integrating by parts in each $\psi_i(U_i)$ the Lebesgue measure,

$$\int_M f P h \mathrm{dvol}_{\boldsymbol{M}} = \sum_{i \in I} \sum_{a,b=1}^{n} \int_{\psi_i(U_i)} \chi_i \cdot f \cdot \left(\frac{1}{\sqrt{|\det g|}} \frac{\partial}{\partial x^a} \sqrt{|\det g|} g^{ab} \frac{\partial h}{\partial x^b} \right) \sqrt{|\det g_{(U,\psi)}|} dx^1 \cdots dx^n$$

$$= \sum_{i\in I}\sum_{a,b=1}^{n}\int_{\psi_i(U_i)} \chi_i \cdot f \cdot \frac{\partial}{\partial x^a}\sqrt{|\det g|}g^{ab}\frac{\partial h}{\partial x^b}dx^1\cdots dx^n$$

$$= -\sum_{i\in I}\sum_{a,b=1}^{n}\int_{\psi_i(U_i)} \frac{\partial \chi_i f}{\partial x^a}\cdot\sqrt{|\det g|}g^{ab}\frac{\partial h}{\partial x^b}dx^1\cdots dx^n \,,$$

where we dropped a boundary term in each domain U_i which vanishes since the relevant integrand smoothly vanishes before reaching ∂U_i in view of the presence of χ_i. Repeating the procedure for the derivative $\frac{\partial}{\partial x^b}$, we end up with

$$\int_M fPh\,\mathrm{dvol}_{\boldsymbol{M}} = \sum_{i\in I}\sum_{a,b=1}^{n}\int_{\psi_i(U_i)}\left(\frac{\partial}{\partial x^b}\sqrt{|\det g|}g^{ab}\frac{\partial \chi_i\cdot f}{\partial x^a}\right)\cdot h dx^1\cdots dx^n$$

$$= \sum_{i\in I}\sum_{a,b=1}^{n}\int_{\psi_i(U_i)}\left(\frac{1}{\sqrt{|\det g|}}\frac{\partial}{\partial x^b}\sqrt{|\det g|}g^{ab}\frac{\partial \chi_i\cdot f}{\partial x^a}\right)\cdot h\sqrt{|\det g|}dx^1\cdots dx^n$$

$$= \sum_{i\in I}\int_M (Pf_i)h\,\mathrm{dvol}_{\boldsymbol{M}} = \int_M \sum_{i\in I}(Pf_i)h\,\mathrm{dvol}_{\boldsymbol{M}} = \int_M (Pf)h\,\mathrm{dvol}_{\boldsymbol{M}} \,,$$

where we defined $f_i = \chi_i\cdot f$, so that $\sum_{i\in I} f_i = f$. $\square$

The obtained result has an important implication concerning the properties of the advanced and retarded operators A, R of the Klein-Gordon operator P.

Proposition 3.68. *The operators $A, R : C^\infty_c(M) \to C^\infty(M)$ as defined in Proposition 3.62 satisfy the following further properties.*

(a) *They are the formal adjoint of each other, in the sense that*

$$\int_M fAh\,\mathrm{dvol}_{\boldsymbol{M}} = \int_M (Rf)h\,\mathrm{dvol}_{\boldsymbol{M}}, \quad \int_M fRh\,\mathrm{dvol}_{\boldsymbol{M}} = \int_M (Af)h\,\mathrm{dvol}_{\boldsymbol{M}} \quad \forall f,h\in C^\infty_c(M). \tag{3.61}$$

(b) *In addition to (3.55), we also have*

$$AP\restriction_{C^\infty_c(M)} = RP\restriction_{C^\infty_c(M)} = id_{C^\infty_c(M)} \,. \tag{3.62}$$

(c) *If $h\in C^\infty_c(M)$, $C^\infty_c(M)\ni f_n\to 0$ uniformly as $n\to+\infty$ and supp$(f_n)\subset K$ for a common compact K, then $\int_M hAf_n\,\mathrm{dvol}_{\boldsymbol{M}}\to 0$ as $n\to+\infty$ and the same is valid for R.*

Proof. (a) and (c). We prove the thesis for R, the case of A has a strictly analogous proof. Take $f,h\in C^\infty_c(M)$. If $S(k) := \{p\in M \mid k(p)\neq 0\}$ when $k: M\to\mathbb{R}$, we have

$$S(hRf) = S(h)\cap S(Rf) \subset J^-(supp(h))\cap J^+(supp(f))$$

where we used $J^{\pm}(supp(h)) \supset supp(h) \supset S(h)$ by definition and $S(R(f)) \subset supp(R(f)) \subset J^{+}(supp(f))$. Taking the closures:

$$supp(hRf) = \overline{S(hRf)} \subset \overline{J^{-}(supp(h)) \cap J^{+}(supp(f))} = J^{-}(supp(h)) \cap J^{+}(supp(f))$$

the latter set being compact according to Proposition 3.57 and thus closed since M is Hausdorff. At this juncture, pick out $\chi \in C_c^{\infty}(M)$ such that $\chi(p) = 1$ if $p \in J^{-}(supp(h)) \cap J^{+}(supp(f))$. Taking (3.55) and Proposition 3.67 into account, we have that

$$\int_M hRf \mathrm{dvol}_{\boldsymbol{M}} = \int_M h\chi Rf \mathrm{dvol}_{\boldsymbol{M}} = \int_M (P(Ah))\chi Rf \mathrm{dvol}_{\boldsymbol{M}} = \int_M (Ah)P(\chi Rf)\mathrm{dvol}_{\boldsymbol{M}} \,. \quad (3.63)$$

With the previous argument we see that

$$S((Ah)P(\chi Rf)) \subset S(Ah) \cap S(P(\chi Rf)) \subset J^{-}(supp(h)) \cap S(Rf) \subset J^{-}(supp(h)) \cap J^{+}(supp(f))$$

and thus

$$supp(AhP(\chi Rf)) \subset J^{-}(supp(h)) \cap J^{+}(supp(f))$$

that implies

$$(Ah)P(\chi Rf) = (Ah)P(Rf) = (Ah)f \,,$$

for the definition of χ. Inserting the found identity in the last integral of (3.63)

$$\int_M hRf \mathrm{dvol}_{\boldsymbol{M}} = \int_M (Ah)f \mathrm{dvol}_{\boldsymbol{M}} \,.$$

This identity is one os the two cases in (a), the other has an identical proof. It immediately implies (c) by a direct use of the dominated convergence theorem.
(b) If $f, h \in C_c^{\infty}(M)$, then $Pf \in C_c^{\infty}(M)$ and thus (a) and Proposition 3.67 yield

$$\int_M hR(Pf)\mathrm{dvol}_{\boldsymbol{M}} = \int_M (Ah)(Pf)\mathrm{dvol}_{\boldsymbol{M}} = \int_M (PAh)f \mathrm{dvol}_{\boldsymbol{M}} = \int_M hf \mathrm{dvol}_{\boldsymbol{M}} \,.$$

Therefore, for every $h \in C_c^{\infty}(M)$,

$$\int_M h(f - R(Pf))\mathrm{dvol}_{\boldsymbol{M}} = 0 \,.$$

The proof ends due to Lemma 3.66. The case of A is strictly analogous. □

Remark 3.69. Noticing that $\mathcal{E}(M) \subset \mathcal{D}'(M)$, (c) of the above proposition immediately implies that A, R extended to complex functions according to Remark 3.63 are sequentially continuous with respect to the natural topologies of maps $\mathcal{D}(M) \to \mathcal{D}'(M)$. As a consequence they admit distributional kernels in $\mathcal{D}(M \times M)$ on account of the *Schwartz kernel theorem.* ■

3.3.7 Divergence and Green theorems

If $\boldsymbol{M} = (M, g)$ is a (pseudo)Riemannian manifold of dimension n, let $S \subset M$ be an $n-1$ dimensional embedded submanifold. The metric g induces on S a smooth assignment of symmetric bilinear forms $g_S : S \ni p \mapsto g_{Sp}$. Here $g_{Sp} : T_pS \times T_pS \to \mathbb{R}$ is defined as $g_{Sp}(u_p, v_p) := g_p(u_p, v_p)$, where $u_p, v_p \in T_pS$ are viewed as elements of T_pM according to the natural injective homomorphism presented in (1) Remark 3.11. If g is Riemannian also (S, g_S) is Riemannian, since positivity is preserved by the said restriction. If g is Lorentzian, non-degenerateness may be not preserved. Also the type of signature may change on S. If non-degenerateness survives the restriction, so that h_S is a metric, it could be either of Euclidean type or of Lorentzian type. If g is not Riemannian nor Lorentzian, several other possibilities may arise.

In all cases, even if h_S is degenerate somewhere, we shall call h_S the **metric induced** by g on S.

There is a Borel measure vol_S associated to h_S that satisfies both Theorem 3.64 and Proposition 3.65 since, in the proof of them, non-degenerateness does not play a role. However Lemma 3.66 may fail since non degenerateness is exploited in its demonstation.

Definition 3.70. If N is a smooth manifold of dimension k, a subset $A \subset N$ is said to be of **zero measure**, if for every local chart (U, ψ) such that $U \cap A \neq \varnothing$, $\psi(U \cap A)$ has zero Lebesgue measure in $\mathbb{R}^k$. ■

We are now in a position to state a pair of identities of fundamental relevance in mathematical physics [3].

Theorem 3.71. *Let $\boldsymbol{M} := (M, g)$ be a Lorentzian of dimension $n \geq 2$. Consider $V \subset M$ an open relatively compact subset such that*

(i) ∂V a $n-1$ smooth embedded submanifold;

(ii) $g_{\partial V}$ is non-degenerate possibly up to a subset of the smooth manifold ∂V of zero measure.

If $X \in \mathfrak{X}(M)$, the **divergence-theorem identity** *holds*

$$\int_V div_{\boldsymbol{M}} X \, \mathrm{dvol}_{\boldsymbol{M}} = \int_{\partial V} g(X, \mathbf{n_S}) \, \mathrm{dvol}_{\partial V} \,. \tag{3.64}$$

If $f, h \in C^\infty(M)$, the **Green identity holds**

$$\int_V f \Box_g h - h \Box f \, \mathrm{dvol}_{\boldsymbol{M}} = \int_{\partial V} f \nabla_{\mathbf{n}_S} h - h \nabla_{\mathbf{n}_S} f \, \mathrm{dvol}_{\partial V} \,. \tag{3.65}$$

$\mathbf{n}_S := \frac{n_S^\sharp}{\sqrt{g(n_S^\sharp, n_S^\sharp)}}$ is the outgoing unit vector normal to S, where it exists, $\nabla_{\mathbf{n}_S} h := g(\mathbf{n}_S, dh^\sharp) = \langle \mathbf{n}_S, dh \rangle$.

If $V = M$ and the latter is compact, then the identites above are still valid with 0 *in the right-hand side.*

Remark 3.72.

(1) The latter identity easily follows form the former.

(2) These identities are vald also for a Riemannian manifolds. In that case g_S is automatically Riemannian and $\Box_g$ is called *Laplace-Beltrami operator*.

(3) The above identities are valid also when strongly relaxing the regularity conditions on ∂V within the approach of the *geometric measure theory*. ■

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