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Facets of Non-Equilibrium in Perturbative Quantum Field Theory

An Algebraic Approach

Ph.D. thesis of

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"... the response to what struck me as beauty, whatever that curious emanation, from a being or an object or a situation or a landscape... That had a very powerful effect on me as it does on everyone. And I prayed to have some response to the things that were so clearly beautiful to me, and they were alive."

Leonard Cohen

Abstract

In this thesis we study some non-equilibrium aspects of an interacting, massive scalar field theory treated perturbatively. This is done analysing some properties of the interacting KMS state constructed by Fredenhagen and Lindner [FL14] in the framework of perturbative Algebraic Quantum Field Theory.

In the first part we treat the stability of KMS states, namely we check whether the free state evolved with the interacting dynamics converges to the interacting state. In the meantime we also analyse the return to equilibrium, that is the analogous property with the role of the free and interacting quantities exchanged. We prove that those two properties hold if the perturbation potential is of spatial compact support and that they fail otherwise, even if an adiabatic mean is considered. While the stability leads to non-curable divergencies, the analysis of return to equilibrium gives something finite, which is interpreted as a non-equilibrium steady state.

The novelty of this non-equilibrium state drove us to try to characterise it in more details. To do so, in the second part we introduce relative entropy and entropy production for perturbative quantum field theory, justifying those definitions by proving their main properties. Furthermore, we showed that they are well-defined in the adiabatic limit if we consider densities. These two definitions allowed to prove that the non-equilibrium steady state is thermodynamically trivial, namely it has zero entropy production.

The present thesis is based on [DFP18a, DFP18b].

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think anything but how I am grateful to him and how lucky I am in having had is guidance all this time. Ti voglio bene Pa, grazie di tutto!

CONTENTS

INTRODUCTION

From many points of view, the status of contemporary theoretical physics is somehow uncertain and full of open problems. Without even mentioning quantum gravity, which up to date is something more than a dream, also the so-called "physics beyond standard model" is not perfectly understood and the present hypothesis are unfortunately only speculations and are not supported by experimental data. Despite all that, Quantum Field Theory (QFT) is without any doubt one of the most important achievements of modern science and still is the theory whose predictions are the most accurate, just to quote one think of the anomalous magnetic moment of the proton. In this (not isolated) case, the agreement between the experimental value is just striking, see [Pa16] for a status report on the experimental results. In spite of its amazing predictive power, QFT has its own problems, for example, in the way it is formulated and used by physicists, it is mathematically non rigorous. For instance, at the present there is no way to make the measures used in the path integral approach well-defined in case of non-linear theories or to make sense out of the Wick rotation for general theories. In particular, conditions on the applicability of the Wick rotation and on the well-posedness of Euclidean QFT has been thoroughly discussed by Osterwalder and Schrader in [OS73, OS75]. Furthermore, the traditional approach to QFT applied on curved backgrounds results pretty involved and complicated.

Several steps towards a rigorous formulation of QFT have been done following the so-called *algebraic approach to quantisation*, first introduced by Haag and Kastler in [HK64], which is the final recollection of several ideas and new contributions arisen in the first years of the 60's and where the two authors formulated the renowned axioms of QFT's. Aside from the conceptual benefit of having a theory posed on solid and rigorous foundations, this more mathematically-oriented approach has been very fruitful in the clarification of numerous obscure spots and it allowed to reach also real improvements and extensions of the theory, see [BDFY15, Ha92] and the bibliography therein for a review. In particular, one of the very first successes of the algebraic approach was the explanation of the particle structure arising in experiments, thanks to the famous *Haag-Ruelle scattering theory* [Ha58, Ru62].

There are many more applications and developments justifying a mathematically rigorous approach, such as the Doplicher-Haag-Roberts analysis [DHR69a, DHR69a, DHR71, DHR74], the new insights in constructive field theories due to Lechner and collaborators [Le08], the applications to bi-dimensional conformal theories or the works pointing towards the formulation of QFT's

on quantum space-time. A modern introduction, with several references, to the status of art can be found in [BDFY15]. Anyway, it must be said that the novelty of this approach is not of physical interest only, but it allowed for several achievements also in many fields of mathematics, such as operator algebras, theory of differential operators, algebraic and differential geometry and category theory. It is not possible to talk about all this in the present thesis, so we are forced to spend some words about few of these topics only.

To start with, we would like to mention that this mathematical approach, now customarily called Algebraic Quantum Field Theory (AQFT), led to a clear explanation of why no preferred vacua exist and, consequently, why the concept of particle loses its meaning on a generic space-time. In particular, the absence of a natural choice of a vacuum state makes the traditional QFT on curved backgrouds very complicated and involved. The problem can be traced back to the lack of the Fourier transform and of a preferred time-direction. Instead, AQFT is insensitive to that since it keeps the fields and the observables as preferred objects, hence this framework turned out to be very well-suited for the description of QFT on curved backgrounds, as pointed out by Dimock [Di80] and Kay and Wald [KW91] (see also references therein).

The reason of these great advantages is that the algebraic quantisation is a two-fold procedure: First the observables of the system are detected and encoded in a topological *-algebra, then the state of the system is specified as a functional over it. The state allows to represent the observables as operators on a Hilbert space via the GNS construction, but since the configurations space on which the algebras are built are typically infinite-dimensional, there are many inequivalent such representations. This implies that there is no reason why the Fock space representation typically used in the physical literature, on which the notion of particle is based, should be the preferred one. We will enter the details of this construction soon. For the moment we want just to mention that, as soon as the background is a globally hyperbolic Lorentzian manifold, the algebra of observables may be found in a state-independent way, so the non-existence of the vacuum does not constitute a real problem. Furthermore, the algebraic approach leads to the formulation of a condition which selects the physical states, which are characterised by the so-called *Hadamard condition*, see [FNW81, Ra96a] or [KW91, Wa94] for a review more oriented on QFT on curved space-time.

In addition, in the seminal work of Brunetti, Fredenhagen and Verch [BFV03], the Haag-Kastler axioms are reformulated and adapted in such a way to make them compatible with the principle of General Relativity, in particular with the principle of *local covariance*. This is done using the language of category theory, defining a QFT as a functor from the category of physical space-times to that of *-algebras. Despite its tremendous importance and its implications, we will avoid the categorical formulation, preferring to keep this work on a less abstract and more pragmatical level.

All this opened the way for the work of Brunetti, Dütsch, Fredenhagen, Hollands and Wald and collaborators, which in a series of works [BDF09, BrFr00, BFK95, HW01, HW02] managed to construct a rigorous framework for interacting theories on curved space-times treated with per-

turbation theory, comprehensive of Wick polynomials, time-ordered products and including also renormalisation. This is nowadays called *perturbative Algebraic Quantum Field Theory* (pAQFT), and it constitutes the framework we used in this work.

The last application we would like to mention concerns a very recent achievement, namely the construction of an interacting thermal equilibrium state for an interacting scalar field theory achieved in [FL14, Li13] by Fredenhagen and Lindner, which brings fresh air in the realm of the so-called Thermal Field Theory, that is QFT developed considering correlation functions at non-zero temperature. In the traditional literature, the construction of thermal correlation functions for interacting theories is problematic due to the presence of infrared divergencies. Such issue is completely avoided using the approach of [FL14], where it is explicitly and rigorously shown that the adiabatic limit, which is the source of IR divergencies, can be taken and it gives a finite result. The methods used in the traditional approach are mainly the Keldysh contour integration or the Matsubara imaginary-time formalism. Using the first construction, infrared divergencies at higher perturbative orders are still present. The Matsubara imaginary-time formalism is more efficient in this respect, in particular it always permits to build the perturbative partition function of the state expanding the propagators over the Matsubara frequencies, but unfortunately, the direct computation of the correlations in position space requires a backward Wick rotation, which is often problematic. We do not insist more on this, demanding an interested reader to the traditional literature, for example [LW87, LeB00].

The goal of this thesis is the study of some of these new thermodynamic features of perturbative QFT which are now available thanks to the work of [FL14], focusing on the simplest case of a real, scalar field on Minkowski space-time. Doing so, we were also able to explore some non-equilibrium aspects of the model whose analysis, to the best of our knowledge, have never appeared in the literature before. In particular, in [DFP18a] we provided an example of non-equilibrium steady state for the interacting theory, while in [DFP18b] we managed to define relative entropy and entropy production for these kind of models.

We devote the rest of the introduction to go deeper and to give further details on what has been said so far.

The Algebraic Description of a Quantum System

The algebraic approach is a particular framework which allows to make quantum theories mathematically rigorous, whose range of application varies from Quantum Mechanics to Quantum Field Theory, passing through Quantum Statistical Mechanics. This framework is based on the fact that the observables of a theory, *i.e.* the quantities one can measure of a physical system, can naturally be described as elements of an algebra. For example, considering a classical system, by common sense it is clear that we can measure two physical quantities performing subsequent measures on the system, for instance we can measure the velocity and the position of the particle. Similarly, scaling the apparatus we are using, we get the property according to which an observable can be multiplied by a scalar. The product is needed to make sense out of some quantities

which are obtained by multiplication of other observables, *e.g.* areas are multiplication of lengths.

This can be expressed in mathematical language by saying that the observables form an algebra, since from the previous discussion we argue that they can be summed (additivity of the observables), multiplied by a scalar and multiplied by themselves. Furthermore, in order to make the theory working, we must add a topology in order to define convergence of sequences of observables, and an involution so to select the positive elements. Despite a classical system being insensitive to the order in which multiple measures are performed, a quantum system is not due to the Heisenberg uncertainty principle. This translates in saying that an algebra of quantum observables is not Abelian, so "quantising" a classical systems means to make the algebra non-commutative in such a way the uncertainty principle is automatically satisfied. Technically, in the case of bosonic systems, this amounts to implement the canonical commutation relations (CCR).

Independently of the system to be quantum or classical, one can ask what "measuring an observable" means. Roughly speaking, a measure is an assignment of a number to any observable. If we think our system to be prepared in a given state this assignment is realised computing the expectation value of the observable we are interested in. In traditional quantum theories this is done following a probabilistic approach where the expectation values are actually the mean values of the results of repeated measurements of a certain observable in a given state. A mathematically reasonable description of the measure process is obtained saying that a state is a functional over the algebra of observables. Indeed, it can not be a generic functional, but it must satisfy certain properties, for instance for a rescaled observable, the value of the measure must be rescaled accordingly, so the functional must be linear. Moreover, we must require it to associate positive expectation values to positive elements, so that self-adjoint elements should have real expectation values, in accordance with the fact that physical observable (which are described by self-adjoint operators) quantities are real and can not assume complex values in nature. A less heuristic argument may be given by introducing two different but physically significant products on the space of observables. The first one is the Jordan product, which is a commutative, non associative product encoding the freedom of exchanging the order of the measurements, while the second is induced by the Poisson brackets of classical mechanics, which corresponds to $\mathrm{i}/\hbar$ times the quantum mechanical commutator, which is an antisymmetric product. Actually, one finds that the two products are strictly related and this bound between the two naturally leads to the algebraic description of the observables developed so far. For a more precise description we refer to [BäFr09, Str08].

To this physically-motivated picture, we need to add some rigour and some technical requirements. First of all we argue that the algebra will be very different according to which kind of system we want to describe, in fact we have that a quantum mechanical system can be very-well formulated in terms of algebras of bounded operators, that is using C^*-algebras or type I von Neumann algebras, while an infinite system such as one given by a free field theory involves type III von Neumann algebras. Instead, interacting fields (as the ones we will deal with in this thesis), requires unbounded elements, so leading to the use of topological *-algebras.

In conclusion, the algebraic quantisation is shaped up to a two-fold procedure: First the alge-

bra of observable is specified, and afterwards the state of the system is assigned as a functional over it. This split is also physically satisfactory because it accommodates very well two peculiar features of relativistic and quantum physics, which may seem to be in contrast at first glance, namely *locality* of classical theory and the existence of *non-local correlations* present in quantum physics (*e.g.* the entanglement). Algebraic quantisation presents these two aspects of the theory as separated, the observables are all local and the non-local aspects are properties of the state. This is why this approach is often referred to as *local quantum physics* [Ha92].

Hitherto, we have explained why the observables of a generic physical system form a (generally infinite) topological *-algebra $\mathscr{A}$, what is missing is how observables evolve in time. This is done assigning a one-parameter group of automorphisms of the algebra, that is a map $\mathbb{R} \ni t \mapsto \tau_t \in \mathrm{Aut}(\mathscr{A})$ such that $\tau_t \circ \tau_s = \tau_{s+t}$ for all $s, t \in \mathbb{R}$. When possible, we will require the time-evolution to be continuous in the relevant topology of the algebra. If a norm is available, in most of the systems this is formulated as $\lim_{t\to 0} \|\tau_t(A) - A\| = 0$ for all $A \in \mathscr{A}$. Notice that in the case studied in this thesis we will not have a norm on our algebra, so the continuity requirement must be imposed in a different way, for example by assigning a state and requiring a weak-* continuity to the dynamics. Anyway the continuity plays a more limited role in those kind of systems.

An example of time-evolution may be obtained by considering a self-adjoint element $H \in \mathscr{A}$ and defining

$$\tau_t(A) \doteq e^{\mathrm{i}tH} A e^{-\mathrm{i}tH} \qquad \forall A \in \mathscr{A}.$$

Physically, we can interpret H as the *Hamiltonian* of the system. Loosely speaking, we are doing nothing but implementing an algebraic counterpart[1] of the Heisenberg picture.

Definition 1 (Dynamical System)**.** The data $(\mathscr{A}, \tau_t)$ of a topological *-algebra $\mathscr{A}$ endowed with a one-parameter group of automorphisms $\{\tau_t\}_{t\in\mathbb{R}}$ is called a *-dynamical system. If in particular $\mathscr{A}$ is a C^*-algebra and if τ_t is strongly-continuous, we call it a C^*-dynamical system, while if $\mathscr{A}$ is a (concrete or abstract) von Neumann one and τ_t is σ-weakly continuous, we call it a W^*-dynamical system.

This consists in the first part of the algebraic approach since the definition of the algebra of observables together with their evolution in time amounts to the specification of all the observables of the physical system. Notice that if the algebra is Abelian we are dealing with classical systems, while if it is not we are describing quantum ones. In order to complete the description of the system, we have to prescribe its physical state. From the physical point of view, assigning a state means that, when we perform a measure to a given observable, we must get a precise and particular numerical value which represents the mean value of repeated experiments. Hence, this naturally leads to the following definition of state (sometimes called *algebraic state*) in the algebraic setting:

Definition 2 (State)**.** A state ω over a unital topological *-algebra $\mathscr{A}$ is a linear functional $\omega : \mathscr{A} \to \mathbb{C}$ which in addition is

[1] Notice that up to now we are using abstract algebras only, the connection with the Hilbert space formalism will be clarified soon.

Positive: $\omega(A^*A) \geq 0$ for all $A \in \mathscr{A}$;

Normalised: $\omega(\mathbb{1}) = 1$, where $\mathbb{1}$ denotes the identity in $\mathscr{A}$.

Notice that, if $\mathscr{A}$ is a C^*-algebra, the normalisation condition can be rewritten as $\|\omega\|_* = \omega(\mathbb{1}) = 1$, where $\|\cdot\|_*$ denotes the usual norm in the dual space. We will always assume that all the algebras we will deal with are unital[2]. Furthermore, the positivity prescription corresponds to the usual requirement according to which the physical observables are self-adjoint.

The assignment of a state permits also to recover unambiguously the Hilbert space picture proper of "traditional" quantum theories using the Gel'fand-Neymark-Segal (GNS) construction, which runs as follows.

First of all, we notice that, given a non-degenerate representation $(\mathscr{H}, \pi)$ of a C^*-algebra $\mathscr{A}$, where $\mathscr{H}$ is a Hilbert space with inner product $\langle\cdot|\cdot\rangle$ and π is the representation map, and a normalised vector $\Omega \in \mathscr{H}$, the linear functional

$$\omega_\Omega(A) \doteq \langle \Omega_\omega \,|\, \pi(A)\Omega_\omega \rangle$$

defines a state over $\mathscr{A}$, customarily called a *vector state*. This means that given an algebra of observables which admits a representation as operators on a certain Hilbert space, one can always find a state over the algebra. We want to show that the converse is also true, *i.e.* that every state defines a representation over a suitably constructed Hilbert space. Furthermore, we will see that the construction is unique up to unitary equivalent representations.

The key observation is that, given a state ω, every *-algebra can be turned into a pre-Hilbert space by endowing it with a positive semidefinite sesquilinear form:

$$\langle A \,|\, B \rangle_\omega^\sim \doteq \omega\left(A^* B\right) \qquad \forall\, A, B \in \mathscr{A}.$$

We denote this pre-Hilbert space as $\tilde{\mathscr{H}}_\omega \doteq \left(\mathscr{A}, \langle\cdot|\cdot\rangle_\omega^\sim\right)$. In order to cope with the fact that the product may be degenerate, we define the ideal

$$\mathscr{I}_\omega \doteq \left\{A \in \mathscr{A} \,|\, \omega\left(A^* A\right) = 0\right\},$$

and afterwards we take the quotient, obtaining the pre-Hilbert space $\mathscr{H}'_\omega \doteq \tilde{\mathscr{H}}_\omega / \mathscr{I}_\omega$, where we have defined the pre-Hilbert product

$$\left\langle \psi_A \,\middle|\, \psi_B \right\rangle_\omega \doteq \langle A \,|\, B \rangle_\omega^\sim = \omega\left(A^* B\right) \qquad \forall\, \psi_A, \psi_B \in \mathscr{H}'_\omega,$$

with ψ_A being the equivalence class generated by A. The Hilbert space of the representation, denoted by $\mathscr{H}_\omega$, is defined as the completion of $\mathscr{H}'_\omega$ with respect to the topology induced by the scalar product $\langle\cdot|\cdot\rangle_\omega$.

The next step consists in defining the representation map of the algebra on $\mathscr{H}_\omega$. The idea is to define it as the left multiplication

$$\pi_\omega(A)[\psi_B] \doteq \psi_{AB},$$

[2]This is not strictly necessary, but we do not want to take over a discussion about approximate identities here.

where ψ_{AB} is defined as the equivalence class generated by the element $AB \in \mathscr{A}$. The proof that this is a well-defined representation is straightforward and may be found, for instance, in [BR97a]. This concludes the construction of the representation $(\mathscr{H}_\omega, \pi_\omega)$, now we are left with the specification of the vector Ω_ω representing the state ω. Actually, since we are working with unital algebras, we put

$$\Omega_\omega \doteq \psi_{\mathbb{1}},$$

which, by definition of the scalar product, gives

$$\langle \Omega_\omega \mid \pi_\omega(A)\Omega_\omega \rangle = \langle \Omega_\omega \mid \psi_A \rangle = \omega(A).$$

The vector Ω_ω is trivially normalised. In addition, we notice that the vector Ω_ω is cyclic for the representation. This can be seen by noticing that the set $\{\pi_\omega(A)\Omega_\omega \mid A \in \mathscr{A}\}$ coincides by construction with the dense set of equivalence classes $\{\psi_A \mid A \in \mathscr{A}\}$, which is dense in $\mathscr{H}_\omega$.

The construction above is a sketch of the proof of the main part of the celebrated *Gel'fand-Neimark-Segal construction*, which we are now going to state as a full theorem. For a rigorous proof and for a complete discussion of what we have hitherto treated, an interested reader may check [**?**, BR97a, JOPP12, Sak98, Ta02] for example. For the development of the construction in the case of a general *-algebra see [KM15].

Theorem 1 (GNS Construction)**.** *Let ω be a state over a *-algebra $\mathscr{A}$. Then there exists a cyclic representation $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$, called the GNS representation, of $\mathscr{A}$ such that $\omega(A) = \langle \Omega_\omega \mid \pi_\omega(A)\Omega_\omega \rangle$ for all $A \in \mathscr{A}$. The GNS representation is unique up to unitary equivalences, namely given two different GNS representations $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ and $\left(\mathscr{H}'_\omega, \pi'_\omega, \Omega'_\omega\right)$ with the properties defined above, there exists a unitary map $U : \mathscr{H}_\omega \to \mathscr{H}'_\omega$ such that $\pi'_\omega(A) = U\pi(A)U^*$ for all $A \in \mathscr{A}$.*

Proof. We are left with the proof of the uniqueness of the representation only. Let us suppose that $\left(\mathscr{H}'_\omega, \pi'_\omega, \Omega'_\omega\right)$ is another GNS representation. Then there exists a unitary operator U defined as

$$U\pi_\omega(A)\Omega_\omega \doteq \pi'_\omega(A)\Omega'_\omega \qquad \forall\, A \in \mathscr{H}'_\omega.$$

This is well-defined since it preserves the scalar product, as can be checked by direct inspection. Moreover it is invertible. Thus, it is closable to a unitary operator satisfying all the desired properties. □

An interesting case occurs when the state ω is pure. In particular the following result holds true, see [BR97a, Section 2.3.]:

Theorem 2. *Let $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ be the GNS representation associated with a C^*-algebra $\mathscr{A}$ and a state ω. Then the following are equivalent:*

1. *ω is pure;*
2. *ω is an extremal element of the cone of the states over $\mathscr{A}$;*
3. *The representation $(\mathscr{H}_\omega, \pi_\omega)$ is irreducible, that is the only invariant subspaces of $\mathscr{H}_\omega$ under the action of $\pi(\mathscr{A})$ are $\{0\}$ and $\mathscr{H}_\omega$ itself.*

It is now interesting to come back to the dynamics and to see how this is implemented in the GNS representation. In general, we say that a one-parameter group of automorphisms $\{\tau_t\}_{t\in\mathbb{R}}$ is implemented by unitary elements $V_t \in \mathscr{H}_\omega$ if

$$\pi_\omega(\tau_t(A)) = V_t \pi_\omega(A) V_t^*.$$

Actually, not every time-evolution is implementable by unitaries, and, if it exists, the implementation may not be unique, hence we need conditions for this to exist.

Something better can be said if we assume that ω is faithful and invariant under the evolution τ_t. In particular, in this case it can be shown that it is unitarily implemented by a strongly continuous one-parameter group of automorphisms $\mathbb{R} \ni t \mapsto V_t^\omega \in \mathscr{B}(\mathscr{H}_\omega)$. The self-adjoint infinitesimal generator of V_t^ω is usually denoted by L^ω, that is

$$V_t^\omega = e^{\mathrm{i}tL^\omega},$$

and it is commonly referred to as the Ω_ω-*Liouvillian*. It can be proven that L^ω is the unique self-adjoint operator such that

$$L^\omega \Omega_\omega = 0, \qquad e^{\mathrm{i}tL^\omega} \pi_\omega(A) e^{-\mathrm{i}tL^\omega} = \pi_\omega(\tau_t(A)) \qquad \forall\, A \in \mathscr{A}.$$

The previous discussion should be sufficient to let the reader understand the main ideas and results about the algebraic approach to quantum theories. Much more may be said about this very broad and interesting topic, but this would be far beyond the purposes of this thesis. Some more words about more specific topics, such as von Neumann algebras and Tomita-Takesaki theory, will be spent further on in the thesis, especially at the beginning of Chapters 3 and 4. Those two subjects are central in the description of algebraic quantum theories since, for instance, it can be shown that the enveloping algebra $\pi_\omega(\mathscr{A})''$, where the double prime denotes the double commutant, is a von Neumann algebra, either if $\mathscr{A}$ is a C^*- or a W^*-algebra. The enveloping algebra is often used in the description of quantum systems because it opens the way for using a very nice feature of von Neumann algebras, which is Tomita-Takesaki modular theory. The importance of modular theory is manifold, both in mathematics and in physics, a beautiful introduction to that may be found in [Ha92, Chapter V]. In particular, Tomita-Takesaki theory is fundamental for the present thesis due to its strict relation with the KMS condition and since it is the building block for Araki's definition of relative entropy [Ar76].

An interested reader may look at some classical textbooks on the subjects, such as [BR97b, Ha92, Str08], which are comprehensive of results about Statistical Mechanics, Quantum Field Theory and Quantum Mechanics. A reader which instead is more into the mathematics of algebraic quantum theories can consult the wide literature on the theory of operator algebras, for example [BR97a, Sak98, Ta02].

Algebraic Quantum Field Theory

The main subject of the present thesis is Quantum Field Theory, so we would like to present here some of its more important and relevant features before going into the explicit details of the scalar

field theory in the main core of the thesis. Actually, a rigorous treatment of QFT is one of the main successes of the algebraic approach described so far. Moreover, QFT played also a prominent role and motivation in the development of this framework.

We would like to start from the *Haag-Kastler axioms*, which are the basic requirement a quantum field theory must fulfill so to be well-posed. They were first formulated in [HK64] for the case of Minkowski space-time, and then extended to a generic curved background in [Di80]. A further reformulation has been given in [BFV03] using category theory in order to implement local covariance, so formulating the notion of *locally covariant quantum field theory*, which we prefer not to treat here, sticking to the "traditional" formulation.

Haag-Kastler Axioms

To each open, bounded region $\mathbb{O} \subseteq \mathbb{M}$ is associated a unital *-algebra $\mathscr{A}(\mathbb{O})$ interpreted as the algebra of observables of the theory supported in the space-time region $\mathbb{O}$.

Locality: Given two arbitrary regions $\mathbb{O}_1 \subseteq \mathbb{O}_2 \subset \mathbb{M}$, then the corresponding algebras satisfy the isotonic relation $\mathscr{A}(\mathbb{O}_1) \subseteq \mathscr{A}(\mathbb{O}_2)$. Given an inducting sequence $\{\mathbb{O}_i\}_{i\in I}$ of increasing subregions $\mathbb{O}_i \subseteq \mathbb{O}_{i+1}$, for a certain (infinite) index set I such that $\bigcup_{i\in I} \mathbb{O}_i = \mathbb{M}$, then we can define the algebra of observables of the whole space-time $\mathbb{M}$ as the inductive limit

$$\lim_{i\in I} \mathscr{A}(\mathbb{O}_i) = \mathscr{A}(\mathbb{M}) \doteq \mathscr{A}.$$

Causality: Let $\mathbb{O}_1, \mathbb{O}_2 \subseteq \mathbb{M}$ two causally separated regions. Then, for any $\mathbb{O} \supset \mathbb{O}_i$, for $i = 1,2$ (possibly $\mathbb{O} \simeq \mathbb{M}$)

$$[\mathscr{A}(\mathbb{O}_1), \mathscr{A}(\mathbb{O}_2)] = \{0_{\mathbb{O}}\}.$$

Time-Slice Axiom: If $\mathbb{O}_1 \subset \mathbb{O}_2$ contains a Cauchy surface of $\mathbb{O}_2$, then the embedding $\mathbb{O}_1 \hookrightarrow \mathbb{O}_2$ is a isomorphism.

These axioms really encode the main facets of a good quantum field theory. Locality implies that the physics of a system should not depend on the size of the laboratory used to experiment it. Causality is a requirement which permits to include relativity in the theory, since it prescribes that spacelike separated observables are independent and can not influence each other. This is why it is often called Einstein causality.

The last axiom is a dynamical one. It reflects the fact that every model that is ruled by an hyperbolic partial differential equation is deterministic. Actually, the solutions to these problems are expected to be uniquely determined by the assignment of the initial data on a Cauchy surface. In algebraic terms this is translated by the fact that the (on-shell) algebra defined on a neighbourhood of a Cauchy surface is isomorphic to the one defined over the whole space-time [CF09].

One of the main improvements reached via the algebraic approach is the existence of several inequivalent representations of the algebra of observables on a Hilbert space. This is due to the

fact that, in order to fulfill the Haag-Kastler axioms, one ends up handling type III von Neumann algebras that violate the validity of the hypothesis of von Neumann theorem, for example the Weyl algebras involved are based on an infinite dimensional symplectic space.

There are also several ways to realise these axioms concretely in the case of a free field theory, while treating the case of interacting theories is more tricky. We chose to work using the *functional approach* to AQFT, which is very-well suited for treating interacting models. In the case of a quantum scalar field theory, the observables are described as functionals over the field configurations space $\mathscr{E} \doteq C^\infty(\mathbb{M};\mathbb{R})$, $\mathbb{M}$ being the space-time. After requiring some regularity hypothesis, the so-called *microcausality*, and endowing them with the pointwise product and with an involution (which is nothing but the complex conjugation), we obtain the classical *-algebra of observables.

The quantisation is performed by *formal deformation* of the pointwise product, defining a $\star$ product using the 2-point function of a Hadamard state ω. This has several nice features and implications: First of all it allows to introduce the Wick ordering and the Wick polynomials avoiding any divergence, so including in the algebra every relevant observable, like the stress-energy tensor or the perturbation potentials needed to describe energy densities and all the other physically interesting quantities. The Wick ordering is taken with respect to the chosen state ω, but it can be shown that all the algebras obtained with different states are *-isomorphic. This makes the construction of the algebra independent of the state. Furthermore, the $\star$ product is designed so that the canonical commutation relations are implemented, that is

$$\big[\phi(x),\phi(y)\big] = \mathrm{i}\hbar\Delta(x,y),$$

Δ being the causal propagator, namely the retarded-minus-advanced fundamental solution to the Klein-Gordon equation.

In this way one obtains the quantisation of the free theory. It must be noticed that this way of proceeding has the effect of turning the observables into *formal power series* in the quantisation parameter $\hbar$, which is the reduced Planck constant. This may be considered quite an ugly feature and a not really elegant way of proceeding, but it actually has a great advantage in the study of interacting models, which at the end of the day is our real goal. It is well-known that, nowadays, it is impossible to solve the equation of motion proper of interacting models, which are therefore treated using perturbation theory. In this respect, the use of formal power series has a deep physical insight: The famous agreement between theory and experiments displayed by quantum field theory is achieved by theoretical computations performed at a finite perturbative order, neglecting the others (for lack of computational power basically) and not caring about the convergence of the perturbative series. Formal power series are the perfect tool to model this situation. One may wonder about how this (somehow rude) approximation is able to provide such striking results: Indeed, this is still an open question, and maybe the mathematical rigor could be able to provide a good answer in the future.

Algebraically, perturbation theory is implemented by selecting a class of interacting observables and representing them into the free algebra, where they are realised as perturbations of free observables, namely formal power series in the coupling constant with zeroth order given by

a free observable. This is done by defining a time-ordered product, out of which we construct the S-matrices as time-ordered exponentials. The S-matrices (to be precise the associated relative S-matrices) are the sought interacting observables, but since they are too involved to be used directly, they are mapped into the free algebra, so exploiting perturbation theory at its best. This is done via the Bogoliubov map. We will explain this soon, first we must point out that the whole interacting construction has to be performed off-shell, due to the fact that the quotient used to build the free, on-shell algebra is not respected by the time-ordering. Heuristically, this is due to the fact that a dynamical interacting observable solves an equation of motion which is not the free one. Nonetheless we will see that the Bogoliubov map manages to implement an off-shell version of the equation of motion, representing dynamical interacting observables as free dynamical observables. Last but not least, this perturbative framework furnishes a well-posed Haag-Kastler net of *-algebras.

Let us give more details on the interacting formalism, starting from the definition of the time-order product. For regular functionals, this can be defined out of the $\star$ product exploiting the *causal factorisation property*:

$$F \cdot_T G = \begin{cases} F \star G & \text{if } \mathrm{spt}(F) \cap J_-(\mathrm{spt}(G)) = \emptyset \\ G \star F & \text{if } \mathrm{spt}(G) \cap J_-(\mathrm{spt}(F)) = \emptyset \end{cases},$$

J_- denoting the causal past. A full definition of the T-product is a complicated and involved procedure, first obtained by Hollands and Wald [HW01, HW02] which requires *renormalisation*. Notice that, after the the extension of the product to generic local functionals is complete, this way of developing the theory rules out the usual ultraviolet divergences present in traditional QFT, which are basically due to the use of a non-renormalised T-product. It must be stressed that the time-ordered product can be extended at most to local fields (or time-ordered products of local fields). The full construction and renormalisation is performed using Epstein and Glaser *causal perturbation theory*, see [EG73], and using Steinmann scaling limits to define the powers of the Feynman propagator required in the time-ordered product, see [BrFr00, BFK95, BDF09].

Once the time-ordering is introduce, we are in the position of describing the interacting quantities, defining the *formal S-matrices*, namely the algebraic analogue of the usual S-matrices, as time-ordered exponentials. The interacting algebra is the one generated by them. Up to now there exists no explicit expression for these objects, hence this construction would remain rather abstract and, after all, empty. A solution is provided by the *Bogoliubov map*, which allows to embed these interacting observables in the free algebra. We will consider as the interacting algebra the one generated by the so-obtained Bogoliubov element, which are nothing but perturbative expansions around free elements depending from the interaction potential. In particular, those interacting observables are double formal power series both in the Planck constant $\hbar$ and in the coupling constant λ.

An important part in the construction is played by the so-called *adiabatic limit*. In order to make the theory ultraviolet and infrared finite, at the beginning we had to put a cutoff on to the

interaction potential, which is then defined as a local functional of the form

$$V_g(\phi) \doteq \int_{\mathbb{M}} \mathrm{P}[\phi](x)\, g(x)\, dx \qquad g \in C_c^\infty(\mathbb{M}, \mathbb{R}),$$

where P is a generic polynomial in the field configurations. Nevertheless, this cutoff is just a mathematical artifact and, at the end of the construction, it must be removed. The limit $g \to 1$ is called the adiabatic limit.

It can be shown that, thanks to the causal factorisation and to the time-slice axiom, the net of interacting algebra does not depend on g, hence the so-called *algebraic adiabatic limit* can be taken without any problem [BrFr00]. In particular, the cutoff may be moved and enlarged. The real issues with the adiabatic limit appear when we try to define states on interacting theories since they explicitly depend on the cutoff g. This means that the problem of the *weak adiabatic limit* is a serious one and it must be discussed case by case. In particular, the weak adiabatic limit is the reason for the presence of infrared divergencies in QFT. The tough nature of the problem is testified by the fact that very few cases are solved. The existence of the interacting vacuum has been proved by Epstein and Glaser themselves in [EG73], while an interacting KMS state in the adiabatic limit was shown to exist only in 2014 in [FL14]. Even more recent is the proof that weak adiabatic limit can be taken in massless theories, at least for ϕ^4 interactions, see [DrHaPi16, Du18].

The true protagonist of this thesis is the interacting KMS state $\omega^{\beta,V}$ of [FL14]: Its construction is based on a generalisation of the Araki's construction [Ar73] performed in Statistical Mechanics and it was possible thanks to a clever implementation of an interacting Hamiltonian formalism based on the time-slice axiom, which circumvents the no-go imposed by Haag theorem. In particular, Fredenhagen and Lindner explicitly built their state as a perturbation of the free, extremal (α_t, β)-KMS one and they proved that it satisfies the KMS condition at the same inverse temperature β and with respect to an interacting time-evolution α_t^V, which is obtained as a Dyson series out of the free one. The free dynamics α_t here is given by the pull-back to functionals of the Minkowski temporal translations.

The state $\omega^{\beta,V}$ is something new in the mathematical and theoretical physics panorama, hence it is worthy to study it in more details, hoping to shed new light in some obscure aspects of thermal field theory. A first interesting peculiarity is that its construction is free of infrared divergencies once a renormalisation scheme is fixed. Moreover, the construction can be performed whatever renormalisation scheme has been chosen. Unfortunately, a clear relation with the physical literature is not available yet, but it is for sure something worthy to be further investigated.

Another interesting aspect is that the construction generalises techniques proper of Statistical Mechanics, hence it may be valuable to take this analogy further and check what else can be translated into pAQFT language. This is exactly what this work is about, in particular here we will discuss the results obtained by myself, in collaboration with Drago and Pinamonti, in [DFP18a] and [DFP18b].

First of all we tackled the problem of *stability* and *return to equilibrium*: Roughly speaking, the question is whether the free KMS state, evolved in time with respect to the interacting dynamics, converges to the interacting equilibrium state in the large-time limit, namely if

$$\lim_{t\to\infty} \omega^{\beta}\left(\alpha_t^V(A)\right) = \omega^{\beta,V}(A)$$

for every interacting observable A. This property is named stability, while, reverting the order of free and interacting quantities we get the return to equilibrium:

$$\lim_{t\to\infty} \omega^{\beta,V}(\alpha_t(A)) = \omega^{\beta}(A).$$

In the analysis of these limit we have to take into account also the role of the adiabatic limit, which is not granted to commute with the temporal one. This is actually not the case, as we have explicitly shown.

We started considering a spacely-compactly supported potential: In this case we proved that, due to some strong clustering properties of the free KMS state, both stability and return to equilibrium hold true.

If instead the adiabatic limit is taken before the large-time one, the situation changes drastically. The analysis of the stability leads to incurable infrared divergencies, which brake the validity of perturbation theory. On the other hand, looking at the return to equilibrium is fruitful and interesting because the result of the limit is finite. We were able to prove that what we obtained is a state for the free theory that is stationary with respect to the free dynamics and that does not satisfy the KMS condition. We interpreted it as a *non-equilibrium steady state* (NESS) according to the definition given by Ruelle [Ru00] and, to our knowledge, this is the first example of this kind of states in the realm of perturbative Quantum Field Theory.

The second generalisation from Statistical Mechanics concerns the notion of relative entropy and entropy production. Unfortunately, definitions as general and powerful as the ones of Statistical Mechanics, see for instance [Ar76, Ar77, JP01, JP02, JP02b], are forbidden in our framework due to the lack of structures on the *-algebras. For instance, the relative modular operator, which is the main ingredient in Araki's relative entropy, is not available. Another issue is the difficulty in the construction of states due to the weak adiabatic limit, which implies that actually very few physically relevant states are known in pAQFT.

This led us in [DFP18b] to adopt a more pragmatic approach, which begins with the observation that the statistical mechanical formulas for perturbed equilibrium states involve only objects which are at disposal also in pAQFT, hence we just assumed these formulas as definitions. We then showed that this definition is well-posed and fulfills all the properties required by the relative entropy. Furthermore, the definition remains finite in the adiabatic limit by considering densities. We stress that, to our knowledge, our definition of relative entropy is the first to be discussed in the realm of perturbative quantum field theories.

Concerning the definition of entropy production, the extension of the definition given by Jakšić and Pillet in [JP01] is more direct. In addition, we shown that also the entropy production per unit volume is actually finite in the adiabatic limit. The main result concerning entropy production is the proof of an analogue of [JP01, Theorem 1.1.], that characterises it as the derivative of

the relative entropy. This proposition is of pivotal importance because it implies that the NESS defined in [DFP18a] has zero entropy production, namely this state is thermodynamically trivial. An interpretation of this curious fact is not available at the moment and requires further investigations. Nonetheless the definition of relative entropy and entropy production for perturbatively constructed quantum field theories is in our humble opinion a remarkable fact, since it constitutes a first step towards some non-equilibrium aspects of this models.

Contents and Organisation of the Thesis

In Chapter 1 we introduce the functional approach to the algebraic quantisation of a free, massive scalar field theory. We start by a quick overview about Lorentzian geometry and about the solution of the Cauchy problem for a Klein-Gordon equation on globally hyperbolic space-times. The second section is devoted to a survey on the classical theory, together with the presentation of the main tools of microlocal analysis and of the functional spaces involved. The chapter is concluded with Section 1.3, where the formal deformation quantisation is performed. To do so, in Section 1.3.3 we introduce the Hadamard condition and the class of physical states which it selects. Finally, we describe the *-algebra of quantum observables.

In this chapter the theory is developed in full generality on curved space-times, but starting from the following one we reduce ourselves to work on Minkowski only, since this is the only case in which the perturbed KMS state is constructed.

The discussion of the interacting theory is the subject of Chapter 2. It starts with the definition of the time-ordered product and with a sketch of the renormalisation problem, which in the context of pAQFT is seen as the problem of extending suitable distributions to the whole space-time. The time-ordered product allows for the definition of the S-matrix as a time-ordered exponential. The algebra of interacting observables is realised by embedding the algebra generated by the S-matrices into the algebra of free observables via the Bogoliubov map. After this, the time-slice axiom is discussed and it is shown how it can be used to identify the two algebras. Section 2.3 contains a discussion about how to construct states on the interacting algebra and a summary of the construction of the interacting KMS state performed in [FL14]. In this chapter we also deal with the problem of taking the adiabatic limit. In the last section we consider the possibility of extending the construction to other situations, such as space-times with compact Cauchy surfaces or to other models, such as a vector boson model.

Chapter 3 treats the stability and return to equilibrium of interacting KMS states. Its first section is devoted to introduce these two properties and it sketches what is known about this topic in Statistical Mechanics and what is different with respect to the field theoretical world. In Section 3.2 we prove that, for a spatially compactly supported interaction potential both stability and return to equilibrium hold true in pAQFT. This is done by showing the validity of certain temporal clustering properties of the free state.

If instead the adiabatic limit is considered, both stability and return to equilibrium fail, even if we take some ergodic averages. While stability leads to infrared divergencies, the study of the

return to equilibrium results in something finite. All this is shown in Section 3.3, while in Section 3.4 we prove that the finite result obtained is well-defined as a non-equilibrium steady state (NESS). This chapter is based on [DFP18a].

In order to pursue the study of the NESS, in Chapter 4 we tackled the problem of the definition of relative entropy and entropy production for a perturbatively defined quantum field theory. After an introductory section about Tomita-Takesaki modular theory and the Araki's definition of relative entropy for W^*-dynamical systems, we present our definition and the proof that it satisfies all the relevant properties required by relative entropy. Our definition is limited to the states known, namely the interacting KMS states, possibly composed with some perturbed dynamics.

Following the work of Jakšić and Pillet, in Section 4.4 we also define entropy production in our framework. We also explicitly prove that these two definitions are compatible with the adiabatic limit by taking densities. All this machinery is used to show that the NESS defined at the end of the previous chapter actually has vanishing entropy production. All the results included in this chapter first appeared in [DFP18b].

The thesis is concluded by some final remarks and an outlook of possible prosecutions of the work.

CHAPTER 1

THE FREE MASSIVE SCALAR FIELD

This chapter is devoted to the quantisation of a free, massive scalar field theory. The literature dealing with this problem, which it can be considered solved to any extent, is wide and various; several techniques and methods have in fact been developed to reach this goal, for example, limiting ourselves to the algebraic quantisation world only, we quote [BäFr09, BeDa15, Ha92]. Remarkably, the problem is solved not only in flat backgrounds, but also in curved ones.
The approach we are going to follow in this thesis is the perturbative one since, at the end of the day, we aim to study interacting models. Anyway, also in this form the quantisation procedure is pretty well understood and it has been completely developed, apart from the resummation of the series, starting from the works of Brunetti, Dütsch, Fredenhagen and collaborators [BDF09, BFK95, BFV03, BFR17, CF09, DF01b, DF04, FR15, HW01, HW02], so in the following we will just collect known results.

The chapter has the following structure: In the first section we introduce the geometric setting and the main results concerning the Cauchy problem for the Klein-Gordon equation, with a particular focus on the properties of its fundamental solutions. The second deals with the formulation of the classical theory. Here all the main classes of functionals over all possible field configurations describing the observables of the theory are defined and, to this avail, a short account on some key results of microlocal analysis is provided, so to make the exposition as more self-contained as possible. The final section deals with the definition of the quantum algebra of observables, which is achieved by formal deformation quantisation of the classical algebra. This section contains also an introduction to the Hadamard condition, which is the criterium by which physical states for a QFT on curved backgrounds are selected.

1.1 The Cauchy problem for the Klein-Gordon equation

1.1.1 Geometric Setting

We start with a brief introduction to Lorentzian differential geometry which will be used in the following, so to fix the notations. Completeness is far from our purposes, so we suggest to an interested reader to refer, for example, to [BEE96, Ne83, Wa84], on which this short dissertation is based.

A *Lorentzian manifold* is a couple (M,g), where M is a n-dimensional smooth manifold and g is a Lorentzian metric, which we will always assume to be of "mostly plus" signature $(-,+,\dots,+)$. Thanks to the Lorentzian structure we can define a *causal structure* on our manifold. Let us start introducing it for the simplest case of Minkowski space $(\mathbb{R}^n,\eta)$, η being the Minkowski metric $\eta_{\mu\nu} \doteq \mathrm{diag}(-1,+1,\dots,+1)$: Given a vector $v \in \mathbb{R}^n$, we say that it is *timelike* if $\eta(v,v) < 0$, *spacelike* if $\eta(v,v) > 0$ and *lightlike* if $\eta(v,v) = 0$, while it will be called *causal* if $\eta(v,v) \leq 0$. Furthermore, it is possible also to determine a time orientation: Fixing the time coordinate versor $e_0 = (1,\mathbf{0})$, we say that a causal vector $v = (v_0,\mathbf{v})$, for $\mathbf{v} \in \mathbb{R}^3$, is *past-directed* ($v \lhd 0$) if $\eta(v,e_0) > 0$, while we call it *future-directed* ($v \rhd 0$) if $\eta(v,e_0) < 0$.

Observing that the tangent space T_pM of a Lorentzian manifold (M,g) at a point $p \in M$ is isomorphic to Minkowski, we can induce a causal structure on (M,g) by saying that a piecewise C^1-curve $\gamma : \mathbb{R} \to M$ is timelike, spacelike, lightlike or causal whenever its tangent vector is of the same character on every point of γ and the time orientation is preserved along γ. We are now in the position of defining the *chronological past*.

Definition 1.1.1 (Chronological Past)**.** The chronological past $I_-(x)$ of a point $x \in M$ is the set of points that are linked to x by past-directed, timelike curves.
The chronological past of a subset $O \subset M$ is defined as $I_-(O) \doteq \bigcup_{x\in O} I_-(x)$.

Similarly, we define the *causal past*:

Definition 1.1.2 (Causal Past)**.** The causal past $J_-(x)$ of a point $x \in M$ is the set of points that are linked to x by past-directed, causal curves.
The chronological past of a subset $O \subset M$ is defined as $J_-(O) \doteq \bigcup_{x\in O} J_-(x)$.

The chronological and the causal futures I_+ and J_+ of a point and of a region are defined replacing "past-directed" with "future-directed". In general, $I_\pm(O)$ is the interior of $J_\pm(O)$, which is thus contained in the closure of $I_\pm(O)$. In addition, the chronological future and past are open subsets of the manifold, while their causal counterparts are not always closed, even though O is. We will denote with $J(O) \doteq J_+(O) \cup J_-(O)$ and $I(O) \doteq I_+(O) \cup I_-(O)$ the causal and chronological *light cones* respectively.

In the following, we will be interested in some particular properties shared by a subset $O \subset M$.

Definition 1.1.3 (Future/Past Compactness)**.** We say that a subset $O \subset M$ is future/past compact if $O \cap J_\pm(x)$ is compact for all $x \in M$. If O is both past- and future-compact, it is called timelike-compact.

Definition 1.1.4 (Achronality/Acausality)**.** A subset $O \subset M$ is called *achronal* (resp. *acausal*) if every timelike (resp. causal) curve crosses O at most once.

Moreover, given a certain physical signal, we are able to characterise geometrically the region of the manifold which can in principle be influenced by it as follows:

Definition 1.1.5 (Domain of Dependence)**.** The future (+), respectively past (−) domain of dependence $D_{\pm}(O)$ of a subset $O \subset M$ is the set of points $p \in M$ such that every past, respectively future inextensible causal curve passing through p intersects O. The set $D(O) \doteq D_{+}(O) \cap D_{-}(O)$ will be called domain of dependence.

Definition 1.1.6 (Cauchy Hypersurface)**.** A Cauchy hypersurface $\Sigma \subset M$ is an achronal surface whose domain of dependence $D(\Sigma)$ coincides with the whole manifold M, *i.e.* $D(\Sigma) = M$.

In the present work we are interested in studying a quantum field theory on a Lorentzian manifold, so we need to control a Cauchy problem over it. To this goal further requirements on the background are needed. In particular, most of the physically interesting models are described by wave equations, whose initial value problem is well-defined on *globally hyperbolic space-times*. A survey on the solution of the Cauchy problem is postponed to the next section, here we want to introduce and specify the backgrounds we are interested in, giving some examples.
Basically, we have to give meaning to the terms "globally hyperbolic" and "space-time": We will do it in two steps, starting from the last one. The definition of space-time requires some more additional ingredients:

Definition 1.1.7. A Lorentzian manifold (M, g) is said to be *orientable* if it admits a nowhere-vanishing volume form.
We say that (M, g) is *time-orientable* if there exists a non-vanishing, continuous timelike vector field $\mathfrak{t}$ on M.

We are now ready to define what a space-time is.

Definition 1.1.8 (Space-time)**.** A space-time is a smooth, Hausdorff, connected, paracompact, 4-dimensional Lorentzian manifold (M, g) endowed with an orientation $d\mu_g$ and a time-orientation $\mathfrak{t}$. We will denote it by $\mathbb{M} \doteq (M, g, d\mu_g, \mathfrak{t})$.

Remark 1.1.1. Of course, it is possible to define a generic n-dimensional space-time. We chose to fix the dimension $n = 4$ just because this is the physically interesting case for a relativistic QFT, so it is the only one that we take into account in this thesis.
When needed, we will specify also the metric, so denoting the space-time by $(\mathbb{M}, g)$.

Let us now switch to global hyperbolicity. This is a requirement that concerns the implementation of the causality principle, so to prevent some science-fiction-situations such as time travels, which *a priori* might be present in the theory[1]. A first possible way to cope with it could be asking that no closed causal curves are present in the space-time (*weak causality condition*). Actually, it turns out that a stronger condition is necessary to avoid particular subtle situations, see [Wa84].

[1] A famous example is the Gödel solution to the Einstein equations, see [Gö49].

Definition 1.1.9 (Strong Causality Condition)**.** We say that a Lorentzian manifold (M,g) satisfies the strong causality condition if, for each $p \in M$ and for every open neighbourhood U_p of p, there exists an open neighbourhood $V_p \subset U_p$ such that every causal curve in M starting and ending in V_p is entirely contained in U_p.

It is straightforward to prove that the strong causality condition implies the weak one. Moreover, every causally convex open subset of (M,g) satisfies the strong causality condition.

Definition 1.1.10 (Global Hyperbolicity)**.** A Lorentzian manifold (M,g) that satisfies the strong causality condition and in which the intersection $J_+(p) \cap J_-(q)$ is compact for all $p,q \in M$ is said to be globally hyperbolic.

Definition 1.1.11 (Globally Hyperbolic Space-Time)**.** A globally hyperbolic space-time is a globally hyperbolic Lorentzian manifold endowed with an orientation and a time-orientation, as per Definition 1.1.8.

It must be said that global hyperbolicity as defined above is a rather abstract concept, so in practice it is almost impossible to check whether a space-time is globally hyperbolic or not using only that definition. Luckily, a very useful and more concrete characterisation has been achieved in [BeSa05] extending results known from [Ge70], which we collect in the following theorem.

Theorem 1.1.1. *Given a Lorentzian manifold (M,g), the following facts are equivalent:*

1. *(M,g) is globally hyperbolic;*
2. *There exists a Cauchy hypersurface Σ in (M,g);*
3. *(M,g) is isometric to $\mathbb{R}\times\Sigma$ with metric $-\alpha\,dt^2 + h_t$, where α is a smooth, positive function and h_t is a Riemannian metric on Σ depending smoothly on $t \in \mathbb{R}$. Furthermore, each $\{t\}\times\Sigma$ is a smooth, spacelike Cauchy hypersurface in (M,g).*

In order to let the reader grasp the importance of this characterisation theorem, we list some examples of physically interesting space-times which are also globally hyperbolic.

Example 1.1.1 (Globally Hyperbolic Space-Times)**.**

1. The simplest example is the Minkowski space-time $(\mathbb{R}^4,\eta)$.
2. A more general class of globally hyperbolic space-times, which includes Minkowski, is that of *ultrastatic space-times*. A space-time $(\mathbb{M},g)$ is ultrastatic if it is isometric to $\mathbb{R}\times\Sigma$, equipped with line element given by $ds^2 = dt^2 + \pi^*(g)$, where $\pi^*(g)$ is the pull-back of the metric under the map $\pi : \mathbb{R}\times\Sigma \to \Sigma$.
3. All *Friedman-Lemaitre-Robertson-Walker* (FLRW) space-times are globally hyperbolic. Such space-times are important in cosmological models, arising as 4-dimensional homogeneous and isotropic solutions to the Einstein equations with matter described by a classical homogeneous and isotropic fluid. Topologically, they are isomorphic to $\mathbb{R}\times\Sigma$ and their line element is
$$ds^2 = dt^2 - a^2(t)\left(\frac{dr^2}{1-\kappa r^2} + r^2 d\mathbb{S}^2(\theta,\phi)\right),$$

where $d\mathbb{S}^2(\theta,\phi)$ is the line element of the unit 2-sphere, $a^2(t)$ is a smooth, strictly positive function of time, called Hubble function. Finally, κ is a constant which can be set, up to normalization, to $0,\pm 1$. Upon this choice depends the nature of the 3-dimensional spacelike Cauchy hypersurfaces. In particular, $\mathbb{R}^3$, the 3-sphere $\mathbb{S}^3$ or the 3-hyperboloid $\mathbb{H}^3$ arise as possible model spaces. The range of the radial coordinate r runs on all $\mathbb{R}^+$ if $\kappa = 0,-1$, while it lies inside the interval $(0,1)$ if $\kappa = 1$. The proof of the global hyperbolicity can be found in [BEE96].

4. Further examples are given by other solutions to the vacuum Einstein equations, such as some black holes space-times like the *Schwarzschild solution*, which characterises a spherically symmetric black hole, or the *Kerr family* of solutions describing rotating, uncharged black holes. Another example is the *de Sitter metric*, which is the maximally symmetric solution. This is often used as a working example in QFT on curved backgrounds. For a more detailed account see [To97, Wa84].

1.1.2 Fields over a Space-Time

The interest in globally hyperbolic space-times is two-fold, on the one hand it rises because, as we saw before, their nature allows to avoid pathological situations. On the other hand, most of the physical field theoretical models are described as initial values problems for wave-like equations, so the presence of Cauchy hypersurfaces is crucial for assigning initial data.
In general, a field is defined as a smooth function with values on a certain vector bundle over a given space-time $\mathbb{M}$, so, in order to fix the notations, we recall the definition of a vector bundle.

Definition 1.1.12. A vector bundle of rank $k < \infty$ over a Lorentzian manifold (M,g) is an assignment $E \equiv E(M,\pi,V)$, where E, called the total space, is a smooth manifold of dimension $k+n$, V, named the typical fibre, is a k-dimensional vector space and $\pi : E \to M$ is a smooth surjective projection. Furthermore, we impose the following requirements:

- There exists a vector space isomorphism between V and the fibre $E_p \doteq \pi^{-1}(p)$ for each $p \in M$;
- Given a generic $p \in M$, there exist an open neighbourhood U_p of p and a diffeomorphism $\varphi : \pi^{-1}(U_p) \to U_p \times V$ such that $\pi_1 \circ \varphi = \pi$ on $\pi^{-1}(U_p)$, for $\pi_1 : U_p \times V \to U_p$ being the projection on the first factor on the Cartesian product;
- The restrictions of φ to each fibre are isomorphisms of vector spaces.

The couple (U_p,φ) fulfilling those conditions is called a local trivialisation of E. We say that a bundle is trivial if it can be expressed globally as a Cartesian product $E = M \times V$.

The causal structure present on a Lorentzian manifold M selects some interesting classes of functions according to their support properties, which are collected in the next definition.

Definition 1.1.13. Given a Lorentzian manifold M and a finite-dimensional vector space V, we call

- $C^\infty(M;V)$ the space of smooth functions on M with values in V;
- $C^\infty_c(M;V)$ the space of smooth, compactly supported functions on M with values in V;
- $C^\infty_{sc}(M;V)$ the space of smooth, spacelike compact functions on M with values in V, that is the space of functions $f \in C^\infty(M;V)$ for which there exists a compact subset $K \subset M$ such that $\mathrm{spt}(f) \subset J(K)$;
- $C^\infty_{fc/pc}(M;V)$ the space of smooth, future/past compact functions on M with values in V. We say that $f \in C^\infty(M;V)$ is future compact if $\mathrm{spt}(f) \cap J_+(p)$ is compact for all $p \in M$. The past compact functions are defined accordingly.
- $C^\infty_{tc}(M;V)$ the space of smooth, timelike compact functions on M with values in V, *i.e.* those functions that are both past and future compact, $C^\infty_{tc}(M;V) \doteq C^\infty_{fc}(M;V) \cap C^\infty_{pc}(M;V)$.

Notations. In this thesis we will denote the spaces of smooth and smooth and compactly supported functions respectively with

$$\mathscr{E}(M;V) \doteq C^\infty(M;V) \quad \text{and} \quad \mathscr{D}(M;V) \doteq C^\infty_c(M;V). \tag{1.1.1}$$

If $V \equiv \mathbb{R}$ we will omit the specification of the co-domain. In particular, we will write $\mathscr{E} \equiv C^\infty(\mathbb{M};\mathbb{R})$ and $\mathscr{D} \equiv C^\infty_c(\mathbb{M};\mathbb{R})$.

The spaces of distributions and of compactly supported distributions are introduced as duals of the previous spaces and denoted with $\mathscr{D}'$ and $\mathscr{E}'$ respectively.

When dealing with bundles, a natural definition encoding the notion of field is that of a section of the bundle.

Definition 1.1.14 (Space of Sections)**.** Given a vector bundle E, we denote with $\Gamma_\bullet(E) \doteq \{s \in C^\infty_\bullet(M;E) \,|\, \pi \circ s = \mathrm{Id}_M\}$ the space of smooth sections of E, where $\mathrm{Id}_M : M \to M$ is the identity map on M. Here, the subscript $\bullet$ stands for the particular choice of the class of functions among the ones given in Definition 1.1.13.

Notice that the space $\Gamma_\bullet(E)$ is an infinite-dimensional vector space and that, for trivial bundles, $\Gamma_\bullet(E) \simeq C^\infty_\bullet(M;V)$. This is the relevant case in this work, as explained by the following example.

Working Example (Real Scalar Field)**.** The prominent example for this thesis is the real scalar field over a globally hyperbolic space-time $\mathbb{M}$. This model is geometrically described by considering the rank $k = 1$ trivial bundle $E \doteq \mathbb{M} \times \mathbb{R}$ with fibre $V \equiv \mathbb{R}$, so that the generic field configuration is a smooth, real-valued function $\phi \in \mathscr{E}$.

Example 1.1.2. There are other possible choices of fields, corresponding to different vector bundles. Here we want to quickly list some of them, without entering too much into details.

- Instead of considering a single scalar bosonic field, it is possible to look at a n-plet of them, namely studying the so-called vector boson model, which is described by the trivial bundle $W \doteq \mathbb{M} \times \mathbb{R}^d$, with fibre $V \equiv \mathbb{R}^d$. The generic configuration then is modeled by a smooth section $\boldsymbol{\varphi} \in \mathscr{E}(\mathbb{M}, \mathbb{R}^d)$.

- In order to construct Fermionic fields one has to take into account the Dirac equation. For doing so, the spinor and co-spinor bundles are necessary. They are given by

$$\mathrm{D}\mathbb{M} \doteq \mathbb{M} \times \mathbb{C}^4, \qquad \mathrm{D}^*\mathbb{M} \doteq \mathbb{M} \times \left(\mathbb{C}^4\right)^* .$$

  The generic spinor and co-spinor are described as sections $\sigma \in \Gamma^\infty(\mathrm{D}\mathbb{M})$ and $\overline{\sigma} \in \Gamma^\infty(\mathrm{D}^*\mathbb{M})$ respectively. For an analysis of the Dirac field we demand to [DaHaPi09], while for a complete account on spin geometry see [LM89].

- Another physically relevant example is Maxwell theory. In this case we must consider a $U(1)$-principal bundle P and its bundle of connections $\mathbf{C}(P)$, which is an affine bundle modeled on the vector space $\mathrm{Hom}(\mathrm{T}\mathbb{M};\mathrm{Ad}(P))$. The electromagnetic field is then described as a smooth section of the bundle of connections, *i.e.* $A \in \Gamma^\infty(\mathbf{C}(P))$. For further details on the construction see [BDS14, BDHS14].

Other examples such as Proca field or Majorana field may be found, for instance, in [BeDa15, BDH13].

For the analysis of the Cauchy problem of the wave equation, some further structures are necessary. Starting from two vector bundles E, F over a Lorentzian manifold M, as per Definition 1.1.12, we consider the *bundle of homomorphisms* $\mathrm{Hom}(E,F)$, which is a vector bundle over M constructed as follows: The fibre over a point $p \in M$ is given by the vector space $\mathrm{Hom}(E_p,F_p) \simeq \mathrm{Hom}(V_E,V_F)$. If $F \equiv E$, we shall call it the *bundle of endomorphisms*, which is a bundle with typical fibre $\mathrm{End}(E)$.

Another remarkable construction is the bundle $E \times_M E$, obtained by taking the Cartesian product fibrewise. This kind of geometrical structures are important as they allow to endow E with an inner product, as shall we do in the following definition:

Definition 1.1.15. Let E be a vector bundle over M. A real, non-degenerate inner product on E is a smooth map $\cdot : E \times_M E \to \mathbb{R}$ such that

- Its restriction to $V_p \times V_p$ is a bilinear form for every point $p \in M$;
- Given $v \in V_p$, then $v \cdot w = 0$ implies $v = 0$ for every $w \in V_p$.

If the inner product is symmetric, we call it *Bosonic*, while, if it is antisymmetric, we name it *Fermionic*.

Any inner product on E induces a non-degenerate pairing

$$(\cdot,\cdot) : \Gamma_c(E) \times \Gamma(E) \to \mathbb{R}; \qquad (s,t) \mapsto \int_M s^* t \, d\mu. \tag{1.1.2}$$

It is also worthy to introduce a pairing between $\Gamma(E)$ and its fibrewise dual $\Gamma(E^\vee)$ as

$$\langle f^\vee, f \rangle \doteq \int_M f^\vee(f) d\mu \tag{1.1.3}$$

for all $f \in \Gamma(E)$ and $f^\vee \in \Gamma(E^\vee)$ whose supports have compact overlap. Notice that, if E is endowed with a non-degenerate inner product, we can identify $E^\vee$ and E^* and, under this identification, the duality pairing (1.1.3) turns out to coincide with (1.1.2).

1.1.3 The Cauchy problem on Globally Hyperbolic Space-Times

All the geometric tools introduced hitherto are needed for addressing the problem of studying wave equations on curved space-times. To this aim, Green hyperbolic operators [Bä15] will play a key role, so we devote this section to define them. A lot has been written about this subject, so we do not even try to give a complete account on it, suggesting to an interested reader to take a look at [BGP07, Fri75, Wal12], or at [BäFr09] for a more QFT-oriented introduction.

Let us fix, once and for all, a vector bundle E (see Definition 1.1.12) over a globally hyperbolic space-time $\mathbb{M}$ as given in Defintions 1.1.12 and 1.1.11.

Definition 1.1.16 (Linear Partial Differential Operators)**.** Let E, F be two vector bundles of ranks k_E, k_F respectively built over the same base space $\mathbb{M}$. A linear partial differential operator of order at most $m \in \mathbb{N}$ is a linear map $D : \Gamma(E) \to \Gamma(F)$ such that, for all $p \in \mathbb{M}$, there exist a coordinate neighbourhood U_p, two local trivialisations (U_p, Ψ_E) and (U_p, Ψ_F) and a collection of local maps $A_\alpha : U \to \mathrm{Hom}(V_E, V_F)$ labeled by a multi-index α such that, for every $s \in \Gamma(F)$, on U we have

$$Ds = \sum_{|\alpha| \leq m} A_\alpha \partial^\alpha s.$$

Here, the sum runs over all multi-indexes $\alpha = (\alpha_0, \dots, \alpha_{m-1}) \in \mathbb{N}^m$ such that $|\alpha| \doteq \sum_{j=0}^{m-1} \alpha_j \leq m$ and $\partial^\alpha \doteq \prod_{j=0}^{m-1} \partial_j^{\alpha_j}$, where ∂_j denotes the partial derivative with respect to the j-th coordinate of the chart U_p. We say that D is of order m when it is of order at most m, but not of order $m-1$.

This definition is very general and it includes a huge variety of operators, most of which can not be associated with a Cauchy problem, so being irrelevant for Physics. Therefore an instrument to classify linear partial differential operators is needed. A suitable notion is that of *principal symbol*:

Definition 1.1.17 (Principal Symbol)**.** Let E, F be two vector bundles over the same base space $\mathbb{M}$. Let $D : \Gamma(E) \to \Gamma(F)$ be a linear partial differential operator of order m. Consider a local chart U_p, with $p \in \mathbb{M}$, and two local trivialisations of E and F, we call principal symbol of D the map $\sigma_D : \mathrm{T}^*\mathbb{M} \to \mathrm{Hom}(E, F)$ locally defined as:

$$\sigma_D(\xi) \doteq \sum_{|\alpha| = m} A_\alpha(p) \xi^\alpha \qquad \forall\, \xi \in \mathrm{T}^*\mathbb{M},$$

where we are using the notation introduced in Definition 1.1.16.

With the principal symbol at disposal, we are able to select the most pertinent class of differential operators, which turns out to be the one of *normally hyperbolic operators*:

Definition 1.1.18 (Normally Hyperbolic Operator)**.** A linear partial differential operator $D : \Gamma(E) \to \Gamma(F)$ is normally hyperbolic if $\sigma_D(\xi) = g(\xi, \xi)\,\mathrm{Id}_{V_p}$ for all $\xi \in \mathrm{T}^*\mathbb{M}$ and $p \in \mathbb{M}$.

The structure of a normally hyperbolic operator D is very peculiar if written in a local trivialisation around a point $p \in \mathbb{M}$ of the bundle E. In particular, for $j = 1, \dots, m-1$, there exist smooth maps $A, A^j : U \to \mathrm{End}(V)$ such that, for every $s \in \Gamma(E)$, on U we have

$$Ds = g^{ij}\,\mathrm{Id}_V\, \partial_i \partial_j s + A^i \partial_i s + As.$$

Another important fact about partial linear differential operators is their relation with the fibre pairing (1.1.2), which is given by means of the formal adjoint of an operator:

Definition 1.1.19 (Formal Adjoint)**.** Let E, F be two vector bundles over $\mathbb{M}$, which we assume to be endowed with non-degenerate inner products $(\cdot,\cdot)_E$ and $(\cdot,\cdot)_F$ as given in Definition 1.1.15. Let $D : \Gamma(E) \to \Gamma(F)$ be a linear partial differential operator. We define the formal adjoint of D as the linear partial differential operator $D^* : \Gamma(F) \to \Gamma(E)$ such that, for any $s \in \Gamma(E)$ and $t \in \Gamma(F)$ with compact $\mathrm{spt}(s) \cap \mathrm{spt}(t)$, the following relation holds

$$\big(D^* t, s\big)_F = (t, Ds)_E \,.$$

If $F \equiv E$ and $D^* = D$, we say that D is formally self-adjoint.

The existence of the formal adjoint is a consequence of the Stokes theorem, while its uniqueness is due to the non-degeneracy of the pairing of F.

There is also a notion of dual of a partial differential operator, which is given using the duality pairing (1.1.3) as follows:

Definition 1.1.20 (Formal dual)**.** Let E be a vector bundle over $\mathbb{M}$ and $E^\vee$ be its dual. Furthermore, let $D : \Gamma(E) \to \Gamma(E)$ be a partial differential operator. We call *formal dual* of D the linear partial differential operator $D^\vee : \Gamma(E^\vee) \to \Gamma(E^\vee)$ defined by

$$\big\langle D^\vee f^\vee, f \big\rangle = \big\langle f^\vee, Df \big\rangle, \tag{1.1.4}$$

where $f \in \Gamma(E)$ and $f^\vee \in \Gamma(E^\vee)$ have supports with compact overlap.

The interest for normally hyperbolic operators has raised in Quantum Field Theory since many (free) physically interesting models are ruled by partial differential equations involving such kind of operators. Moreover, if the background space-time is globally hyperbolic, it can be proven that the Cauchy problem is well-posed and that Green fundamental solutions exist. This key fact, summed up in the following proposition, is one of the key ingredients in the algebraic formulation of QFT on curved backgrounds.

Proposition 1.1.1. *Let $(\mathbb{M}, g)$ be a globally hyperbolic space-time and $\Sigma \subset \mathbb{M}$ be any of its spacelike Cauchy hypersurfaces, with future-pointing normal vector field $\mathbf{n}$. Consider a vector bundle E over $\mathbb{M}$, a normally hyperbolic operator $D : \Gamma(E) \to \Gamma(E)$ and a D-compatible[2] covariant derivative ∇ on E. Furthermore, let $E_{|\Sigma}$ the restriction of E to Σ. Then, for any $s \in \Gamma(E)$ and for any $u_0, u_1 \in \Gamma(E_{|\Sigma})$, the following initial value problem admits a unique solution $u \in \Gamma(E)$:*

$$\begin{cases} Du = s & \text{on } \mathbb{M} \\ u = u_0 & \text{on } \Sigma \\ \nabla_{\mathbf{n}} u = u_1 & \text{on } \Sigma \end{cases} . \tag{1.1.5}$$

If we set $\Omega \doteq \mathrm{spt}(u_0) \cup \mathrm{spt}(u_1) \cup \mathrm{spt}(s)$, then $\mathrm{spt}(u) \subset J(\Omega)$.

[2] We say that a covariant derivative is D-compatible if there exists $A \in \Gamma(\mathrm{End}(E))$ such that $\Box_\nabla + A = D$.

In the rest of this chapter we will consider free theories only, so we will set $s \equiv 0$, so making the equation linear. It must be said that much can be done even if $s \neq 0$.

In order to quantise a free theory, the first step consists in finding a solution to the equation $Du = 0$, possibly avoiding to solve the Cauchy problem (1.1.5) directly. What makes normally hyperbolic operators particularly nice in this respect, is the fact that, on globally hyperbolic manifolds, they admit unique *Green operators* [Bä15, BG12, BGP07], that are defined as follows:

Definition 1.1.21 (Green Operators)**.** Let E be a vector bundle over a globally hyperbolic space-time $\mathbb{M}$. Furthermore, let $D : \Gamma(E) \to \Gamma(E)$ be a linear partial differential operator. We call retarded and advanced Green operators the two linear maps

$$\Delta^R : \Gamma_{pc}(E) \to \Gamma(E), \qquad \Delta^A : \Gamma_{fc}(E) \to \Gamma(E), \tag{1.1.6}$$

satisfying the following properties:

1. $D \circ \Delta^R(f) = f = \Delta^R \circ D(f)$ and $\mathrm{spt}(\Delta^R f) \subset J^+(\mathrm{spt}\, f)$ for all $f \in \Gamma_{pc}(E)$;
2. $D \circ \Delta^A(f) = f = \Delta^A \circ D(f)$ and $\mathrm{spt}(\Delta^A f) \subset J^-(\mathrm{spt}\, f)$ for all $f \in \Gamma_{fc}(E)$.

Moreover, the retarded-minus-advanced operator

$$\Delta \doteq \Delta^R - \Delta^A : \Gamma_{tc}(E) \to \Gamma(E) \tag{1.1.7}$$

will be referred to as causal propagator. A linear partial differential operator admitting both Δ^R and Δ^A is called Green hyperbolic.

An interesting fact is that the advanced and the retarded operators are in formal duality, in the sense of Definition 1.1.20.

Proposition 1.1.2. *Let E be a vector bundle over a globally hyperbolic space-time $\mathbb{M}$ and let $E^\vee$ be its dual. Suppose $D, D^\vee$ be two Green hyperbolic operators on E and $E^\vee$ respectively, with retarded and advanced Green operators given by $\Delta^{R/A}$ and $(\Delta^\vee)^{R/A}$. Then*

$$\left\langle (\Delta^\vee)^{R/A} f^\vee, f \right\rangle = \left\langle f^\vee, \Delta^{A/R} f \right\rangle \quad \forall\, f \in \Gamma(E) \text{ and } f^\vee \in \Gamma(E^\vee).$$

Proof. For any $f^\vee \in \Gamma_0(E^\vee)$ and $f \in \Gamma_0(E)$ and using Definition 1.1.21 we get the equalities

$$\left\langle (\Delta^\vee)^{R/A} f^\vee, f \right\rangle = \left\langle (\Delta^\vee)^{R/A} f^\vee, D \circ \Delta^{A/R} f \right\rangle = \left\langle D^\vee \circ (\Delta^\vee)^{R/A} f^\vee, \Delta^{A/R} f \right\rangle = \left\langle f^\vee, \Delta^{A/R} f \right\rangle,$$

which proves the thesis. □

By Definition 1.1.21, we argue that a Green hyperbolic operator D admits left-inverses Δ^R and Δ^A on respectively past- and future-compact supported sections, hence D is injective thereon. This implies that, if they exist, they are unique and are specified by their support properties and by the condition of being right-inverses also on $\Gamma_{pc}(E)$ and $\Gamma_{fc}(E)$. Since the support is unique, they are unique too, see [Bä15, BeDa15] and references therein for further details.

Proposition 1.1.3. *Let E be a vector bundle over a globally hyperbolic space-time $\mathbb{M}$ endowed with a non-degenerate inner product, as per Definition 1.1.15. Let $D : \Gamma(E) \to \Gamma(E)$ and let D^* be its formal adjoint, and assume that both are Green hyperbolic operators with advanced and retarded Green operators given by $\Delta^{A/R}$ and $(\Delta^*)^{A/R}$ respectively. Then*

$$\left((\Delta^*)^{A/R} f', f\right) = \left(f', \Delta^{R/A} f\right) \quad \forall\, f', f \in \Gamma_0(E).$$

Proof. As noticed before, thanks to the presence of a non-degenerate inner product on E, we can identify the duality pairing (1.1.3) with the inner product (1.1.2). Under this identification, we get $D^\vee = D^*$, so the hypothesis of Proposition 1.1.2 are verified and hence the assert is proven. □

As showed in [Bä15, BGP07], all normally hyperbolic operators are Green hyperbolic, in particular, in our discussion we followed the convention used in the first reference. Notice also that there are Green hyperbolic operators which are not globally hyperbolic. A physically relevant example is the Dirac operator [BG12]. Indeed, we will not deal with those in the present work, which is concerned with the Klein-Gordon operator only.

Working Example. As an example, we compute the advanced and retarded Green functions for the Klein-Gordon operator $P \doteq -\Box + m^2$ on Minkowski space-time $\mathbb{M} = (\mathbb{R}^4, \eta)$. By Definition 1.1.21, we look for two operators Δ^R and Δ^A which weakly solve

$$\left(-\Box_x + m^2\right) \Delta^{R/A}(x, y) = \delta(x, y),$$

and share the correct support properties. Here, $\Box_x = g^{\mu\nu}\nabla_\mu \nabla_\nu$ is the d'Alembert operator with respect to the x variable. The standard way to solve is by Fourier transform, noticing that the two solutions $\Delta^{R/A}$ depend only on $x - y$ due to translation invariance on Minkowski. Hence we have

$$\Delta^{R/A}(x - y) = \frac{1}{(2\pi)^4} \int \widehat{\Delta^{R/A}}(k) e^{-\mathrm{i}k(x-y)}\, d^4k$$

in the sense of distributions. The corresponding equation in Fourier transform becomes

$$\left(k^2 + m^2\right) \widehat{\Delta^{R/A}}(k) = 1.$$

This means that

$$\widehat{\Delta^{R/A}}(k) = \frac{1}{k^2 + m^2},$$

so, in order to get an explicit formula for $\Delta^{R/A}$, we insert this expression in the inverse Fourier transform, choosing an appropriate contour of integration for the k^0-integration. In particular, according to Cauchy's theorem, the choice which leads to the correct support properties is given by the so-called ε-prescription, which allows to perform the complex-integration, selecting the correct contour:

$$\widehat{\Delta^{R/A}}(k) = -\frac{1}{(k^0 \pm \mathrm{i}\varepsilon)^2 - \mathbf{k}^2 - m^2}.$$

Furthermore, performing the integral over k^0 explicitly, we get an explicit formula for the advanced and retarded propagators:

$$\Delta^{R/A}(x - y) = \mp \mathrm{i} \frac{\theta(\pm(x^0 - y^0))}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{e^{-\mathrm{i}E(\mathbf{k})(x^0 - y^0) + \mathrm{i}\mathbf{k}\cdot\mathbf{x}} - e^{\mathrm{i}E(\mathbf{k})(x^0 - y^0) + \mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{2E(\mathbf{k})}\, d^3\mathbf{k}, \tag{1.1.8}$$

where $\mathbf{k}\cdot\mathbf{x}$ denotes the Euclidean product on $\mathbb{R}^3$ between the 3-vectors $\mathbf{k}$ and $\mathbf{x}$ and $E(\mathbf{k}) \doteq \sqrt{\mathbf{k}^2+m^2}$. By subtracting, we get also an expression for the causal propagator:

$$\Delta(x-y) = -\frac{\mathrm{i}}{(2\pi)^3}\int_{\mathbb{R}^3} \frac{e^{-\mathrm{i}E(\mathbf{k})(x^0-y^0)+\mathrm{i}\mathbf{k}\cdot\mathbf{x}} - e^{\mathrm{i}E(\mathbf{k})(x^0-y^0)+\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{2E(\mathbf{k})}\, d^3\mathbf{k}. \tag{1.1.9}$$

The reason why we introduced advanced and retarded Green operators is the observation that they allow to assign to every $f \in \Gamma(E)$, with E any vector bundle over $\mathbb{M}$, a solution of the equation via the causal propagator. That is, given the equation $Du = 0$, a solution can be written as $u = \Delta f$. Up to now, this does not guarantee that all solutions can be characterised in this way. This result needs some additional work.

Lemma 1.1.1. *Let E be a vector bundle over a globally hyperbolic space-time $\mathbb{M}$ and let $D : \Gamma(E) \to \Gamma(E)$ be a Green hyperbolic operator, $\Delta^{A/R}$ being its associated advanced and retarded operators and Δ the resulting causal propagator. Then $f \in \Gamma_{tc}(E)$ is such that $\Delta f = 0$ if and only if $f = Dh$ for some $h \in \Gamma_{tc}(E)$. Furthermore, $f \in \Gamma_{tc}(E)$ is such that $Df = 0$ if and only if $f = 0$ and, moreover, for any $f \in \Gamma(E)$ there exists $h \in \Gamma(E)$ such that $Dh = f$.*

Proof. By definition of Green operators, $\Delta \circ D(h) = 0$ for all $h \in \Gamma_{tc}(E)$. So, it remains to show that, given $f \in \Gamma_{tc}(E)$ such that $\Delta f = 0$, then one can find $h \in \Gamma_{tc}(E)$ such that $f = \Delta h$.

Given any such f, $\Delta f = 0$ implies $\Delta^A f = \Delta^R f$, so, by the support properties of Δ^A and Δ^R, $\mathrm{spt}(\Delta^A f) \subset J^+(\mathrm{spt}\, f) \cap J^-(\mathrm{spt}\, f)$, which means $h = \Delta^A f \in \Gamma_{tc}(E)$. Hence, applying D, we get

$$D(h) = D \circ \Delta^A(f) = f.$$

Assume now that there exists $f \in \Gamma_{tc}(E)$ such that $Df = 0$, then one gets

$$f = \Delta^{A/R} \circ D(f) = 0.$$

Finally, consider $f \in \Gamma(E)$ and a partition of unity $\{\chi_+, \chi_-\}$ on $\mathbb{M}$ such that $\chi_\pm = 1$ on a past/future-compact region, we can write $h = \Delta^R(\chi_+ f) + \Delta^A(\chi_- f) \in \Gamma(E)$. So, since $\chi_+ + \chi_- = 1$ on the whole $\mathbb{M}$, we get $Dh = f$. □

This last result allows for the sought characterisation of the space of solutions to the equation $Du = 0$ in terms of the causal propagator.

Theorem 1.1.2. *Let E be a vector bundle over a globally hyperbolic space-time $\mathbb{M}$ and let $D : \Gamma(E) \to \Gamma(E)$ be a Green hyperbolic operator, $\Delta^{A/R}$ being its associated advanced and retarded operators and Δ the resulting causal propagator. Then the map*

$$\frac{\Gamma_{tc}(E)}{D(\Gamma_{tc}(E))} \to \mathbf{Sol}, \qquad [f] \mapsto \Delta f \tag{1.1.10}$$

is a vector space isomorphism between the vector space of smooth solutions **Sol** *to the linear partial differential equation $Du = 0$, $u \in \Gamma(E)$, and the quotient of $\Gamma_{tc}(E)$ by the image of D acting on $\Gamma_{tc}(E)$.*

Proof. We start noticing that $\Delta : \Gamma_{tc}(E) \to \Gamma(E)$ induces the desired map. Moreover, thanks to Lemma 1.1.1, its image does not depend on the representative of the equivalence class $[f]$, and $u = \Delta f$ solves $Du = 0$.

To prove that this map is injective, let us suppose $f, f' \in \Gamma_{tc}(E)$ to be such that $\Delta f = \Delta f'$. By linearity and by Lemma 1.1.1, there exists $h \in \Gamma_{tc}(E)$ such that $Dh = f - f'$, which means that f and f' lay in the same equivalence class in $\Gamma_{tc}(E)/D(\Gamma_{tc}(E))$, so proving injectivity.

Regarding surjectivity, let $u \in \mathbf{Sol}$ and take a partition of unity as in proof of Lemma 1.1.1. Then $D(\chi_+ u + \chi_- u) = Du = 0$, so $h = D(\chi_- u) = -D(\chi_+ u)$ is timelike compact. We conclude the proof using the properties of advanced and retarded Green functions:

$$\Delta h = \Delta^A D(\chi_- u) + \Delta^R D(\chi_+ u) = \chi_- u + \chi_+ u = u. \qquad \square$$

Even if we reached a complete characterisation of the solutions, we are not fully satisfied because for our purposes, we need a particular subspace of the space of solutions, introduced in the next proposition.

Proposition 1.1.4. *In the hypothesis of Theorem 1.1.2, the following statements hold true:*

1. *If $f \in \Gamma_0(E)$ satisfies $Df = 0$, then $f = 0$;*
2. *Given $f \in \Gamma_0(E)$ such that $\Delta f = 0$, there exists $h \in \Gamma_0(E)$ such that $Dh = f$;*
3. *For each $h \in \Gamma_0(E)$ there exists $f \in \Gamma_{sc}(E)$ such that $Df = h$.*

Furthermore, let $\mathbf{Sol}_{sc} \subset \mathbf{Sol}$ be the vector space of smooth, spacelike compact solutions of $Du = 0$. Then the map

$$\frac{\Gamma_0(E)}{D(\Gamma_0(E))} \to \mathbf{Sol}_{sc}, \qquad [f] \mapsto \Delta f \tag{1.1.11}$$

is an isomorphism between $\mathbf{Sol}_{sc}$ and the quotient of $\Gamma_0(E)$ by the image of D acting on $\Gamma_0(E)$.

We omit the proof of this Proposition since it is similar to the one of Theorem 1.1.2. It can be found for instance in [BGP07].

The reason why spacelike compact solutions are so interesting for Quantum Field Theory is that they can naturally be endowed with a symplectic structure, so allowing for the construction and the quantisation of the algebra of observables, see for example [BäFr09, BGP07, BeDa15, BDH13, Wa94].

Proposition 1.1.5. *Let E be a vector bundle over a globally hyperbolic space-time $\mathbb{M}$ endowed with a non-degenerate inner product. Consider a formally self-adjoint Green hyperbolic operator $D : \Gamma(E) \to \Gamma(E)$, with corresponding advanced and retarded fundamental solutions Δ^A and Δ^R respectively, and with causal propagator Δ. Then the following map defines a non-degenerate bilinear form on $\Gamma_0(E)$*

$$\tau : \frac{\Gamma_0(E)}{D(\Gamma_0(E))} \times \frac{\Gamma_0(E)}{D(\Gamma_0(E))} \to \mathbb{R}, \qquad ([f],[f']) \mapsto \tau([f],[f']) \doteq (f, \Delta f'). \tag{1.1.12}$$

Here, $(\cdot,\cdot)$ is the inner product defined in equation (1.1.2)*, while $f \in [f]$ and $f' \in [f']$ are two arbitrary representatives in the equivalence classes. Furthermore, if the inner product is a bosonic one, τ is a symplectic form, while τ is a scalar product in the fermionic case.*

Notations. Notice that $\tau([f],[f'])$ is often denoted with $\Delta(f,f')$. Along this thesis, we will usually follow this last convention.

Proof. First, notice that the definition of τ does not depend on the choice of the representatives because $\Delta \circ D(h) = 0$ for all $h \in \Gamma_0(E)$ and it is formally self-adjoint. The bilinearity is also immediate.

Let us analyse the non-degeneracy in more detail: Suppose $f \in \Gamma_0(E)$ is such that $\tau([f],[f']) = 0$ for all $f' \in \Gamma_0(E)$. By Lemma 1.1.1 this would imply

$$(f, \Delta f') = -(\Delta f, f) = 0 \qquad \forall\, f' \in \Gamma_0(E).$$

But the pairing $(\cdot,\cdot)$ is non-degenerate by definition, so it must be $\Delta f = 0$, that is $f \in D(\Gamma_0(E))$, meaning that $[f] = 0$. The same reasoning leads to the non-degeneracy in the other argument.

To conclude, let us suppose the pairing being bosonic, the fermionic case be addressed in a similar fashion. So τ is anti-symmetric, in fact

$$-\tau([f],[f']) = -(f, \Delta f') = (\Delta f, f') = (f', \Delta f) = \tau([f'],[f]),$$

where the self-adjointness of Δ and the anti-symmetry of the inner-product have been used. □

1.2 The Classical Algebra of Observables

Before starting with the quantisation procedure we must specify the objects we want to quantise, hence we devote this section to the construction of the algebra of classical observables for a massive scalar field theory. Even though very much can be said about the classical scalar field theory and many interesting mathematical and physical structures are involved in its study, we will limit ourselves to present the main objects and results only, suggesting an interested reader to look at [BFR17] for a more detailed analysis. For sake of generality, we will still work on a general globally hyperbolic space-time $(\mathbb{M}, g)$.

Several ways of formulating and quantising the algebra of observables for a scalar field have been developed in the literature. The method we will follow in the present thesis is the so-called *functional approach to AQFT*, in which the observables are modelled as functionals over the space of field configurations. This choice is motivated by the fact that this procedure is very-well suited for working with perturbation theory and, consequently, to deal with interacting models. As we will see, these functionals are selected so that it is possible to extract information about any given field configuration (*separability*). Furthermore, the information provided by a functional will not be detected by any other functional (*optimality*). Even though the choice of these functionals can be made rather abstract, in order to describe a physical theory we must make contact with the dynamics: This goal is achieved by defining a symplectic structure out of the partial differential equation describing our model, as we did at the end of the previous section.

1.2.1 Linear Functionals

The configurations space for a real scalar field is $\mathscr{E} \doteq C^\infty(\mathbb{M},\mathbb{R})$, the space of real-valued smooth functions on the space-time $\mathbb{M}$. To start with, we define the most simple observables, *i.e.* the *linear functionals* on $\mathscr{E}$.

Definition 1.2.1 (Linear Functionals)**.** Given $f \in \mathscr{D}(\mathbb{M},\mathbb{C}) \doteq C^\infty_c(\mathbb{M},\mathbb{C})$, we call linear functional the map $F_f : \mathscr{E} \to \mathbb{R}$ defined by

$$F_f(\phi) \doteq \int_{\mathbb{M}} f\phi \, d\mu_g, \tag{1.2.13}$$

where $d\mu_g$ is the standard volume form defined out of the orientation and of the metric present on the space-time $(\mathbb{M},g)$.

These functionals are well-defined thanks to the non-degenerate, bilinear pairing between $\mathscr{D}(\mathbb{M};\mathbb{C})$ and $\mathscr{E}$. Furthermore, due to the injectivity of the map $f \mapsto F_f$, it is possible to identify the space of linear functionals $\mathscr{F}_{\text{lin}} \doteq \{F_f : f \in \mathscr{D}(\mathbb{M};\mathbb{C})\}$ with $\mathscr{D}(\mathbb{M};\mathbb{C})$ itself. Due to the non degeneracy of the pairing between $\mathscr{D}(\mathbb{M};\mathbb{C})$ and $\mathscr{E}$ it descends that, given $\phi \in \mathscr{E}$ and for all $f \in \mathscr{D}(\mathbb{M};\mathbb{C})$, $F_f(\phi) = 0$ implies $\phi \equiv 0$. This means that the class of linear functionals is big enough to separate the off-shell field configurations: Given $\phi,\psi \in \mathscr{E}$ there exists $f \in \mathscr{D}(\mathbb{M};\mathbb{C})$ such that $F_f(\phi) \neq F_f(\psi)$. Nevertheless, we stress that the off-shellness of the configurations is a necessary condition for this identification, when we will move to dynamical configurations this will not hold true any longer.

The linear functionals are not enough for describing all the physics of a quantum field theory, so it will be necessary to introduce other classes of functionals in order to give meaning, for instance, to the Wick polynomials. Before doing that we prefer to deal with the dynamics. In fact, in order to develop an interacting QFT using perturbation theory it is necessary to work off-shell since the time-ordered product does not respect the on-shell observables, so it is convenient to talk about the dynamics now, once and for all.

A real scalar field is ruled by the Klein-Gordon equation on a globally hyperbolic space-time $\mathbb{M}$

$$(-\Box + m^2 + \xi R)\phi = 0, \tag{1.2.14}$$

where R is the scalar curvature of $\mathbb{M}$ and $\Box \doteq g_{\mu\nu}\nabla^\mu\nabla^\nu$ is the Laplace-Beltrami operator. m represents the mass of the field[3], while ξ is a coupling constant which accounts for the magnitude of backreaction of the scalar curvature of the manifold on the field itself. At the end of the day we will be interested in working on Minkowski space-time only, so for sake of simplicity we assume $\xi = 0$ (*minimal coupling*), nevertheless everything will hold true also using non-vanishing constants. For notational simplicity, we will introduce the *Klein-Gordon operator*

$$P \doteq -\Box + m^2; \qquad P\phi = 0. \tag{1.2.15}$$

An on-shell configuration is a (strong) solution to the Klein-Gordon equation. We recollect all the solutions in the space

$$\mathbf{Sol} \doteq \{\phi \in \mathscr{E} : P\phi = 0\}. \tag{1.2.16}$$

[3]We do not require any constraint on its sign since it will be of no interest in this thesis.

The operator P is a linear normally hyperbolic differential operator, as per Definition 1.1.18. Moreover, it is formally self-adjoint (see Definition 1.1.19): Given two configurations $\phi, \psi \in \mathscr{E}$ with supports with compact overlap, if we apply integration by parts twice we obtain:

$$\int_{\mathbb{M}} (P\phi)\psi \, d\mu_g = \int_{\mathbb{M}} \phi(P\psi) \, d\mu_g.$$

Being normally hyperbolic, P admits unique retarded and advanced Green operators Δ^R and Δ^A as per Definition 1.1.21. We have also explicitly computed them in the case of Minkowski, see equation (1.1.8).

The linear functionals are still able to separate the points in **Sol**, these being contained in $\mathscr{E}$, so the functionals F_f can detect any information also on off-shell configurations. On the contrary, restricting to on-shell field configurations, it is possible to find functionals which give no information at all. An example can be easily constructed as follows: Given $f \in \mathscr{D}(\mathbb{M};\mathbb{C})$, than Pf is a smooth and compactly-supported function on its own, so it is possible to construct a linear functional associated to it as $F_{Pf} : \mathscr{E} \to \mathbb{R}$. In general, integration by parts implies that $F_{Pf}(\phi) = F_f(P\phi)$ for all $\phi \in \mathscr{E}$, hence $F_{Pf}(\phi) = 0$ for all $\phi \in \mathbf{Sol}$. This example shows that the linear functionals, after restriction to solutions, are not injectively labeled by compactly-supported smooth functions anymore due to the presence of redundant functions in $\mathscr{D}(\mathbb{M};\mathbb{C})$.
This issue is solved by taking a proper quotient, ridding out the unwanted elements. Hence we define

$$N \doteq \left\{ f \in \mathscr{D}(\mathbb{M};\mathbb{C}) : F_f(\phi) = 0 \ \ \forall \, \phi \in \mathbf{Sol} \right\}.$$

Lemma 1.2.1. *The subspace N coincides with $P(\mathscr{D})$.*

Proof. Consider $f \in \mathscr{D}$ such that $F_f(\phi) = 0$ for every on-shell field configuration ϕ. According to Proposition 1.1.4, the causal propagator $\Delta : C^\infty_{tc}(\mathbb{M}) \to \mathscr{E}$ associated with P maps surjectively onto **Sol**, so the condition on f can be reformulated as

$$F_f(\Delta h) = 0 \qquad \forall \, h \in C^\infty_{tc}(\mathbb{M}).$$

We have already proved that $\left(\Delta^{A,R}\right)^* = \Delta^{R,A}$, so we have

$$F_f(\Delta h) = \int_M f(\Delta h) \, d\mu_g = -\int_{\mathbb{M}} (\Delta f) \cdot h \, d\mu_g = 0,$$

where it vanishes by hypothesis. So we conclude that $\Delta f = 0$. By definition of causal propagator, we can find $f' \in \mathscr{D}(\mathbb{M};\mathbb{C})$ such that $Pf' = f$, so $f \in N$ implies $f \in P(\mathscr{D})$. Since the inclusion $P(\mathscr{D}(\mathbb{M};\mathbb{C})) \subset N$ is obvious, the thesis follows. □

As per proposition 1.1.4, we consider the quotient

$$\mathscr{O} \doteq \frac{\mathscr{D}(\mathbb{M};\mathbb{C})}{P(\mathscr{D}(\mathbb{M};\mathbb{C}))}, \tag{1.2.17}$$

where an equivalence class $[f] \in \mathscr{O}$ generates a functional $F_{[f]} : \mathbf{Sol} \to \mathbb{R}$ defined by $F_{[f]}(\phi) \doteq F_f(\phi)$ for all $\phi \in \mathbf{Sol}$ and for any choice of the representative f of the class $[f]$. In addition, by passing

to the quotient, we manage to obtain a one-to-one correspondence between points in $\mathscr{O}$ and linear functionals of the form $F_{[f]}$, without losing the separation property for **Sol**. This motivates the choice of $\mathscr{O}$ as the space of *classical observables* for the scalar field. Furthermore, we point out that the quotient implements the dynamics at the level of observables, so that the functionals weakly solve the equation of motions. We will refer to the observables in $\mathscr{O}$ as to the *on-shell observables*.

Still, there is some work left to do to obtain the full classical scalar field theory, in particular we need to induce a symplectic structure on $\mathscr{O}$. To this avail, we apply Proposition 1.1.5 and we obtain

$$\tau : \mathscr{O} \times \mathscr{O} \to \mathbb{R}; \qquad ([f],[h]) \mapsto \tau([f],[h]) \doteq F_f(\Delta h) = \int_{\mathbb{M}} f \Delta h \, d\mu_g, \tag{1.2.18}$$

for two generic representative f, h of the two equivalence classes $[f],[h]$. Thus, the data $(\mathscr{O},\tau)$ is the symplectic space of observables of a real scalar field on the globally hyperbolic space-time $\mathbb{M}$, which is the starting point for the quantisation procedure. Indeed, the classical observables share already two properties analogous to the Haag-Kastler axioms, namely *causality* and the *time-slice axiom*, as proved in the next theorem:

Theorem 1.2.1. *Given a globally hyperbolic space-time $(\mathbb{M}, g)$, let $(\mathscr{O},\tau)$ be the symplectic space of classical observables for a real scalar field. Then the following properties hold:*

Causality *Given $f, h \in \mathscr{D}$ such that $\mathrm{spt}(f) \cap J(\mathrm{spt}(h)) = \emptyset$, then $\tau([f],[h]) = 0$.*

Time-slice axiom *Let $U_\Sigma \subset \mathbb{M}$ be a globally hyperbolic open neighbourhood of a spacelike Cauchy hypersurface Σ. If we denote with $(\mathscr{O},\tau)$ and $(\mathscr{O}_U,\tau)$ the symplectic spaces of observables for $\mathbb{M}$ and U_Σ respectively, then the map*

$$L : \mathscr{O}_U \to \mathscr{O}; \qquad L[f] = [f]_0 \quad \forall f \in \mathscr{D}(U_\Sigma)$$

is an isomorphism of symplectic spaces. Here $[f]_0$ denotes the extension by zero of $[f]$ to the whole $\mathbb{M}$.

Proof. See [BeDa15] and reference therein. □

Remark 1.2.1. In the literature, it is very often used another approach for inducing a symplectic structure for the classical scalar field, which in the end turns out to be equivalent to ours. In particular, one considers $\mathbf{Sol}_{sc}$, the space of solution to (1.2.14) with spacelike compact support, and define the following symplectic structure on it:

$$\sigma : \mathbf{Sol}_{sc} \times \mathbf{Sol}_{sc} \to \mathbb{R}; \qquad (\phi,\psi) \mapsto \sigma(\phi,\psi) \doteq \int_\Sigma \left(\phi \nabla_{\mathbf{n}} \psi - \psi \nabla_{\mathbf{n}} \phi\right) d\Sigma, \tag{1.2.19}$$

for a spacelike Cauchy surface $\Sigma \subset \mathbb{M}$, where $\mathbf{n}$ is the future-pointing unit normal vector field on Σ and $d\Sigma$ is the induced volume form on Σ. Implicitly, we are restricting the integrand to the Cauchy surface. Moreover, it can be proven that σ does not depend on the choice of Σ. The isomorphism then its realized by the map

$$i : \mathscr{O} \to \mathbf{Sol}_{sc}; \qquad [f] \mapsto i([f]) \doteq \Delta f,$$

for any representative $f \in \mathscr{D}(\mathbb{M};\mathbb{C})$ of $[f] \in \mathscr{O}$. Such a map arises quite naturally considering that the causal propagator enters in the definition of the space $\mathscr{O}$ through the quotient.

What is left to check is that $\sigma(\Delta f, \Delta h) = \tau([f],[h])$ for all $f, h \in \mathscr{D}(\mathbb{M};\mathbb{C})$. First, we notice that $\phi = \Delta f$ and $\psi = \Delta h$ are both solutions of the equations of motion by definition of causal propagator. Hence we get

$$\begin{aligned}
\int_{\mathbb{M}} f\,\Delta h\, d\mu_g &= \int_{J_+(\Sigma)} f\psi\, d\mu_g + \int_{J_-(\Sigma)} f\psi\, d\mu_g \\
&= \int_{J_+(\Sigma)} (P\Delta^A f)\psi\, d\mu_g + \int_{J_-(\Sigma)} (P\Delta^R f)\psi\, d\mu_g \\
&= -\int_\Sigma \Big(\nabla_{\mathbf{n}}(\Delta^A f)\Big)\psi\, d\Sigma + \int_\Sigma (\Delta^A f)\nabla_{\mathbf{n}}\psi\, d\Sigma \\
&\quad + \int_\Sigma \Big(\nabla_{\mathbf{n}}(\Delta^R f)\Big)\psi\, d\Sigma - \int_\Sigma (\Delta^R f)\nabla_{\mathbf{n}}\psi\, d\Sigma \\
&= \int_\Sigma \big(\phi\nabla_{\mathbf{n}}\psi - \psi\nabla_{\mathbf{n}}\phi\big)\, d\Sigma,
\end{aligned}$$

where in the third step we used integration by parts twice, exploiting the support properties of Δ^A and Δ^R. In this procedure, the boundary terms vanish since they depend on $P\psi = 0$. Adding together all the boundary terms the thesis follows.

1.2.2 The Kinematical Algebra of Observables

Even though the picture achieved using the linear functionals is satisfactory from several points of view, still it is not enough for describing an interacting model. In fact, all the physically interesting interactions are described by non-linear functions of the fields, think for instance to the $\lambda\phi^4$-model or to the sine-Gordon model. For taking them into account, we have to enlarge the class of functionals. The price we pay for dealing with more complicated functionals is that we have to cope with their distributional and microlocal features.

The Spaces of Functionals

The first class of functionals we introduce are the polynomial functionals, that correspond to the simpler way to extend linear functionals one can think of.

Definition 1.2.2 (Polynomial Functionals)**.** A monomial functional of degree n is a map $F : \mathscr{E} \to \mathbb{C}$ of the form

$$F(\phi) \doteq \langle f, \phi^{\otimes n}\rangle = \int_{\mathbb{M}^n} f(x_1,\dots,x_n)\phi(x_1)\cdots\phi(x_n)\, d\mu_g(x_1)\cdots d\mu_g(x_n), \tag{1.2.20}$$

where $f \in \mathscr{E}'(\mathbb{M}^n,\mathbb{C})$ is a compactly supported distribution and $\langle\cdot,\cdot\rangle$ is the duality pairing between $\mathscr{E}'(\mathbb{M}^n,\mathbb{C})$ and $\mathscr{E}(\mathbb{M}^n,\mathbb{C})$. We call polynomial functional of degree n a linear combination of monomial functionals of various degrees lower than n. The vector space generated by polynomial functionals of various degree is named $\mathscr{F}_{\mathrm{pol}}$.

Particularly interesting classes of functionals contained in $\mathscr{F}_{\mathrm{pol}}$ are the following:

- Linear functionals defined in Definition 1.2.1 are polynomial functionals of degree $n = 1$. Given a point $x \in \mathbb{M}$, we call *evaluation functional* a linear functional that is smeared with $f = \delta(x) \in \mathscr{E}'(\mathbb{M}, \mathbb{C})$, that is:
$$\mathrm{Ev}_x(\phi) \doteq \phi(x). \tag{1.2.21}$$
It is possible to define n-fold products of linear fields by taking $f(x_1, \dots, x_n) = f_1(x_1) \cdots f_n(x_n)$, with $f_k \in \mathscr{D}(\mathbb{M}, \mathbb{C})$ for all $k = 1, \dots, n$, obtaining
$$\left[F_{f_1} \cdots F_{f_n}\right](\phi) \doteq \int_{\mathbb{M}^n} f_1(x_1) \cdots f_n(x_n)\, \phi(x_1) \cdots \phi(x_n)\, d\mu_g(x_1) \cdots d\mu_g(x_n)$$
- The prototypical example of interactions for a real scalar field theory is given by the *field monomials*
$$F(\phi) \doteq \int_{\mathbb{M}} h\, \phi^n\, d\mu_g. \tag{1.2.22}$$
They are polynomial functionals of the form of (1.2.20) smeared with
$$f(x_1, \dots, x_n) = h(x_1)\, \delta(x_1 - x_2) \cdots \delta(x_{n-1} - x_n).$$

Even though much can be done using polynomial functionals, we need something more refined and general. Sometimes in fact non-polynomial interactions are needed (*e.g.* for some constructive models like the Liouville or the sine-Gordon ones). Actually, it must be said that the non-polynomiality will cause also some topological issues, which can nonetheless be solved as we will show later on, see also [BFR17]. In particular, a non-polynomial observable has to be described as a series, hence a notion of convergence must be introduced. Moreover, once two such observables are constructed, in order to preserve the algebraic structure we shall specify how the multiplication between them is done, *i.e.* how the two series can be combined and resummed. A good way out can be found by characterising the functionals directly through their differentiable and singular behaviour. In addition, owing those techniques in our tool box is really helpful in order to develop the quantisation and the construction of the time-ordered product. The first thing to do is to clarify what is the "derivative of a functional":

Definition 1.2.3 (Functional Derivative)**.** We say that a functional $F : \mathscr{E} \to \mathbb{C}$ is differentiable if the function $\mathbb{R} \ni \lambda \mapsto F(\phi + \lambda\psi)$ is differentiable for every $\phi, \psi \in \mathscr{E}$. Its first derivative is defined by
$$F^{(1)}(\phi)[\psi] \doteq \frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} F(\phi + \lambda\psi). \tag{1.2.23}$$
We say that F is continuously differentiable if the map $F^{(1)} : \mathscr{E} \times \mathscr{E} \to \mathbb{C}$ is continuous. A functional which is continuous and continuously differentiable is said a C^1-functional.
Accordingly, we define C^n-functionals and the n^{th}-functional derivative of F as
$$F^{(n)}(\phi)[\psi_1, \dots, \psi_n] \doteq \frac{\partial^n}{\partial\lambda_1 \cdots \partial\lambda_n}\bigg|_{\lambda_1 = \cdots = \lambda_n = 0} F\left(\phi + \sum_{j=1}^{n} \lambda_j \psi_j\right), \tag{1.2.24}$$
where $\psi_j \in \mathscr{E}$ for every $j = 1, \dots, n$ and where the continuity for $F^{(n)}$ is meant as the joint continuity as a functional on $\mathscr{E} \times \mathscr{E}^{\otimes n}$. We say that a functional is *smooth* if it is C^n for every $n \in \mathbb{N}$.

Example 1.2.1. An explicit computation shows that the k^{th}-functional derivative ($k \leq n$) of a polynomial functional of the form (1.2.20) is given by

$$F^{(k)}(\phi)[x_1,\dots,x_k] = \frac{n!}{(n-k)!}\int_{\mathbb{M}^{n-k}} f(x_1,\dots,x_k,y_1,\dots,y_{n-k})\phi(y_1)\cdots\phi(y_{n-k})d\mu_g(y_1)\cdots d\mu_g(y_{n-k}),$$

where $F^{(k)}(\phi)[x_1,\dots,x_k]$ denotes the integral kernel of the k-distribution $F^{(k)}(\phi)[\psi_1,\dots,\psi_k]$, that is given by:

$$F^{(k)}(\phi)[\psi_1,\dots,\psi_k] = \int_{\mathbb{M}^k} F^{(k)}(\phi)[x_1,\dots,x_k]\psi_1(x_1)\cdots\psi_k(x_k)d\mu_g(x_1)\cdots d\mu_g(x_k).$$

In particular, this implies that every polynomial functional is smooth because every k^{th}-functional derivative, with $k > n$ vanishes.

Another important feature we must introduce is the notion of the *support of a functional*: In order to study a Quantum Field Theory it turned out to be convenient to restrict the potential describing the self-interaction to a compact region of the space-time, extending it in the end by taking the so-called adiabatic limit (see Section 2.2). Moreover, in general we will assume the observables to have compact support. The definition of support of a functional was given in [BDF09] and it arises as an extension of the definition of the support of a distribution (see [Hö03]) to the non-linear case. It goes as follows:

Definition 1.2.4 (Support)**.** The support[4] of a functional $F : \mathscr{E} \to \mathbb{C}$ is defined as the closure of the set

$$\mathrm{spt}(F) \doteq \left\{x \in \mathbb{M} : \forall U_x \, \exists \phi,\psi \in \mathscr{E} \text{ with } \mathrm{spt}(\psi) \subset U_x \text{ s.t. } F(\phi+\psi) \neq F(\phi)\right\}, \tag{1.2.25}$$

where U_x denotes a generic neighbourhood of $x \in \mathbb{M}$. If $\mathrm{spt}(F)$ is compact, we say that F is *compactly supported* and we will write $F \in \mathscr{F}_c$.

Notice that this definition is not restricted to polynomial functionals, but it applies to more general ones. It tells us that the functional F is insensitive to local changes of the field configuration $\phi(x)$, for $x \notin \mathrm{spt}(F)$. Moreover, we stress that $\mathrm{spt}(\phi) \cap \mathrm{spt}(F) = \emptyset$ does not imply $F(\phi) = 0$. In [BFR17] it is proved that the support of smooth functionals is characterised by the support of its first functional derivative, *i.e.*

$$\mathrm{spt}(F) = \overline{\bigcup_{\phi\in\mathscr{E}} \mathrm{spt}\left(F^{(1)}(\phi)\right)},$$

where $\bar{\cdot}$ stands for the closure.

Yet, the compactness of the support is not enough to entail the locality required to model the interactions. In fact, functionals are defined as distributional objects, so in order to define a meaningful theory we also need to give conditions on their singular behaviour. The most natural object for addressing this kind of questions comes from Microlocal Analysis and is the following (see [Hö03, FJ98]):

[4] We will always denote the support of a functional and the support of every generic function in the same way, *i.e.* with spt. The distinction with the various notions of support is natural.

Definition 1.2.5 (Wave-Front Set)**.** Let $X \subset \mathbb{R}^n$ be an open set, $u \in \mathscr{D}'(X,\mathbb{C})$ and $x \in X$. $k \in \mathbb{R}^n \setminus \{0\}$ is not a singular direction for u at the point x if there exist an open conic[5] neighbourhood V_k of k and a test function $f \in \mathscr{D}(X,\mathbb{C})$ non-vanishing at x such that the f-localized Fourier transform of u

$$\widehat{fu}(p) \doteq u\left(fe^{-\mathrm{i}x\cdot p}\right)$$

is rapidly decreasing in V_k, that is for every $N \in \mathbb{N}$ there exists a constant $c_N > 0$ such that

$$\left|\widehat{fu}(p)\right| \leq c_N \frac{1}{(1+|p|)^{N/2}} \quad \forall\, p \in V_k.$$

The collection of the singular directions of u at x is denoted by $\Sigma_x(u)$. The wave-front set of u is then defined as

$$\mathrm{WF}(u) \doteq \left\{(x,k) \in \mathbb{R}^n \times (\mathbb{R}^n \setminus \{0\}) : k \in \Sigma_x(u)\right\}. \tag{1.2.26}$$

The wave-front set entered as a fundamental ingredient of QFT on curved background thanks to the seminal work of Radzikowski [Ra96a] and of Brunetti, Fredenhagen and Köhler [BFK95], in which the condition for selecting physical interesting states is successfully reformulated in terms of the celebrated *microlocal spectrum condition*, see also Section 1.3.3. Loosely speaking, the wave-front set tells us how regular a distribution is by looking at the decay of its Fourier transform in an arbitrarily small neighbourhood of a point x. Despite the wave-front set being an interesting object on its own, we limit ourselves in listing some features which will be useful for our purposes. A complete account on the subject can be found in [Hö03, Chapter 8] or in the more introductory text [FJ98, Chapter 11].

Two first basic properties concern the wave-front set of smooth functions and of a linear combination of distributions.

- Given $u \in \mathscr{D}'(X,\mathbb{C})$, $\mathrm{WF}(u) = \emptyset$ if and only if $u \in \mathscr{E}(X,\mathbb{C})$;
- For all $u, v \in \mathscr{D}'(X,\mathbb{C})$ and all $\alpha, \beta \in \mathbb{C}$ we have

$$\mathrm{WF}\left(\alpha u + \beta v\right) \subset \mathrm{WF}(u) \cup \mathrm{WF}(v). \tag{1.2.27}$$

The next result, known as the *Theorem of propagation of singularities*, deals with the behaviour of the wave-front set of a distribution u under the evolution driven by a differential operator P:

Proposition 1.2.1. *Given $u \in \mathscr{D}'(X,\mathbb{C})$ and $f \in \mathscr{E}(\mathbb{M},\mathbb{C})$ and a smooth linear differential operator $P : \mathscr{E}(\mathbb{M},\mathbb{C}) \to \mathscr{E}(\mathbb{M},\mathbb{C})$ we have*

$$\mathrm{WF}(fu) \subseteq \mathrm{WF}(u), \qquad \mathrm{WF}(Pu) \subseteq \mathrm{WF}(u) \subseteq \mathrm{WF}(Pu) \cup \mathrm{Ch}(P),$$

where $\mathrm{Ch}(P)$ is the characteristic set of P, which corresponds to the locus of the zeros of the principal symbol σ_P of P (see Definition 1.1.17). Furthermore, if σ_P is real-valued, the set $\mathrm{WF}(u) \setminus \mathrm{WF}(Pu)$ is invariant under the characteristic flow generated by the Hamiltonian vector field associated with σ_P.

[5] We say that $\Gamma \subset \mathrm{T}^*\mathbb{M}$ is a conic neighbourhood if, given $\xi = (x,p) \in \Gamma$, then $(x,\lambda p) \in \Gamma$ for all real $\lambda > 0$.

The following proposition furnishes a sufficient condition for the multiplication of two distributions, and it will play a pivotal role all along this thesis.

Proposition 1.2.2 (Hörmander criterium)**.** *Let $u, v \in \mathscr{D}'(X,\mathbb{C})$ be two distributions such that the Whitney sum of their wave-front sets*

$$\mathrm{WF}(u) + \mathrm{WF}(v) \doteq \left\{(x, k+k') \in \mathrm{T}^*\mathbb{M} : (x,k) \in \mathrm{WF}(u) \text{ and } (x,k') \in \mathrm{WF}(v)\right\}$$

is such that $\mathrm{WF}(u) + \mathrm{WF}(v) \cap \{0\} = \{\emptyset\}$, 0 being the zero section in $\mathrm{T}^*\mathbb{M}$. Then the product uv is well-defined as an element of $\mathscr{D}'(X,\mathbb{C})$ and its wave-front set satisfies

$$\mathrm{WF}(uv) \subseteq \left\{(x, k+k') \in T^*\mathbb{M} \setminus \{0\} : (x,k) \in \mathrm{WF}(u) \text{ or } k = 0,\ (x,k') \in \mathrm{WF}(v) \text{ or } k' = 0\right\}.$$

With these tools at our disposal, we can define all the functionals of interest. To do so, let us first fix some notations: We will denote by $\mathscr{F}$ the space of smooth and compactly supported functionals, as per Definitions 1.2.3 and 1.2.4.

We start with the definition of the *regular functionals*, namely those that exhibit no singular behaviour.

Definition 1.2.6 (Regular Functionals)**.** We define the space of regular functionals as

$$\mathscr{F}_{\mathrm{reg}} \doteq \left\{F \in \mathscr{F} : \mathrm{WF}\left(F^{(k)}(\phi)\right) = \emptyset,\ \forall\, k \in \mathbb{N}, \forall\, \phi \in \mathscr{E}\right\}. \tag{1.2.28}$$

This definition implies that every functional derivative of a regular functional is well-defined as a compactly supported function in $\mathscr{D}(\mathbb{M},\mathbb{C})$. Examples of regular functionals are the linear ones, actually regular functionals are spanned by them. Unfortunately, the interactions are meant to be singular objects, so they can not be described by functionals of this kind, hence we need to work a bit more.

Definition 1.2.7 (Microcausal Functionals)**.** We define the space of microcausal functionals as

$$\mathscr{F}_{\mu c} \doteq \left\{F \in \mathscr{F} : \mathrm{WF}\left(F^{(n)}(\phi)\right) \cap \left(\overline{V}_+^k \cap \overline{V}_-^k\right) = \emptyset,\ \forall\, k \in \mathbb{N}, \forall\, \phi \in \mathscr{E}\right\}, \tag{1.2.29}$$

where $\overline{V}_\pm^n$ are the future/past light cones in $(\mathrm{T}^*\mathbb{M})^n$, with respect to the metric g.

The microcausal functionals satisfy all the regularity property we need and, in addition, they can be given the structure of a topological *-algebra[6], so they will serve as observables for the real scalar field theory. In particular, the quantisation procedure and the Hörmander criterium 1.2.2 will motivate the condition imposed on their wave-front set. In order to cast them into a topological *-algebra, we need to define an involution, a product and a topology. The algebraic structure is easily handled by appealing to the pointwise product of functions. Actually, given $F, G \in \mathscr{F}_{\mathrm{loc}}$, $\phi \in \mathscr{E}$ and $\lambda \in \mathbb{C}$ we define

$$(F+G)(\phi) \doteq F(\phi) + G(\phi), \qquad (\lambda F)(\phi) \doteq \lambda \cdot F(\phi), \qquad (F \cdot G)(\phi) \doteq F(\phi)G(\phi). \tag{1.2.30}$$

[6]Recall that a topological *-algebra is an algebra endowed with an involution and with a locally convex topology with respect to which the product is a continuous map.

In particular, the constant functional $\mathbb{1}(\phi) \equiv \mathbb{1} \doteq 1$ is the unit of this set. The involutive structure is given by the complex conjugation $\bar{\cdot}$:

$$F^*(\phi) \doteq \overline{F(\phi)}. \tag{1.2.31}$$

Concerning the topology, a natural choice would have been the topology of the pointwise convergence of functionals together with their derivatives of all orders. However, it does not take into account the extra information about the wave-front set of microcausal functionals, see [BFR17]. This issue is solved using the *Hörmander pseudo-topology*, which we briefly introduce now (see [Hö03, Section 8.2] for a complete account).

Let $X \subset \mathbb{R}^N$ be an open subset (indeed, the construction holds true for a general manifold) and let $\Gamma \subset \mathrm{T}^*X$ be a conic subset (see the footnote 5). Then we define

$$\mathscr{D}'_\Gamma(X,\mathbb{C}) \doteq \{u \in \mathscr{D}'(X,\mathbb{C}) : \mathrm{WF}(u) \subseteq \Gamma\}.$$

Since it is possible to prove that this sets are not close in the usual weak *-topology, then we must define a more-suited notion of convergence: We say that $\{u_n\}_{n\in\mathbb{N}} \subset \mathscr{D}'_\Gamma(X,\mathbb{C})$ converges to $u \in \mathscr{D}'_\Gamma(X,\mathbb{C})$ if

1. u_n converges to u in $\mathscr{D}'(X,\mathbb{C})$;
2. For all $f \in \mathscr{D}(X,\mathbb{C})$, all $\alpha \in \mathbb{N}$ and for some open cone $V \subset \mathbb{R}^N$ such that $\Gamma \cap (\mathrm{spt}(f) \times V) = \emptyset$, it holds that
$$\sup_V |k|^\alpha \left|\widehat{fu_n}(k) - \widehat{fu}(k)\right| \to 0 \quad \text{as } n \to \infty.$$

This prescription defines the Hörmander pseudo-topology. Our goal is to adapt this definition to functionals in $\mathscr{F}_{\mu\mathrm{c}}$: To do so, consider a sequence $\Gamma = \{\Gamma_j\}_{j\in\mathbb{N}}$ where $\Gamma_j \subseteq \mathrm{T}^*\mathbb{M}^j$ are conic subsets (see footnote 5) for all j defined as the complement of $\left(\overline{V_+}^j \cap \overline{V_-}^j\right)$ in $\mathrm{T}^*\mathbb{M}^j$, as per Definition 1.2.7. Then we define

$$\mathscr{F}_{\Gamma_j} \doteq \left\{F \in \mathscr{F} : \mathrm{WF}\left(F^{(j)}(\phi)\right) \subseteq \Gamma_j, \ \ \forall\, j \in \mathbb{N} \text{ and } \forall\, \phi \in \mathscr{E}\right\}.$$

We say that a sequence of functionals $\{F_n\}_{n\in\mathbb{N}}$ converges to F in $\mathscr{F}_\Gamma$ if and only if $F_n^{(j)}(\phi) \to F^{(j)}(\phi)$ in $\mathscr{D}'_\Gamma(\mathbb{M},\mathbb{C})$ for all $j \in \mathbb{N}$ and all $\phi \in \mathscr{E}$. This is realised by considering the inductive limit

$$\mathscr{F}_\Gamma \doteq \varinjlim_{j\nearrow\mathbb{N}} \mathscr{F}_{\Gamma_j}$$

endowing it with the locally convex inductive limit topology induced by the Hörmander topology present on every space $\mathscr{F}_{\Gamma_j}$. Slightly abusing the terminology, we call it the Hörmander pseudo-topology for functionals. This is the sought topology which allows to make sense to non-polynomial functionals, see [BDF09, BFR17, Re16] for further details. The second problem we need to consider is that of taking multiplications of non-polynomial observables, so to have a well-defined algebra structure. This means that we should prescribe how to combine order by order the various terms of the two series defining these observables. This is done by noticing that the $\star$ product we will define in the following (which is used to define the non-polynomial observables and to multiply them) is sequentially continuous with respect to this topology, see [BDF09, BFR17, Re16]. Anyway, we will not deal with this class of observables, as we shall specify later.

We are in position to define the classical algebra of observables. To do so, we will not consider the full algebra of functionals, but we will limit ourselves to the polynomial ones, *i.e.* we will consider the algebra $\mathscr{F}_{\mu c} \cap \mathscr{F}_{\text{pol}}$ consisting of the microcausal functionals which have a finite number of non-vanishing functional derivatives only. The motivation for this choice is two-fold: First, the interactions one deals with when studying the real scalar field are of polynomial kind only, so this restriction causes no loss of generality. Second, the Hörmander pseudo-topology we defined is in contrast with the Poisson structure one wants to define on the classical algebra. This problem can be fixed, see [BFR17], but this goes beyond the goal of this work. Hence, from now on, we will only consider algebras of polynomial observables in $\hbar$.

Notations. For sake of simplicity, we will not change the notation used for the various functionals space, even if from now on we will refer to space of polynomials only. So, unless otherwise stated, we will write

$$\mathscr{F}_{\mu c} \equiv \mathscr{F}_{\mu c} \cap \mathscr{F}_{\text{pol}} \quad \text{or} \quad \mathscr{F}_{\text{reg}} \equiv \mathscr{F}_{\text{reg}} \cap \mathscr{F}_{\text{pol}}. \tag{1.2.32}$$

Definition 1.2.8 (Classical Algebra)**.** The classical off-shell topological *-algebra of the observables for a free, real, massive scalar field theory is given by the triple $\mathscr{A}_{\text{cls}} \doteq \left(\mathscr{F}_{\mu c}, \cdot, ^*\right)$, where the pointwise product $\cdot$ is defined in (1.2.30), the involution * is given by the complex conjugation as per (1.2.31) and $\mathscr{F}_{\mu c}$ is endowed with the Hörmander pseudo-topology.
Similarly, we define the subalgebra of regular functionals as $\mathscr{A}_{\text{cls,reg}} \doteq \left(\mathscr{F}_{\text{reg}}, \cdot, ^*\right)$.

Local Functionals

Interesting interactions are usually non linear potentials. However, regular non-local interactions lead in general to non-unitary S-matrices (this will be clarified in Section 2.1). In order to restore the desired unitarity, it is convenient to require them to be local objects. In this case, the unitarity of the S-matrix can be restored assigning a renormalisation condition. This motivates the introduction of the *local functionals*.

The concept that really captures the locality of a functional is the *additivity*, which *a posteriori* motivates Definition 1.2.4:

Definition 1.2.9 (Additivity)**.** A functional $F : \mathscr{E} \to \mathbb{C}$ is said to be additive if

$$F(\phi + \psi + \chi) = F(\phi + \psi) - F(\psi) + F(\psi + \chi) \tag{1.2.33}$$

for all $\phi, \psi, \chi \in \mathscr{E}$ such that $\text{spt}(\phi) \cap \text{spt}(\chi) = \emptyset$.

Recalling that, for a general functional, $F(0) \neq 0$[7], this definition tells us that, for $\psi \equiv 0$, an additive functional over a sum of configurations with disjoint support splits up to a constant, which is equal to $F(0)$. Roughly speaking, additive functionals separate the points in $\mathscr{E}$ and non-interacting configurations are detected as separate by any additive functional. Hence, in general, we define a local functional as follows:

[7] For example, take the Weyl functional $F(\phi) = \int e^{i\phi(f)} d\mu_g$.

Definition 1.2.10 (Local Functionals)**.** A functional $F : \mathscr{E} \to \mathbb{C}$ is said to be local if:

1. F is additive;
2. F is smooth as per Definition 1.2.3;
3. $\mathrm{WF}\left(F^{(n)}(\phi)\right) \perp \mathrm{T}\,\mathrm{diag}(n)$, the tangent space of the thin diagonal of $\mathbb{M}^n$, which is defined as

$$\mathrm{diag}(n) \doteq \left\{(x_1,\dots,x_n) \in \mathbb{M}^n : x_1 = \dots = x_n\right\}. \tag{1.2.34}$$

We call $\mathscr{F}_{\mathrm{loc}}$ the space of local functionals.

Notice that the space of local functionals is not closed under the pointwise product of functionals defined in (1.2.30) and that it is not possible to endow it with a *-algebra structure. Nonetheless it can be given the topology induced by the coefficients.

To start with, we give a useful characterisation of the local functionals (see [BDF09, BFR17]).

Proposition 1.2.3. *The n^{th}-functional derivative of a local functional F is supported on the thin diagonal* $\mathrm{diag}(n)$ *for every $n \in \mathbb{N}$, in formulae*

$$\mathrm{spt}\left(F^{(n)}\right) \subset \mathrm{diag}(n) \quad \forall\, n \in \mathbb{N}. \tag{1.2.35}$$

Proof. Given a local functional F, by Definition 1.2.3 of functional derivative we may assume that $\mathbf{x} \equiv (x_1,\dots,x_n) \in \mathbb{M}^n$ is a point in $\mathrm{spt}\left(F^{(n)}(\phi)\right)$. Let us suppose that, for some $j \neq k$, we can find $x_j \neq x_k$, then there exist $\phi_j, \phi_k \in \mathscr{E}$ such that $x_j \in \mathrm{spt}(\phi_j)$, $x_k \in \mathrm{spt}(\phi_k)$ and $\mathrm{spt}(\phi_j) \cap \mathrm{spt}(\phi_k) = \emptyset$. Referring to formula (1.2.24), by additivity we can split the function appearing on the right hand side of that equation as

$$F\left(\phi + \sum_{m=1}^{n} \lambda_m \psi_m\right) = F\left(\phi + \sum_{\substack{m=1 \\ m\neq k}}^{n} \lambda_m \psi_m\right) - F\left(\phi + \sum_{\substack{m=1 \\ m\neq j,k}}^{n} \lambda_m \psi_m\right) + F\left(\phi + \sum_{\substack{m=1 \\ m\neq j}}^{n} \lambda_m \psi_m\right),$$

so not every term contains all λ_m, forcing the functional derivative to be identically zero. Hence, we conclude that the support of $F^{(n)}$ must be contained in the thin diagonal of $\mathbb{M}^n$. □

This proposition implies that every[8] local functional is microcausal, so being a well-defined observable as expected. Another important result about local functionals is the following:

Lemma 1.2.2 ([BDF09])**.** *Any local functional F can be written as a finite sum of local functionals of arbitrarily small support.*

Proof. Given $\epsilon > 0$, consider a finite covering $\{B_j\}_{j=1}^n$ of $\mathrm{spt}(F)$ made by balls of radius $r = \epsilon/4$. Take also $\{\rho_j\}_{j=1}^n$ a subordinate partition of unit. Additivity implies that we can decompose F as

$$F = \sum_J \sigma_J F_J, \qquad F_J(\phi) \doteq F\left(\phi \sum_{j\in J} \rho_j\right),$$

[8] This holds true in the non-polynomial case also.

where $\sigma_J = \pm 1$ and J runs over all the partitions of $\{1,\dots,n\}$ such that $B_j \cap B_k \neq \emptyset$. By definition 1.2.4 we get that

$$\mathrm{spt}(F_J) \subset \bigcup_{j\in J} B_j \doteq B_J.$$

But two generic points in B_J are distant at most $\epsilon/2$, hence every B_J is contained in a ball of radius ϵ. □

This result in fact motivates the real local nature of those functionals. In addition we specify that, since polynomial local functionals are enough for our purposes, in what follows we call $\mathscr{F}_{\mathrm{loc}} \equiv \mathscr{F}_{\mathrm{pol}} \cap \mathscr{F}_{\mathrm{loc}}$, with the usual abuse of the notation.

1.2.3 The Dynamical Algebra of Observables

Having the local functionals at disposal, we can define actions and Lagrangians in the functional framework. In order to obtain well-defined objects, one must integrate the Lagrangian against a test function, so to obtain a local element. With a Renormalization Group approach in mind, one understands that it acts in a non-linear fashion on functionals, so it is convenient to allow also non-linear dependance on the test functions (see [BDF09]). This leads us to define a *generalised Lagrangian* as a functional over the test functions taking values in $\mathscr{F}_{\mathrm{loc}}$.

Definition 1.2.11 (Generalised Lagrangian)**.** A generalised Lagrangian is a map $\mathscr{L} : \mathscr{D} \to \mathscr{F}_{\mathrm{loc}}$ which fulfills the following properties

1. $\mathrm{spt}(\mathscr{L}(f)) \subset \mathrm{spt}(f)$ for all $f \in \mathscr{D}$;
2. $\mathscr{L}(0) = 0$;
3. $\mathscr{L}$ is an additive functional;
4. For a QFT on Minkowski, $\mathscr{L}$ is covariant under the action of the Poincaré group.

Example 1.2.2. The more relevant example to us is the Lagrangian of the free scalar field

$$L_0(f)(\phi) \doteq \frac{1}{2}\int_{\mathbb{M}} \left(\nabla_\nu \phi \nabla^\nu \phi - m^2\phi^2\right) f \, d\mu_g. \tag{1.2.36}$$

The generic interaction can be again formulated as a generalised Lagrangian as follows:

$$L_I(f)(\phi) \equiv V_f(\phi) \doteq \int_{\mathbb{M}} \mathrm{P}[\phi] f \, d\mu_g,$$

for a generic polynomial P.

By considering different algebras of observables and different configurations spaces, it is possible to accommodate different Lagrangians also, such as the Yang-Mills one

$$L_{YM}(f)(A) \doteq -\frac{1}{2}\int_{\mathbb{M}} f \,\mathrm{Tr}(F \wedge *F), \qquad F = dA + \frac{1}{2}[A,A]$$

where $A \in \Lambda^1(\mathbb{M},\mathfrak{g})$, $*$ is the Hodge dual and the trace is taken with respect to the adjoint representation given by the Killing-Cartan metric.

Actually, it must be stressed that the test function f is only a mathematical tool which makes the theory rigorous which has no direct physical interpretation. At the same time, the Lagrangian depends non-trivially on it, hence we have to define a test-function-independent quantity. This is achieved as follows (see [Re16]):

Definition 1.2.12 (Euler-Lagrange Derivative)**.** The Euler-Lagrange derivative of a generalised Lagrangian $\mathscr{L}$ is a map $\mathfrak{S}' : \mathscr{E} \to \mathscr{D}'$ defined by

$$\langle \mathfrak{S}'(\phi), h \rangle \doteq \left\langle \mathscr{L}^{(1)}(f)(\phi), h \right\rangle \tag{1.2.37}$$

where $h \in \mathscr{D}$ and $f \in \mathscr{D}$ is such that $f \equiv 1$ on $\mathrm{spt}(h)$.

The fact that $\mathfrak{S}'$ does not depend on f is a consequence of the local nature of $\mathscr{L}$, which also implies that $\mathfrak{S}'$ would not change adding to $\mathscr{L}$ another generalised Lagrangian $\mathscr{L}'$ supported in the region where f is non-constant. This leads us to define an equivalence class of generalised Lagrangians, which corresponds to what, in physical terms, is called an "action". This equivalence class is defined according to the fact that two Lagrangians induce the same dynamics if they differ by a boundary term (or, in other words, if they differ by a total divergence). In this framework, this feature is captured by the following definition:

Definition 1.2.13 (Action)**.** Two generalised Lagrangians $\mathscr{L}$ and $\mathscr{L}'$ are said to induce the same dynamics, $\mathscr{L} \sim \mathscr{L}'$, if

$$\mathrm{spt}\big(\big(\mathscr{L} - \mathscr{L}'\big)(f)\big) \subset \mathrm{spt}(df) \qquad \forall f \in \mathscr{D}.$$

An equivalence class of generalised Lagrangians under the equivalence relation $\sim$ is called an action and it will be denoted with $\mathfrak{S}$.

Then it is possible to define the equations of motion as extremal points of the variation of the action (*i.e.* through the principle of least action) as follows:

Definition 1.2.14 (Equation of Motion)**.** The equations of motion corresponding to an action $\mathfrak{S}$ are defined as

$$\mathfrak{S}'(\phi) \equiv 0, \tag{1.2.38}$$

which has to be understood as a condition on the field configurations $\phi \in \mathscr{E}$.

It is easy to check that, considering the Euler-Legrange derivative $\mathfrak{S}'_{\mathrm{KG}}(\phi)$ obtained using the Klein-Gordon action (1.2.36), Definition 1.2.14 produces the Klein-Gordon equation (1.2.14). This can be obtained by looking at the second functional derivative of the action $\mathfrak{S}$ as follows:

$$\langle \mathfrak{S}''(\phi), h_1 \otimes h_2 \rangle \doteq \left\langle \mathscr{L}^{(2)}(f)(\phi), h_1 \otimes h_2 \right\rangle, \tag{1.2.39}$$

where $f \equiv 1$ on $\mathrm{spt}(h_1)$ and $\mathrm{spt}(h_2)$. By definition $\mathfrak{S}'' : \mathscr{E} \to L(\mathscr{D} \times \mathscr{D}, \mathbb{C})$, where $L(\mathscr{D} \times \mathscr{D}, \mathbb{C})$ denotes the space of the linear functionals on $\mathscr{D} \times \mathscr{D}$. In particular, due to the locality of $\mathscr{L}$, it follows that we can extend $\mathfrak{S}''(\phi)$ to a functional on $\mathscr{E} \times \mathscr{D}$ by linearity. Moreover, by the Schwartz kernel theorem ([Hö03, Chapter 5]), it induces a continuous linear operator $\mathfrak{P}_{\mathfrak{S}}(\phi) : \mathscr{E} \to \mathscr{D}'$, called the *Euler-Lagrange operator* (see [Re16, BFR17]). For a quadratic action, such as the free Klein-Gordon one (see equation (1.2.14)), one has $\mathfrak{P}_{\mathfrak{S}}(\phi) \equiv P$, which is the same for all $\phi \in \mathscr{E}$ and, obviously $\mathfrak{S}'(\phi) = P\phi$, as expected.

Remark 1.2.2. A crucial assumption for a generic model of pAQFT is that $\mathfrak{P}_{\mathfrak{S}}(\phi)$ must be a normally hyperbolic operator for every field configuration ϕ, as per Definition 1.1.18.

We aim now to define the algebra of on-shell observables as done before concerning linear functionals, that is we want to identify the ideal generated by the functionals that (weakly) solve the equation of motion. To this avail we define the space of on-shell configurations as follows:

$$\mathscr{E}_{\mathrm{KG}} \doteq \left\{\phi \in \mathscr{E} : \mathfrak{S}'_{\mathrm{KG}}(\phi) = 0\right\}. \tag{1.2.40}$$

Following the strategy used for local functionals (cfr. equation (1.2.17)), we define the ideal $\mathscr{F}_{\mathrm{KG}}$ of functionals vanishing on $\mathscr{E}_{\mathrm{KG}}$ as

$$\mathscr{F}_{\mathrm{KG}} \doteq \left\{F \in \mathscr{F}_{\mu\mathrm{c}} : F(\phi) = 0,\ \forall\, \phi \in \mathscr{E}_{\mathrm{KG}}\right\},$$

and we take the quotient $\mathscr{F}_{\mu\mathrm{c}}/\mathscr{F}_{\mathrm{KG}}$, so obtaining the *classical on-shell algebra of observables*:

$$\mathscr{A}_{\mathrm{cls,on}} \doteq \left(\frac{\mathscr{F}_{\mu\mathrm{c}}}{\mathscr{F}_{\mathrm{KG}}}, \cdot, {}^*\right). \tag{1.2.41}$$

Following what we did for the linear functionals in Section 1.2.1, we want to endow the algebra of observables with a *Poisson structure*, see [BFR17, DF03, FR15]. Actually, in the non-linear case we will act differently due to the fact that, in order to implement them algebraically, it turns out to be more convenient to work with the off-shell algebra. In particular, we will work with multilocal functionals only, the extension to every microcausal functional is nonetheless possible, but it has to be addressed carefully. We will not dwell on this, demanding an interested reader to the references quoted above. Due to its generality, we will present the construction for a general action $\mathfrak{S}$, not limiting ourselves to the scalar field. Anyway, we will assume that $\mathfrak{S}$ admits solvable equation of motion $\mathfrak{P}_{\mathfrak{S}}(\phi) = 0$ with associated Green operators $\mathfrak{D}^R$ and $\mathfrak{D}^A$, out of which we construct the causal propagator $\mathfrak{D}$.

Definition 1.2.15 (Poisson brackets)**.** Given two local functionals $F, G \in \mathscr{A}_{\mathrm{loc}}$, we define the retarded and advanced products $\mathrm{R}_{\mathfrak{S}}(F,G)$ and $\mathrm{A}_{\mathfrak{S}}(F,G)$ with respect to a generalised Lagrangian $\mathfrak{S}$ as

$$\mathrm{R}_{\mathfrak{S}}(F,G)(\phi) \doteq \left\langle F^{(1)}(\phi), \mathfrak{D}^R G^{(1)}(\phi)\right\rangle, \qquad \mathrm{A}_{\mathfrak{S}}(F,G)(\phi) \doteq \left\langle F^{(1)}(\phi), \mathfrak{D}^A G^{(1)}(\phi)\right\rangle.$$

A Poisson structure on $\mathscr{A}_{\mathrm{loc}}$ is defined by the following Poisson brackets

$$\{F,G\}_{\mathfrak{S}}(\phi) \doteq \mathrm{R}_{\mathfrak{S}}(F,G)(\phi) - \mathrm{A}_{\mathfrak{S}}(F,G)(\phi) = \left\langle F^{(1)}(\phi), \mathfrak{D}\, G^{(1)}(\phi)\right\rangle \qquad \forall\, \phi \in \mathscr{E},\ \forall\, F,G \in \mathscr{A}_{\mathrm{loc}}. \tag{1.2.42}$$

Notice that $\mathrm{R}_{\mathfrak{S}}(F,G) = \mathrm{A}_{\mathfrak{S}}(G,F)$, so we can equivalently rewrite

$$\{F,G\}_{\mathfrak{S}}(\phi) \doteq \mathrm{R}_{\mathfrak{S}}(F,G)(\phi) - \mathrm{R}_{\mathfrak{S}}(G,F)(\phi),$$

highlighting the antisymmetric nature of the so-defined Poisson brackets.

Remark 1.2.3. This definition, which has been given in the general case, for the Klein-Gordon equation reduces to

$$\{F,G\}(\phi) \doteq \left\langle F^{(1)}(\phi), \Delta G^{(1)}(\phi) \right\rangle \qquad \forall\, \phi \in \mathscr{E},\ \forall\, F,G \in \mathscr{A}_{\mathrm{loc}}, \tag{1.2.43}$$

Δ being the causal propagator of the Klein-Gordon operator given in Definition 1.1.21

Actually, from the definition above alone, it is impossible to argue that $\{\cdot,\cdot\}_{\mathfrak{S}}$ are well-defined Poisson brackets. The full proof of all the required properties may be found in [BFR17].

Although this way of defining a Poisson structure is perfectly consistent and satisfactory, it has the disadvantage of heavily relying on the linearity of the free Klein-Gordon equation. In general, it is not known whether a non-linear equation admits or not Green operator solutions, so it is impossible to define a Poisson structure in this way for an interacting model. A way out was found by Peierls (see [Pe52, Ma94]) introducing the so-called *Peierls brackets*. The first step towards our goal is the definition of the *advanced and retarded Møller maps*.

Definition 1.2.16 (Møller Maps)**.** Let $V \in \mathscr{F}_{\mathrm{loc}}$ be a smooth and compactly supported functional and let $\mathscr{E}_{\mathfrak{S}}$ be the space of solutions of the equation of motion associated to the action $\mathfrak{S}$. We define the retarded Møller map as the linear map

$$\mathrm{r}_{\lambda V} : \mathscr{E}_{\mathfrak{S}} \to \mathscr{E}_{\mathfrak{S}+\lambda V^{(1)}} \tag{1.2.44}$$

which to every solution for $\mathfrak{S}$ associates a solution for $\mathfrak{S} + \lambda V^{(1)}$ in such a way that the two solutions coincide on $J_-(\mathrm{spt}(V))$. Analogously, we defined the advanced Møller map

$$\mathrm{a}_{\lambda V} : \mathscr{E}_{\mathfrak{S}} \to \mathscr{E}_{\mathfrak{S}+\lambda V^{(1)}}, \tag{1.2.45}$$

that connects two solutions in $\mathscr{E}_{\mathfrak{S}}$ and $\mathscr{E}_{\mathfrak{S}+\lambda V^{(1)}}$ respectively which coincide in $J_+(\mathrm{spt}(V))$.

For an explicit computation of those operators it is necessary to explicitly solve the equations of motion for the action $\mathfrak{S} + \lambda V^{(1)}$, which are in general non linear. The advantage of the Peierls prescription is that it requires to know the Møller maps only up to the second order in λ.
Given F,G smooth and compactly supported functionals over $\mathscr{E} \supset \mathscr{E}_{\mathfrak{S}}$, then for all solutions $\phi \in \mathscr{E}_{\mathfrak{S}}$, with $\mathfrak{S}$ arbitrary but fixed, we introduce

$$\mathrm{R}_F G \doteq \frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} G\left(\mathrm{r}_{\lambda \mathrm{F}}(\phi)\right) \quad \text{and} \quad \mathrm{A}_F G \doteq \frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} G\left(\mathrm{a}_{\lambda \mathrm{F}}(\phi)\right), \tag{1.2.46}$$

by which we finally define the Peierls brackets as

$$\{F,G\}_{\mathrm{Pei}}(\phi) \doteq \mathrm{R}_F G(\phi) - \mathrm{A}_F G(\phi) \quad \forall\, \phi \in \mathscr{E}_{\mathfrak{S}}. \tag{1.2.47}$$

The Peierls brackets, as we have just defined them, are well-posed over on-shell configurations only, and this makes the proof of the Jacobi identity a pretty hard task. Morally, the maps defined in (1.2.46) are analogous to the retarded and advanced classical Møller maps given in Definition 1.2.15, hence we expect the Peierls brackets to be equivalent to the Poisson structure

introduced in (1.2.42) when this last one is restricted to on-shell configurations. A proof of this fact may be found in [FR15, Re16], here we limit ourselves to sketch the main steps.

Given a free solution $\phi \in \mathscr{E}_{\mathfrak{S}}$, we name $\phi_{r,G} \doteq \mathrm{r}_{\lambda G}(\phi) \in \mathscr{E}_{\mathfrak{S}+\lambda G^{(1)}}$ and $\phi_{a,F} \doteq \mathrm{a}_{\lambda F}(\phi) \in \mathscr{E}_{\mathfrak{S}+\lambda F^{(1)}}$. Taking the functional derivative of the equations of motion for $\phi_{r,G}$ and $\phi_{a,F}$ respectively, we obtain

$$0 = \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\mathfrak{S}'\left(\phi_{r,G}\right) + \lambda G^{(1)}(\phi_{r,G})\right)\Big|_{\lambda=0} = \mathfrak{P}_{\mathfrak{S}}(\phi)\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\phi_{r,G}\right)\Big|_{\lambda=0} + G^{(1)}(\phi),$$
$$0 = \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\mathfrak{S}'\left(\phi_{a,F}\right) + \lambda F^{(1)}(\phi_{a,F})\right)\Big|_{\lambda=0} = \mathfrak{P}_{\mathfrak{S}}(\phi)\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\phi_{a,F}\right)\Big|_{\lambda=0} + F^{(1)}(\phi).$$

The hypothesis made on $\mathfrak{P}_{\mathfrak{S}}(\phi)$ and the conditions $\phi_{r,G} = \phi$ and $\phi_{a,F} = \phi$ on $J_-(\mathrm{spt}(G))$ and on $J_+(\mathrm{spt}(F))$ respectively, necessarily imply

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\phi_{r/a,V}\right)\Big|_{\lambda=0} = \mathfrak{D}^{R/A}V^{(1)}(\phi).$$

Hence, by direct computation we have

$$\{F,G\}_{\mathrm{Pei}}(\phi) = \left\langle F^{(1)}(\phi), \mathfrak{D}\,G^{(1)}(\phi)\right\rangle \doteq \{F,G\}_{\mathfrak{S}}(\phi), \qquad \forall, \phi \in \mathscr{E}_{\mathfrak{S}}, \quad \forall\, F,G \in \mathscr{F}$$

for $\mathfrak{D} \doteq \mathfrak{D}^A - \mathfrak{D}^R$ and $\mathscr{F}$ being the space of smooth, compactly supported functionals. If $\mathfrak{S}$ coincides with the Klein-Gordon action, we recognise the desired equality with the Poisson brackets defined in equation (1.2.42), which we already know how to extend to kinematical configurations. Concerning the general case, more work must be done, yet it is possible to prove that the extension is possible. Furthermore, this form of the brackets allows to prove the Jacobi identity by direct inspection. We will not go into details, an interested reader can consult [BFR17].

Remark 1.2.4. We stress that the functionals used hitherto are all off-shell, so the functional $\phi \mapsto \langle F^{(1)}(\phi), \mathfrak{D}\,G^{(1)}(\phi)\rangle$ is a well-defined Poisson bracket on the off-shell algebra for all $F,G \in \mathscr{F}_{\mu\mathrm{c}}$, for non-polynomial observables also. In general, unfortunately, it fails to define a Poisson structure if we limit ourselves to $\mathscr{F}_{\mu\mathrm{c}} \cap \mathscr{F}_{\mathrm{pol}}$ due to the fact that the dependence of $\mathfrak{D}$ from ϕ is non-polynomial. Notwithstanding, if we consider a free quadratic action, such as the Klein-Gordon one (see (1.2.36)) and a polynomial local interaction potential $V \in \mathscr{F}_{\mathrm{loc}} \cap \mathscr{F}_{\mathrm{pol}}$, we can consider V as a perturbation and apply the formal power series technology expanding in the coupling constant. With this approach, one deals with polynomial quantities at every order in λ, that is one switches to the space of formal power series with values in the polynomial microcausal functionals, which we denote with $\mathscr{F}_{\mu\mathrm{c}}[\![\lambda]\!]$, see [Re16] for more details.

Locally Covariant Nets of Classical Algebras

As a conclusive remark, we would like to briefly address the question of the axioms for a classical field theory. Even if no quantisation is performed, yet a classical field theory should fit with the principle of relativity, in particular with the finite-speed propagation of physical signals. Indeed, it is possible to formulate an analogue of the Haag-Kastler-Dimock axioms for a classical field theory. To this avail, it is convenient to notice that one could have equivalently formulated the theory limiting to a subregion $\mathbb{O} \subseteq \mathbb{M}$ of the full space-time. The Poisson *-algebra obtained this

way is denoted with $\mathscr{A}_{\mathrm{cls}}(\mathcal{O})$, and its Poisson brackets are denoted by $\{\cdot,\cdot\}_{\mathcal{O}}$. With this language, the axioms of classical scalar field theory are formulated as follows:

Definition 1.2.17 (Axioms of Locally Covariant Classical Field Theory)**.** A classical scalar field over a globally hyperbolic space-time $\mathbb{M}$ is described as a net $\{\mathscr{A}_{\mathrm{cls}}(\mathcal{O}) : \mathcal{O} \subset \mathbb{M}\}$ of unital Poisson *-algebras which satisfies the following properties:

Isotony: To every isometry $i_{12} : \mathcal{O}_1 \to \mathcal{O}_2$, we can associate a unital *-homomorphism $\alpha_{i_{12}} : \mathscr{A}_{\mathrm{cls}}(\mathcal{O}_1) \to \mathscr{A}_{\mathrm{cls}}(\mathcal{O}_2)$ in such a way that, given another isometry $i_{23} : \mathcal{O}_2 \to \mathcal{O}_3$, $\alpha_{i_{23}\circ i_{12}} = \alpha_{i_{23}} \circ \alpha_{i_{12}}$.

Causality: If $\mathcal{O}_1$ and $\mathcal{O}_2$ are spacelike separated, then $\{\mathscr{A}_{\mathrm{cls}}(\mathcal{O}_1), \mathscr{A}_{\mathrm{cls}}(\mathcal{O}_2)\}_{\mathcal{O}_3} = \{0\}$, for any $\mathcal{O}_3$ such that $\mathcal{O}_1, \mathcal{O}_2 \subset \mathcal{O}_3$.

Time-slice Axiom: Let $i_{12} : \mathcal{O}_1 \to \mathcal{O}_2$ and suppose that $i_{12}(\mathcal{O}_1)$ contains a Cauchy surface Σ for $\mathcal{O}_2$. Then the map $\alpha_{i_{12}}$ is surjective and, in particular, it follows that, for every time-slice $\Sigma_\varepsilon \doteq (-\varepsilon, \varepsilon) \times \Sigma$, $\mathscr{A}_{\mathrm{cls}}(\Sigma_\varepsilon) = \mathscr{A}_{\mathrm{cls}}$.

The validity of the axioms for the scalar field theory on curved backgrounds is proven in [Di80].

Notice that, in our case, the full algebra $\mathscr{A}_{\mathrm{cls}} \equiv \mathscr{A}_{\mathrm{cls}}(\mathbb{M})$ can be defined directly, as shown all along the present section. In a more general situation, one has information on the net only: In this case, the isotony axiom allows to get the full algebra as the inductive limit

$$\mathscr{A}_{\mathrm{cls}} \doteq \varinjlim_{\mathcal{O} \nearrow \mathbb{M}} \mathscr{A}_{\mathrm{cls}}(\mathcal{O}). \tag{1.2.48}$$

Remark 1.2.5. We built here a net of off-shell algebras, but one could have equivalently considered the on-shell ones without any drastic change in the construction or in the axioms.

1.3 Quantisation

In this section we will develop the quantisation of the free scalar field on a globally hyperbolic space-time $(\mathbb{M}, g)$. If one looks at the literature, she/he will discover that there are several ways to do so, even restricted to the algebraic quantum world. In particular, there exist many constructionS of the algebras of observables: For instance, one may use a Weyl algebraic approach, as done in [KW91], otherwise it is possible to develop a Borchers-Uhlmann approach (see [BDH13]). The problem with those methods is that they do not allow for taking interactions into consideration because they are on-shell formalisms and they are not explicit enough to describe interactions, so despite being interesting on their own, we will not treat them in this thesis, referring to the literature.

The approach we follow is the functional one, based on *formal deformation quantisation*. The idea behind it is to add quantum corrections to the classical product, so to obtain a non-commutative one which takes into account the canonical commutation relations. The price one has to pay is that the deformation turns the algebra into an algebra of formal power series built over the algebra of microcausal functionals.

1.3.1 Overview

Formal deformation quantisation is one of the most important and well-developed quantisation schemes and it has been applied successfully in both Quantum Mechanics and in Quantum Field Theory. A standard reference where the formalism is developed is [BFFLS78], while some more introductory material may be found, for example, in [Wal02]. In this section we aim to give a general introduction and motivation to the subject, in order to give the reader an idea about the reason why this formalism is well-suited and physically motivated in the study of perturbative quantum field theories.

Formal Power Series

First we would like to spend some words on formal power series and their mathematical description, so to make clear why they are the right tool to rigorously formulate perturbative quantum field theories. The basic idea is that a formal power series is a polynomial of infinite degree, so the way we construct them resembles the definition of polynomials. A good introduction of the algebraic construction and properties can be found in [No69], to which we adhere strictly.
Given a ring R, we build the ring $R[\![\hbar]\!]$ of formal power series on R as the set $R^{\mathbb{N}}$ of infinite sequences of elements of R indexed by the naturals. We denote them with $\{a_j\}$, a_j being the j^{th} term of the sequence. The ring structure on $R^{\mathbb{N}}$ is achieved by defining a sum and a product in the following way:

Addition: $\{a_n\}+\{b_n\} \doteq \{a_n+b_n\}$;

Product: $\{a_n\}\times\{b_n\} \doteq \left\{\sum_{k=0}^{n} a_k b_{n-k}\right\}$,

for any $\{a_n\},\{b_n\} \in R^{\mathbb{N}}$. The reason why we defined the product as the usual Cauchy product between series will be clear soon. The multiplicative ring structure is completed by defining the zero element and the identity:

$$\{0_n\} \doteq (0,0,0,\dots,0\dots) \qquad \{1_n\} \doteq (1,0,0,\dots,0,\dots).$$

Furthermore, we observe that the map $R \ni a_0 \mapsto (a_0,0,0,\dots,0\dots)$ allows to embed R into $R[\![\hbar]\!]$. We now define $\hbar \doteq (0,1,0,\dots,0\dots)$, and we notice that, by definition of the product,

$$\hbar^n = (\underbrace{0,\dots,0}_{n-1},1,0,\dots) \quad \text{and} \quad \hbar^0 = \{1_n\}.$$

With this notation, every sequence with finitely many non-zero terms can be written as a polynomial in $\hbar$, that is

$$\{a_n\} = (a_0,a_1,\dots,a_n,0,\dots) = a_0 + a_1\hbar + \dots + a_n\hbar^n = \sum_{k=0}^{n} a_k\hbar^k$$

where the a_j may as well be zero for some j. Slightly abusing the notation, we denote a generic element $\{a_n\} \in R[\![\hbar]\!]$ as

$$\{a_n\} \doteq \sum_{k=0}^{\infty} a_k\hbar^k.$$

This notation justifies the use of the Cauchy product, in fact the ring operations in the new notation become

$$\{a_n\}+\{b_n\}=\sum_{k=0}^{\infty}a_k\hbar^k+\sum_{k=0}^{\infty}b_k\hbar^k=\sum_{k=0}^{\infty}(a_k+b_k)\hbar^k,$$
$$\{a_n\}\times\{b_n\}=\left(\sum_{k=0}^{\infty}a_k\hbar^k\right)\times\left(\sum_{k=0}^{\infty}b_k\hbar^k\right)=\sum_{k=0}^{\infty}\left(\sum_{j=0}^{k}a_jb_{k-j}\right)\hbar^k.$$

Anyway, we must stress that this notation is purely formal and can not be derived using the operations defined above. Moreover, we do not make any clue concerning the convergence of the series and, in general we do not expect it to happen. In any case, for talking about convergence one needs to have a topology, so the next step would be to define one on $R[\![\hbar]\!]$.

To define a topology, the idea is to stick to what happens in the polynomial case: Let R be a topological ring and let $R[\hbar]$ be the polynomial ring over it. In general, two polynomials are equal if all their coefficients coincide. Given a sequence of polynomials $\left\{P_n=\sum_{j=1}^{N}a_{j,n}\hbar^j\right\}$ in $R[\hbar]$, we say that it converges to a polynomial $P=\sum_{j=1}^{N}a_j\hbar^j$ if $a_{j,n}\overset{n\to\infty}{\longrightarrow}a_j$ for every $j=1,\dots,N$ in the topology of R.
Concerning formal power series $R[\![\hbar]\!]$, the idea is the same. Rigorously speaking, this topology is realized as the R_0-adic topology, where R_0 is the ideal in $R[\![\hbar]\!]$ generated by the sequences $\{a_n\}$ with $a_0\equiv 0$.

Concerning the case of our interest, we take the ring R to be the algebra of polynomial microcausal functionals $\mathscr{F}_{\mu c}$, endowed with the Hörmander topology and we construct the algebra $\mathscr{F}_{\mu c}[\![\hbar]\!]$ with the deformed product, which we are going to define soon. We stress that, from the physical point of view, a formal power series approach is very well-suited, in fact, when doing perturbation theory, it is almost impossible to look at the whole series, but rather physicists are able to make computations at a fixed order, still getting predictions which are in striking accordance with the experimental results. The definition of the star product will motivate the introduction of the formal power series machinery also from a mathematical point of view.

Why Quantisation using Star Products?

Before starting, it is probably good and legitimate to leave small room to philosophy and wonder about the question "what do we mean with quantisation?". Actually, an answer is hard to give. It must be said that the quantisation is a somehow artificial procedure because the classical description of the world must be thought as an approximation, which arises form the more fundamental quantum one.

According to the *correspondence principle*, classical physics must arise as a proper limit out of the quantum description of the system. This is usually encoded in the so-called *classical limit*, which formally allows to recover the classical equations from the quantum one. Very often in the literature this is given by sending the quantisation parameter $\hbar$ to zero. This feature is necessary if we want to experimentally verify the theory. Unfortunately, the (full) understanding of a theory which is fundamentally quantum (still) escapes our knowledge, so we have to be pragmatic and start from the classical world and, afterwards, develop its quantisation. Indeed, this is the

approach followed in this thesis.

Several quantisation schemes have been invented in order to solve the issue, such as the Dirac canonical quantisation, the path integral formulation or the geometric quantisation. Unfortunately, none of them is fully satisfactory, them being or mathematically non-rigorous or too technically involved in order to study non-trivial physical models. Hence, due to the complexity and subtlety of the problem, it is maybe better to make a step back and analyse which features we expect from a satisfactory quantisation scheme, keeping the physical content of the classical limit in mind.

In general, the quantisation amounts to build a quantum (non-commutative) algebra $\mathfrak{A}_{\mathrm{QM}} \equiv \big(\mathfrak{A}_{\mathrm{QM}}, \star, [\cdot,\cdot]_\star\big)$, where $\star$ is the quantum product and $[\cdot,\cdot]_\star$ is the commutator computed with respect to $\star$, out of a Poisson classical (commutative) algebra $\mathfrak{A}_{\mathrm{cls}} \equiv (\mathfrak{A}_{\mathrm{cls}}, \cdot, \{\cdot,\cdot\})$, $\cdot$ being the classical product and $\{\cdot,\cdot\}$ the Poisson bracket. This assignment must satisfy the following requirements, mostly motivated by the classical limit:

- The classical algebra should arise as classical limit of the quantum one, that is $\mathfrak{A}_{\mathrm{QM}} \rightsquigarrow \mathfrak{A}_{\mathrm{cls}}$. This implies that the classical theory must have a reminder of the quantum one, so for instance the algebraic product and the commutator must be preserved in the classical limit, that is
$$\hat{A} \star \hat{B} \rightsquigarrow A \cdot B, \qquad \frac{1}{\mathrm{i}\hbar}\big[\hat{A},\hat{B}\big]_\star \rightsquigarrow \{A,B\}.$$
This discussion motivates *a posteriori* the need of a Poisson structure on the classical algebra, which has to be considered as a "reminiscence" of the quantum non-commutativity. The presence of the factor $(\mathrm{i}\hbar)^{-1}$ is motivated by the reality condition of the Poisson bracket and by dimensional considerations, in fact the quantisation parameter $\hbar$ (which usually corresponds to the Planck constant) is dimensional. This explains why we preferred to avoid the usual notation $\hbar \to 0$ for the classical limit.

- Since we expect the classical observables to arise as classical limits of the quantum ones, the quantum algebra should be at least as big as the classical one. In particular, every classical observable should descend as classical limit of a quantum one.

- Accordingly, we expect also that every classical state can be obtained as classical limit of a state over the quantum algebra. Anyway, the notion of classical limit for states is delicate and we prefer not to enter the details of the question.

- The non-commutativity property of the quantum algebra is governed by the Planck constant, so the size of this effect can not be arbitrarily big and uncontrolled. This idea is supported by the fact that one needs quite accurate instruments to physically detect the quantum aspects of nature. Of course, since the Planck constant is dimensional, talking about size means to compare quantities with the same dimension. By the way, we must also stress the fact that quantum corrections are to all extents significant in various physical situations and are fundamental in the explanations of a huge number of phenomena, such as radiation or the stability of matter.

All these requirements lead to the idea of quantising the classical algebra by deforming the classical product to a non-commutative one in such a way which keeps into account the canonical commutation relations. The corrections are seen as a perturbative series in the quantisation parameter, but those series hardly converge, so that formal power series are naturally involved. In general, given a Poisson manifold M, the algebra of classical observables is given by $C^\infty(M)$. Following [BFFLS78], the deformed product is defined as:

Definition 1.3.1 (Star Product)**.** A star product for the Poisson manifold M is an associative product $\star$ defined on the algebra of formal power series $C^\infty(M)[\![\hbar]\!]$ given by

$$f \star g \doteq \sum_{k=0}^{\infty} \hbar^k C_k(f,g) \tag{1.3.49}$$

satisfying the following properties:

1. $C_0(f,g) = f \cdot g$;
2. $C_1(f,g) - C_1(g,f) = \mathrm{i}\{f,g\}$;
3. $C_k(1,f) = C_k(f,1) = 0$ for all f and all $k \geq 1$;
4. $C_k(f,g)$ is a bi-differential operator.

The product is called Hermitian if, in addition,

$$\overline{f \star g} = \bar{g} \star \bar{f}.$$

Condition (1) amounts to the fact that there are no quantum corrections at the zeroth order, while the second guarantees the correct relation between the quantum commutator and the Poisson structure. The associativity of the product has to be checked order by order in $\hbar$, which here has to be considered more as a formal parameter than as the Planck constant itself. At the level of the C_k's the associativity requires that

$$\sum_{k=0}^{n} C_k(f, C_{n-k}(g,h)) = \sum_{k=0}^{n} C_k(C_{n-k}(f,g),h) \quad \forall\, f,g,h \in C^\infty(M),\ \forall\, n \in \mathbb{N}.$$

Now the natural question of existence and uniqueness of $\star$ product on a generic Poisson manifold M arises. The existence problem was solved by Kontsevich in [Kon03], who proved it for finite-dimensional Poisson manifolds. The uniqueness is even more tricky and requires additional work. In particular, it is useful to define a notion of equivalence between star products. This is motivated, for instance, by the simple case of $M \equiv \mathbb{R}^2$ where it is possible to define two star products (by standard ordering or Weyl ordering, see [Wal02]), which, in the end, turn out to result in the same physical theory.

Definition 1.3.2. Given two star products $\star$, $\star'$ over $C^\infty(M)$, we say that they are equivalent if there is a formal power series

$$\Gamma = \mathrm{Id} + \sum_{k=1}^{\infty} \Gamma_k \hbar^k$$

of differential operators Γ_k such that

$$f \star' g = \Gamma^{-1}(\Gamma f \star \Gamma g) \quad \text{and} \quad \Gamma 1 = 1.$$

Γ is called an equivalence transformation. Furthermore, if $\star, \star'$ are Hermitian, then we require also that $\overline{\Gamma f} = \Gamma \overline{f}$.

So it is clear that, in general, the $\star$ products are not unique, but still one may ask itself wether there is at least a classification of them up to equivalence. The answer is affirmative, and it turns out that the classification is related to some geometric properties of the underlying Poisson manifold M, see [Kon03]. Unfortunately, working with equivalence classes is not enough from the physical point of view since one would like to look at a particular model, which should correspond to one product only. Unfortunately, there is no general solution to this issue and a physical choice of a representative among an equivalence class must be done case by case. We do not linger on this aspect any longer, in order to address the question in the particular case of the deformation quantisation of the scalar field.

1.3.2 Deformation quantisation of $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$

The classical algebra of observables of a scalar field theory $\mathscr{A}_{\mathrm{cls}}$ defined in Definition 1.2.8, endowed with the Poisson structure defined in (1.2.47) fits perfectly in the framework required for developing formal deformation quantisation. The use of polynomial functionals only allows us to work with polynomials with value in $\mathscr{A}_{\mathrm{cls}}$, so avoiding the use of formal power series. That is, we will limit ourselves to deal with the polynomial algebra $\mathscr{A}_{\mathrm{cls}}[\hbar] \hookrightarrow \mathscr{A}_{\mathrm{cls}}[\![\hbar]\!]$[9].

The deformation quantisation of the free scalar field was first performed in [DF01a, DF01b, DF04, Dit90]. The first step consists in the quantisation of the algebra of regular functionals $\mathscr{A}_{\mathrm{cls,reg}}$ by defining the following star product

$$(F \star G)(\phi) \doteq (F \cdot G)(\phi) + \sum_{n=1}^{\infty} \frac{\hbar^n}{n!} \left\langle F^{(n)}(\phi), \left(\frac{\mathrm{i}}{2}\Delta\right)^{\otimes^n} G^{(n)}(\phi) \right\rangle \qquad \forall F, G \in \mathscr{F}_{\mathrm{reg}}[\![\hbar]\!], \tag{1.3.50}$$

where Δ is the causal propagator associated with the free Klein-Gordon equation. Notice that the pairing is well-posed due to the smooth microlocal behaviour of the regular functionals. Furthermore, notice that the series in the right hand side is indeed a finite sum due to the polynomial nature of the functionals. In order to check the associativity, it is helpful to rewrite the product in the form:

$$F \star G \equiv \mathbf{m} \circ e^{\Gamma}(F \otimes G).$$

Here $\otimes$ stands for the tensor product between functionals, $(F \otimes G)(\phi_1, \phi_2) \doteq F(\phi_1)G(\phi_2)$. We have defined also the following operators:

$$\mathbf{m}(F \otimes G)(\phi) \doteq (F \cdot G)(\phi) \tag{1.3.51}$$

$$\Gamma(F \otimes G)(\phi_1, \phi_2) \doteq \frac{\mathrm{i}\hbar}{2} \left\langle F^{(1)}(\phi_1), \Delta G^{(1)}(\phi_2) \right\rangle. \tag{1.3.52}$$

[9] Even if we will work with polynomials only, we prefer to keep the formal power series notation for uniformity with the rest of the literature. Furthermore, when interactions will be taken into account, the obtained functionals will not be polynomial anymore.

Hence it holds that

$$\mathbf{m}\circ\Gamma(F\otimes G)(\phi)=\frac{\mathrm{i}\hbar}{2}\left\langle F^{(1)}(\phi),\Delta G^{(1)}(\phi)\right\rangle. \tag{1.3.53}$$

We also extend the definition of Γ to the generic n-tensor product as

$$\Gamma_{ij}(F_1\otimes\cdots\otimes F_n)\doteq\frac{\mathrm{i}\hbar}{2}\left\langle F_i^{(1)},\Delta F_j^{(1)}\right\rangle\prod_{\substack{k=1\\k\neq i,j}}^{n}F_k. \tag{1.3.54}$$

The associativity can then be checked by direct inspection, making use of the Leibniz rule. We also verify that the $\star$ product we defined respects the criteria introduced in the previous section by explicitly showing how it is related to the Canonical Commutation Relations and how the Poisson structure naturally corresponds to the commutator. To do so, we limit ourselves to consider linear functionals:

$$\left[F_f,F_g\right]_\star\doteq F_f\star F_g-F_g\star F_f=\mathrm{i}\hbar\Delta(f,g)\mathbb{1}. \tag{1.3.55}$$

Definition 1.3.3. The quantum, off-shell algebra of regular observables for a real, massive scalar field theory is the topological *-algebra defined by $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]\doteq\left(\mathscr{F}_{\mathrm{reg}}[\![\hbar]\!],\star,^*\right)$, where $\mathscr{F}_{\mathrm{reg}}$ is the set of polynomial regular observables, $\star$ is defined in (1.3.50) and * is the complex conjugation.

In order to obtain the on-shell algebra, we repeat what we did for the classical theory, namely we consider the two-sided *-ideal $\mathscr{I}_{\mathrm{reg,KG}}\subset\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ generated by the linear functionals of the form F_{Pf} and completed in the Hörmander topology. Then we define the *quantum on-shell algebra of observables* as

$$\mathscr{A}_{\mathrm{reg,KG}}[\![\hbar]\!]\doteq\frac{\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]}{\mathscr{I}_{\mathrm{reg,KG}}}.$$

In the classical theory there were no need of taking a two-sided ideal since the algebra was commutative, but in the quantum case this property is strictly needed in order to get a well-defined quotient. As already said before, in order to give an effective definition of time-ordered product, we must work in the off-shell formalism, so we will consider the algebra $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ only.

Unfortunately, the algebra $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ is not rich enough to describe a scalar field since, as already pointed out, most of the physically interesting observables are characterised by a singular behaviour. At the same time, the $\star$ product defined in (1.3.50) can not be used to quantise the algebra $\mathscr{A}_{\mathrm{cls}}$ because the pairing between the causal propagator and microcausal functionals is in general ill-defined. To solve this issue, we have to extend the algebra of observables, and this requires a discussion about the states of the algebra.

1.3.3 States in pAQFT

In this section we discuss states defined on the quantum algebra $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$. We have already seen in the Introduction that states are positive, normalised and linear functionals over the algebra. Since in the present framework we are dealing with formal power series, some clarifications are necessary.

The definition of states over an algebra of formal power series does not depend on the singular structure of the functionals under consideration and it is not strictly related to the algebra $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$, so, for the sake of generality, we formulate it for a general algebra $\mathscr{A}[\![\hbar]\!]$:

Definition 1.3.4. A state on $\mathscr{A}[\![\hbar]\!]$ is a linear functional $\omega : \mathscr{A}[\![\hbar]\!] \to \mathbb{C}[\![\hbar]\!]$ which is:

Normalized: $\omega(\mathbb{1}) = \{1_n\}_{n\in\mathbb{N}}$;

Positive: Given $A \in \mathscr{A}[\![\hbar]\!]$, we say that ω is positive if there exists $k \in \mathbb{N}$ such that

$$\omega\left(A \star A^*\right) = \sum_{j=0}^{\infty} \hbar^j a_j \quad \Rightarrow \quad a_j \in \mathbb{R} \text{ for all } j \text{ and } a_j = 0 \text{ for all } j < k \text{ and } a_k > 0.$$

It is easy to see that every state ω on $\mathscr{A}$ induces a state $\omega[\![\hbar]\!]$ on $\mathscr{A}[\![\hbar]\!]$ which can be expressed as

$$\omega[\![\hbar]\!](A) = \sum_{j=0}^{\infty} \hbar^j \omega\left(A_j\right),$$

where $A = \left\{A_j\right\}_{j\in\mathbb{N}}$. Roughly speaking, we can obtain states on an algebra of formal power series $\mathscr{A}[\![\hbar]\!]$ starting from states on the initial algebra $\mathscr{A}$. In the rest of the present thesis, we will always consider such states. This definition is satisfactory also from the point of view of the GNS representation. Despite its conceptual importance, this aspect is of little interests for the purposes of the present work, hence for details and definitions we refer an interested reader to [Wal05].

Now, we return to the main topic of states on $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$. This algebra is generated by linear functionals, hence a state ω on $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ is completely characterised by its n-point functions, defined by

$$\omega_n(f_1,\dots,f_n) \doteq \omega\left(F_{f_1} \star \cdots \star F_{f_n}\right) \qquad \forall F_{f_1},\dots,F_{f_n} \in \mathscr{F}_{\mathrm{lin}}. \tag{1.3.56}$$

Due to the continuity of ω in the topology induced by the topology of $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$, the n-point functions are n-distributions $\omega_n \in \mathscr{D}'(\mathbb{M}^n, \mathbb{C})$ for all $n \in \mathbb{N}$. Some additional requirements are put on the n-point functions due to the positivity of the states and on the implementation of the canonical commutation relations.

Giving conditions on the n-point functions, it is possible to select a particularly interesting class of states, namely the so-called *quasi-free states*. Roughly speaking, a quasi-free state is characterised by its 2-point function only, in particular it has vanishing $(2n+1)$-point functions for all $n \in \mathbb{N}$, while every even-point function is factorised in terms of the 2-point function. This definition can be made precise by introducing the *connected functions*. Again, this works for a generic algebra $\mathscr{A}[\![\hbar]\!]$ of formal power series.

Definition 1.3.5. A state ω on a formal power series algebra $\mathscr{A}[\![\hbar]\!]$, admits a decomposition in terms of connected correlation functions given by:

$$\omega(F_1 \star \ldots \star F_n) \doteq \sum_{P\in\mathscr{P}} \prod_{J\in P} \omega^c_{|J|}\left(\bigotimes_{j\in I} F_j\right) \qquad \forall F_1,\dots,F_n \in \mathscr{A}[\![\hbar]\!], \tag{1.3.57}$$

where $\mathscr{P}$ is the set of partitions of $\{1,\dots,n\}$ into non-empty, pairwise disjoint subsets.
If we specialize to $\mathscr{A}[\![\hbar]\!] \equiv \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$, we define the truncated n-point functions of ω as multilinear maps $\omega^T_n : \mathscr{D}(\mathbb{M},\mathbb{C})^{\otimes^n} \to \mathbb{C}$ given by

$$\omega^T_n(f_1 \otimes \cdots \otimes f_n) \doteq \omega^c_n\left(F_{f_1} \otimes \cdots \otimes F_{f_n}\right) \qquad \forall F_{f_1},\dots,F_{f_n} \in \mathscr{F}_{\mathrm{lin}},\ \forall n \in \mathbb{N}.$$

We say that ω is quasi-free (or Gaussian) if $\omega^T_n \equiv 0$ for all $n \neq 2$.

As we will see later, most of the physically significant states are quasi-free, such as the vacuum or the KMS ones. In general, those kind of states are interesting for physical applications because their associated GNS representation is of Fock type [KW91, KM15]. This motivates the fact that, in what follows, we will mainly use Gaussian states.

Indeed, the quasi-free condition is not enough for selecting reasonable physical states, that is states that allows for the definition of expectation values of physically relevant observables, such as the ϕ^2 or the stress-energy tensor. Traditionally, the problem was formulated as follows [Wa94]: A quantum field ϕ is modeled as an operator-valued distribution, so in order to define, say, the expectation value of the ϕ^2 observable, one should multiply two distributions, and this operation is in general ill-defined. There are two possible solutions then: The first is to enlarge the algebra of observables so to include the physically-relevant observables, while the second consists in limiting ourselves to define expectation values. In particular, in this thesis we will stick to the first approach, in which the relevant observables are considered as generators of the algebra and are constructed using a deformed product. Anyway, as we will see, the two approaches are compatible, namely we will obtain the same quantities at the end of the construction. Historically, the second way has been initially followed, so we will take this one as a starting point for our discussion, also due to the fact that it gave important insights in the development of the first, more algebraic approach.

Defining expectation values of physical observables such as Wick polynomials means to give sense to limits of the following type:

$$\text{“}\langle\phi^2(x)\rangle = \lim_{x\to y}\langle\phi(x)\phi(y)\rangle\text{”}.$$

Unfortunately, such quantities are usually pathological since the bi-distributions like $\langle\phi(x)\phi(y)\rangle$ blow up in the coincident-points limit, therefore a regularisation procedure is required. In traditional QFT on Minkowski space-time, the regularisation issue is solved by the normal ordering [PS95], which amounts to recognise that the singular part in the coincidence limit $x \to y$ is given by the vacuum expectation value, which then is subtracted, so that leading to

$$\text{“}\langle\phi^2(x)\rangle = \lim_{x\to y}\left[\langle\phi(x)\phi(y)\rangle - \langle 0\,|\,\phi(x)\phi(y)0\rangle\right]\text{”}.$$

Unluckily, this procedure does not generalise to every curved background for several reasons, one for all the absence of a preferred notion of a vacuum state. So a more general procedure is needed. Heuristically, one can notice that the troubles arise in the ultraviolet regime (*i.e.* in the coincident-point limit, or in other words for high momenta), so that the evaluation on the state amounts to make a measurement in a small region of the space-time. Since every small region of a space-time is diffeomorphic to Minkowski, one expects that a good physical state should possess the same behaviour (in the UV regime) of the Minkowski vacuum. Moreover, we have to require that such a state grants finite fluctuations to the expectation value of the Wick powers of fields and of their derivatives. It is clear now how this condition on states will play a prominent role in the sought extension of the algebra of observables, which exactly amounts for the inclusion of Wick polynomials.

The idea then is to subtract a suitable local bi-distribution $H(x,y)$ possessing the sought singularity structure in the limit $x \to y$. The construction of such distributions amounts to an problem of finding the *Hadamard parametrix* for the free Klein-Gordon equation (1.2.14). The method was found by Hadamard in 1923 [Had23] in order to prove existence and uniqueness of solution for elliptic and hyperbolic equations, and, for the relevant case, can be found in [BGP07, Fri75]. We avoid here the explicit construction due to its length and its highly-technical nature, limiting ourselves to give an overview on the main results.

Let $\mathcal{O} \subset \mathbb{M}$ be a geodesically complete neighbourhood and let $\ell > 0$ be a fixed length scale: Given any $x, y \in \mathcal{O}$, the Hadamard parametrix $H_\ell(x,y)$ is defined as

$$H_\ell(x,y) \doteq \frac{u(x,y)}{(2\pi)^2\,\sigma(x,y)} + v(x,y)\log\left(\frac{\sigma(x,y)}{\ell^2}\right), \tag{1.3.58}$$

where $v(x,y) \doteq \sum_{j=0}^{\infty} v_j(x,y)\frac{\sigma(x,y)^j}{\ell^j}$ and $\sigma(x,y)$ is half the squared geodesic distance (the so-called *Synge's function*), given by

$$\sigma(x,y) \doteq \frac{1}{2} g\left(\exp_x^{-1}(x), \exp_x^{-1}(y)\right),$$

$\exp_x : \mathrm{T}_x M \to M$ being the exponential map defined on the space-time $\mathbb{M} \equiv (M,g)$. The Hadamard parametrices are formal power series, since the convergence in v is in general not granted. Anyway, the functions u, v_j, called *Hadamard coefficients*, are uniquely determined by requiring H_ℓ to be a formal bi-solution of the free Klein-Gordon equation and it can be shown that the series converges at least for analytic space-times. Indeed, to reach our goal, it is enough to regularise v [HW01], for instance by taking

$$v_{\chi,\theta} \doteq \sum_{j=0}^{\infty} v_j\, \chi\left(\frac{\sigma}{\ell\theta_j}\right)^j,$$

where $\chi \in \mathscr{D}$ such that $\mathrm{spt}(\chi) = [-1,1]$, with $\chi(x) = 1$ for $|x| < 1/2$ and $\theta_j \in \mathbb{R}$ for all j define a sequence which converges to 0 fast enough as $j \to \infty$. So, by inserting $v_{\chi,\theta}$ in (1.3.58) we obtain a modified Hadamard parametrix $H_\ell[\chi,\theta]$ which is convergent and solves the free Klein-Gordon equation up to smooth terms.

In order to use the modified Hadamard parametrices to regularise expectation values of observables, we need to work a bit more and regularise the inverse of the Synge's function too, since the coincidence limit $x \to y$ would necessarily lead to singularities. To do so, we define a *time function* $T : \mathbb{M} \to \mathbb{R}$ such that its gradient is everywhere past-directed. Due to Bernal-Sanchez Theorem 1.1.1, the level sets of a time function are given by Cauchy surfaces. For any time function T and real $\epsilon > 0$, we define an ϵ-regularised Synge's function as

$$\sigma_\epsilon(x,y) \doteq \sigma(x,y) + 2\mathrm{i}\epsilon\,(T(x) - T(y)) + \epsilon^2. \tag{1.3.59}$$

Substituting σ with σ_ϵ in (1.3.58), we get to the modified Hadamard parametrix $H_\ell\left[\epsilon,\chi,\theta\right]$, which now can be used to define a bi-distribution $H_\ell\left[0,\chi,\theta\right] \in \mathscr{D}'(\mathcal{O}\times\mathcal{O},\mathbb{C})$ as

$$H_{0,\ell}(f,g) \doteq \lim_{\epsilon \searrow 0} \left\langle f, H_\ell\left[\epsilon,\chi,\theta\right] g\right\rangle \qquad \forall\, f,g \in \mathscr{D}(\mathcal{O},\mathbb{C}).$$

The bi-distribution $H_{0,\ell}$ then is the natural candidate to play the role of the vacuum expectation value in Minkoski space-time, so we have the following definition:

Definition 1.3.6 (Local Hadamard Form)**.** Let T be a time function on M and $\ell > 0$ be a fixed length scale. We say that $u \in \mathscr{D}'(\mathbb{M}^2, \mathbb{C})$ is of local Hadamard form if for any $p \in \mathbb{M}$ there exist a geodesically convex neighbourhood $\mathbb{O}$ and a smooth function $w \in \mathscr{E}(\mathbb{O} \times \mathbb{O}, \mathbb{C})$ such that

$$\big[u(x,y) - H_{0,\ell}(x,y)\big] = w(x,y) \qquad \forall\, x, y \in \mathbb{O}, \tag{1.3.60}$$

where $H_{0,\ell}(x,y)$ is the integral kernel of $H_{0,\ell}$.

The idea then is to implement the normal ordering by subtracting a suitable Hadamard parametrix, so the expectation value of a physical observable of a scalar field theory on a globally hyperbolic space-time is defined as

$$\big\langle \phi^2(x) \big\rangle = \lim_{x \to y} \big[\big\langle \phi(x)\phi(y) \big\rangle - H_{0,\ell}(x,y) \big] .$$

Actually, the whole procedure iterated hitherto can be used to give meaning to expectation values containing derivatives of the fields, such as the stress-energy tensor, see for instance [HW05, Mo03, Wa94].

This characterisation leads naturally to a mathematical definition of physical state: We said before that quasi-free states are completely characterised by their 2-point function, which indeed is a bi-distribution. Therefore we ask the physical states to have a 2-point function which is of local Hadamard form, as per the following definition:

Definition 1.3.7. A quasi-free state ω on $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ satisfies the local Hadamard condition if ω_2 is of local Hadamard form, as per Definition 1.3.6.

Remark 1.3.1. Roughly speaking, the local Hadamard condition tells us that locally every physical state shares the same singular behaviour, which is the one prescribed by the Hadamard parametrix. In particular, every 2-point function of a physical state is equal to H_ℓ up to smooth terms.

Remark 1.3.2. The definition of a 2-point function of a physical state is not affected by the choice of the regularisations χ and θ or by the choice of the time function T. This is due to the fact that the difference

$$H_\ell[\chi,\theta](x,y) - H_\ell[\chi',\theta'](x,y)$$

is a smooth function for every $\ell, \ell' > 0$ and for every possible choice of χ', θ' fulfilling the same hypotheses of χ, θ. This implies also that ω_2 is insensitive to the choice of the length scale ℓ.

In [KW91], in order to characterise physical states, a different, but strictly related requirement is introduced, which goes under the name of *global Hadamard condition*, see [KW91, Ra96a, Ra96b]. To define it, we need the notion of causal normal neighbourhood $\mathbb{O} \subset \mathbb{M}$ of a Cauchy surface Σ, which means that $\mathbb{O}$, considered as a space-time on its own, admits Σ as a Cauchy surface and that, given any $x, y \in \mathbb{O}$ such that $x \in J_+(y)$, there exists a convex normal neighbourhood containing $J_-(x) \cap J_+(y)$. It can be shown that every Cauchy surface Σ of every globally hyperbolic space-time $\mathbb{M}$ admits a causal normal neighbourhood and it can be covered by a countable number of them, see [KW91, Ra96a]. Then the global Hadamard condition asks the local Hadamard one to

hold in any causal normal neighbourhood $\mathbb{O}$ of a Cauchy surface in such a way that no additional singularities appear in ω_2 but the one originating from the local Hadamard condition. The global nature of the condition derives from the fact that one can glue the Hadamard functions defined on every neighbourhood. Thanks to the theorem of propagation of singularities (Proposition 1.2.1), it is possible to show that a bi-distribution satisfying the global Hadamard condition on $\mathbb{O}$ is a bi-solution of the free Klein-Gordon equation satisfying the same condition on every causal normal neighbourhoods of any Cauchy surfaces of $\mathbb{M}$. In addition, the global Hadamard condition ensure the bi-distribution to be positive up to smooth functions.

Up to now, we successfully selected a class of states which allows to give meaning to most of the more relevant physical observables starting from the regular ones. Unfortunately, in practice it may be hard to verify both the local and the global Hadamard conditions, hence it would be nice to have a more explicit characterisation. A breakthrough in this direction came from the work of Radzikowski [Ra96a, Ra96b], where the two conditions are shown to be equivalent to a third one, formulated in terms of the microlocal behaviour of the 2-point function. This is the well-known *microlocal spectrum condition* (μSC), which selects the correct singular behaviour of a physical state in terms of a restriction on the wave-front set of its 2-point function. This condition arises as a generalisation of the positive spectrum condition which characterises the Minkowski vacuum, which has no direct counterpart on a generic curved background. Actually, the μSC is the real reason which motivates the introduction of the microlocal description of the functionals given in Section 1.2.2, see [BFK95].

From the former discussion about the definition of Wick polynomials, we argue that for any physical state ω for a scalar field in Minkowski space-time, $\omega_2 - \omega_2^{\text{vac}} \in \mathscr{E}\left(\mathbb{M}^2\right)$, where ω^{vac} is the vacuum state. Due to the properties of the wave-front set introduced in Subsection 1.2.2, we get that

$$\mathrm{WF}\left(\omega_2 - \omega_2^{\text{vac}}\right) = \emptyset \quad \Rightarrow \quad \mathrm{WF}(\omega_2) = \mathrm{WF}\left(\omega_2^{\text{vac}}\right).$$

It can be shown (see [Fe08, Section 6] for example) that the 2-point function of the Minkowski vacuum satisfies

$$\mathrm{WF}\left(\omega_2^{\text{vac}}\right) \subseteq \mathscr{N}_+ \times \mathscr{N}_-, \tag{1.3.61}$$

where we have defined

$$\mathscr{N}_+ \doteq \left\{(x,k) \in \mathrm{T}^*\mathbb{M} \,|\, k \rhd 0\right\} \quad \text{and} \quad \mathscr{N}_- \doteq \left\{(x,k) \in \mathrm{T}^*\mathbb{M} \,|\, k \lhd 0\right\}.$$

Following the rule of thumb that a state on a curved background should maintain the short-distances singular behaviour of the Minkowski vacuum, we promote equation (1.3.61) to a general requirement to be put on the 2-point function of a general state ω. This requirement states that the singular behaviour of the 2-point function of a physical state is positive-frequency in the first entry and negative-energy in the second one, so the present condition generalises the positive spectrum condition[10] proper of ω^{vac}.

[10] Recall that this condition heavily relies on the invariance under Poincaré transformations proper of Minkowski space, which is no more available on a generic space-time.

The present condition seems unsatisfactory at first glance, since what we really need in order to define Wick polynomials is a condition granting that the difference of between two 2-point functions is a smooth function. Indeed, the issue have been solved in [Ra96a]:

Proposition 1.3.1. *Given two states ω, ω' whose 2-point functions obey the condition* (1.3.61)*, then* $\omega_2 - \omega_2' \in \mathscr{E}\left(\mathbb{M}^2\right)$.

This result in fact states that the condition (1.3.61) defines an equivalence class of 2-point functions modulo smooth terms. Moreover, it implies that every 2-point function of a physical state has the same wave-front set. This observation allows for a refinement of the condition (1.3.61). First, we notice that the CCR (1.3.55) put a constraint on the antisymmetric part on the 2-point function, namely, given two linear functionals $F_f, F_g \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$:

$$\omega\left(\left[F_f, F_g\right]_\star\right) = \omega\left(F_f \star F_g\right) - \omega\left(F_g \star F_f\right) = \omega_2(f,g) - \omega_2(g,f),$$

but $\left[F_f, F_g\right]_\star = \mathrm{i}\hbar\Delta(f,g)\mathbb{1}$, $\mathbb{1}$ being the identity in $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$, so we obtain

$$\omega_2(f,g) - \omega_2(g,f) = \mathrm{i}\hbar\Delta(f,g) \qquad \forall\, f,g \in \mathscr{D}(\mathbb{M},\mathbb{C}). \tag{1.3.62}$$

This observation leads directly to the following result:

Proposition 1.3.2. *For a state ω fulfilling the condition* (1.3.61)*, we have that*

$$\mathrm{WF}(\omega_2) = \mathrm{WF}(\Delta) \cap (\mathscr{N}_+ \times \mathscr{N}_-). \tag{1.3.63}$$

Proof. Let us define $\omega'(x,y) \doteq \omega(y,x)$, so that $\mathrm{WF}(\omega_2') \subseteq \mathscr{N}_- \times \mathscr{N}_+$ by (1.3.61). Due to the commutation relations (1.3.62) and to the properties of the wave-front set of the linear combination of two distributions (1.2.27), we have

$$\mathrm{WF}(\Delta) \subset \mathrm{WF}(\omega_2) \cup \mathrm{WF}\left(\omega_2'\right) \subset \mathrm{WF}\left(\omega_2'\right) \cup \mathrm{WF}(\Delta).$$

Using equation (1.3.61) again, we have

$$\mathrm{WF}(\Delta) \subset \mathrm{WF}(\omega_2) \cup (\mathscr{N}_- \times \mathscr{N}_+) \subset (\mathscr{N}_- \times \mathscr{N}_+) \cup \mathrm{WF}(\Delta).$$

The thesis follows by taking the intersection with $\mathscr{N}_+ \times \mathscr{N}_-$, and observing that $(\mathscr{N}_+ \times \mathscr{N}_-) \cap (\mathscr{N}_- \times \mathscr{N}_+)$ consists of the zero section only. □

Actually, the wave-front set for the causal propagator of the free Klein-Gordon equation has been computed in [DH72], so we arrive at a final form for the microlocal spectrum condition, which is the one introduced in [Ra96a].

Definition 1.3.8 (Microlocal Spectrum Condition)**.** A distribution $u \in \mathscr{D}'(\mathbb{M}^2,\mathbb{C})$ satisfies the microlocal spectrum condition (μSC) if

$$\mathrm{WF}(u) \doteq \left\{\left(x,k_x;y,-k_y\right) \in \mathrm{T}^*\mathbb{M}^2 \setminus \{0\} \,|\, (x,k_x) \sim (y,k_y),\, k_x \rhd 0\right\}, \tag{1.3.64}$$

where $(x,k_x) \sim (y,k_y)$ means that there exists a lightlike geodesics connecting x and y with tangent covector k_x at x and such that k_y is the co-parallel transported of k_x at y.
We will say that a state ω satisfies the microlocal spectrum condition if its 2-point function does.

Actually, Radzikowski managed to do more, in particular he proved in [Ra96a, Ra96b] that the μSC is indeed equivalent to the Hadamard condition.

Theorem 1.3.1 (Radzikowski)**.** *If $\omega \in \mathscr{D}'\left(\mathbb{M}^2, \mathbb{C}\right)$ solves the free Klein-Gordon equation up to smooth terms and if its antisymmetric part satisfies equation* (1.3.62)*, then the following conditions are equivalent:*

- *ω satisfies the local Hadamard condition;*
- *ω satisfies the global Hadamard condition;*
- *ω satisfies the microlocal spectrum condition.*

Thanks to Proposition 1.2.1, it is possible to see that if the μSC holds on a geodesically convex neighbourhood of a Cauchy surface Σ, then it holds on all $\mathbb{M}$.

This equivalence theorem finally selects the physically interesting states for a QFT on a globally-hyperbolic space-time, which are customarily called *Hadamard states*.

Definition 1.3.9 (Hadamard State)**.** We say that a quasi-free state ω is Hadamard if its 2-point function satisfies the hypothesis of Theorem 1.3.1 plus one of the equivalent conditions there stated.

We have discussed the regularity requirement only for the 2-point function, but originally, in [BFK95], the μSC was defined as a condition on the wave-front set of the generic n-point function, and there the authors proved that such a condition is met by all quasi-free Hadamard states. Later on, in [San10], it has been shown that this condition is equivalent to the one we have stated. Furthermore, the author showed that every Hadamard state has smooth truncated n-point functions.

More precisely, the generalisation of the μSC to non-Gaussian states goes as follows [San10]: Consider a graph G_n with n vertices and finitely many edges. We say that G_n is immersed in $\mathbb{M}$ if to every vertex v_i corresponds a point $x_i \in \mathbb{M}$, for every edge connecting v_i and v_j there exists a piecewise smooth curve γ_{ij} linking x_i and x_j and if we may find a causal, future-directed co-vector ξ_{ij} on γ_{ij} which is covariantly constant along γ_{ij} itself.

Moreover, we say that a vector $(x_1, k_1; \ldots; x_n, k_n) \in \mathrm{T}^*\mathbb{M}^n \setminus \{0\}$ is instantiated by an immersion of G if and only if the immersion sends every vertex v_i, $i = 1, \ldots, n$, to one of the x_i and if

$$k_i = \sum_{\substack{i \to j \\ j > i}} \xi_{ij}(x_i) - \sum_{\substack{j \to i \\ j < i}} \xi_{ij}(x_i)$$

where the notation $\sum_{i \to j}$ means that the sums run over the edges (or the corresponding curves) joining v_i and v_j. This condition on k_i has to be understood as a singularity propagating from x_i to x_j, so it is natural to define a set encoding the singular behaviour allowed for the n-point function of a distribution as

$$\Xi_n \doteq \left\{(x_1, k_1; \ldots; x_n, k_n) \in \mathrm{T}^*\mathbb{M}^n \setminus \{0\} \,|\, \exists G_n \text{ which instantiates } (x_1, k_1; \ldots; x_n, k_n)\right\}.$$

Definition 1.3.10. A state ω satisfies the μSC with smooth immersions if $\mathrm{WF}(\omega_n) \subset \Xi_n$ for all $n \in \mathbb{N}$. In particular, ω is called a generalised Hadamard state if $\mathrm{WF}(\omega_2) \subset \Xi_2$.

Notice that the previous definition does not require ω to be Gaussian, hence it represents an extension of Definition 1.3.8. The equivalence of the two, together with some more details about this more general definition can be found in the original paper [San10].

To conclude this short analysis of states, we would like to briefly discuss the existence of Hadamard states and to provide some examples, so to justify the μSC also from a "practical" point of view. Due to the large extent of this subject, we will not enter too much in details of the constructions, limiting ourselves to present the examples needed for the present work, giving frequent references to the literature.

The problem of existence of Hadamard states was first addressed in [FNW81], with the introduction of the so-called *deformation argument*: Roughly speaking, any globally hyperbolic space-time $\mathbb{M}$ can be deformed in the past of any Cauchy surface in such a way to contain a causal normal neighbourhood of a Cauchy surface of an ultrastatic space-time, where Hadamard states are known to exist [Fu89]. Later on, several techniques and constructions have been developed in order to study Hadamard states for different curved space-times and different theories, some (not all) examples can be found in [DMP09, DMP11, FV13, GW14, GW16, SV00, San13, San15]. Furthermore, there are attempts to extend the Hadamard condition to non-globally hyperbolic backgrounds, for instance considering space-times with boundaries, see for instance [BDFK17, DFJ18, DNP16, Wr17]. Originally, the idea of considering non globally hyperbolic space-times was started by Kay, who introduced the notion of F-locality [Ka92].

In order to provide examples of states, we reduce to the case of a free, massive scalar field on Minkowski space-time. This simplification is not strictly necessary, but this will be the relevant case for this thesis, so it is more convenient to stick with it.

The first, and most simple example of state on $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ is given by the *evaluation functionals*, which are defined as follows

$$\mathrm{Ev}_\phi(F) \doteq F(\phi) \qquad \forall F \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!], \tag{1.3.65}$$

where ϕ is a solution to the equation of motion. Indeed, these states have to be considered as the ones corresponding to classical states.

The next examples we want to introduce are the *vacuum state* and the (free), extremal *KMS state*. They can be defined in a generic ultrastatic space-time also because their definition requires the existence of a one-parameter group of time translations, which in the case of Minkowski is given by the Poincaré translation of the x_0 coordinate. At the level of field configurations, this is defined as $\phi_t(x_0,\mathbf{x}) \doteq \phi(x_0+t,\mathbf{x})$, and it can be transposed at the level of functionals, so defining a one-parameter group of automorphisms of $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$, given by:

$$[\alpha_t(F)](\phi) \doteq F(\phi_t) \qquad \forall F \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]. \tag{1.3.66}$$

For a linear functional F_f this reads

$$[\alpha_t(F_f)](\phi) = \int f(x_0,\mathbf{x})\phi(x_0+t,\mathbf{x})\,dx_0\,d^3\mathbf{x} = \int f(x_0-t,\mathbf{x})\phi(x_0,\mathbf{x})\,dx_0\,d^3\mathbf{x}. \tag{1.3.67}$$

In the following, we will often refer to α_t as the free time-evolution or as the free dynamics. We can get the dual action of α_t on states by pull-back:

$$\alpha_t^* \omega \doteq \omega \circ \alpha_t$$

for every state ω. Of particular interest are the *invariant states* (or *stationary states*), *i.e.* those ones satisfying

$$\alpha_t^* \omega = \omega \qquad \forall\, t \in \mathbb{R}.$$

Many examples of physically relevant states are indeed invariant, the first one we present is the vacuum state (or ground state) [Ha92]. This is of fundamental importance in relativistic QFT and, from the physical point of view, it is the unique state of lowest energy of the system. In the case of Minkowski space-time, this is tantamount to ask the state to be Poincaré-invariant[11]. The construction we sketch here is general and not limited to the scalar field.

Actually, the concept of "lowest energy" needs an explanation, in fact in the relativistic setting the notion of energy is ambiguous. This notion is indeed encoded in the so-called *relativistic spectrum condition*: A translation invariant state ω is called a vacuum if the joint spectrum of the 4-momentum operator P_ω satisfies

$$\mathrm{spec}(P_\omega) \subset J_+(0).$$

Here P_ω is defined as the (self-adjoint) generator of the unitaries $U_\omega(x)$ implementing the translations in the GNS representation associated with the state ω. Its existence is granted by the Stone theorem. This condition can be reformulated by the condition

$$\mathrm{spt}\left(\hat{F}^\omega_{A,B}\right) \subset J_+(0), \qquad F^\omega_{A,B}(x) \doteq \omega(A\,\alpha_x(B))$$

for all observables A, B. Here $\hat{\cdot}$ represents the distributional Fourier transform.

Concerning a free scalar field theory, the construction of the vacuum state, which from now on we call ω^{vac}, is developed by cutting off the negative energies by putting a step function in the momentum space expression of the causal propagator, given in equation (1.1.9). In particular, we have an explicit expression for the (integral kernel) of the 2-point function:

$$\omega_2^{\mathrm{vac}}(x-y) = \frac{1}{(2\pi)^3} \int \theta(p_0)\,\delta\left(p^2 - m^2\right) e^{-\mathrm{i}p(x-y)}\, d^4p. \tag{1.3.68}$$

The integration over p_0 leads to a more explicit expression:

$$\omega_2^{\mathrm{vac}}(x-y) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{e^{\mathrm{i}(E(\mathbf{p})(x_0-y_0) - \mathbf{p}\cdot(\mathbf{x}-\mathbf{y}))}}{2E(\mathbf{p})}\, d^3\mathbf{p},$$

where $E(\mathbf{p}) \doteq \sqrt{\mathbf{p}^2 + m^2}$ and $\cdot$ stands for the 3-dimensional Euclidean product.

The other class of invariant states which is important in this thesis is that of Kubo-Martin-Schwinger (KMS) states. They were first introduced in [HHW67] as a generalization of Gibbs

[11] Poincaré transformations are implemented exactly as done for the free dynamics, so defining one-parameter groups of automorphisms α_{P} of the algebra. One then defines the action of the Poincaré group on states by pull-back, so obtaining invariant states.

states to infinite systems, so they play the role of thermal equilibrium states. The generalization of usual Gibbs states is achieved by highlighting and selecting their main features, and eventually encoding them in what now is customarily called the *KMS condition*, which reads as follows:

Definition 1.3.11 (KMS Condition)**.** Let α_t be a one-parameter group of automorphisms of a topological *-algebra $\mathscr{A}$. A state ω on $\mathscr{A}$ satisfies the KMS condition with inverse temperature β with respect to α_t if the function

$$\mathbb{R} \ni t \mapsto \omega(A\alpha_t(B)) \qquad \forall\, t \in \mathbb{R}$$

admits an analytic continuation to the strip

$$\mathfrak{I}(\beta) \doteq \{z \in \mathbb{C} \,|\, 0 < \Im(z) < \hbar\beta\},$$

is continuous on the boundary and fulfills the boundary condition

$$\omega\left(A\alpha_{i\hbar\beta}(B)\right) = \omega(BA) \qquad \forall\, A, B \in \mathscr{A}. \tag{1.3.69}$$

(α_t, β)-KMS states will be denoted with ω^β.

In the following we will always assume the inverse temperature $\beta = \frac{1}{\kappa_B T}$, with κ_B the Boltzmann constant, to be positive; despite this being the most physically meaningful choice, very often (above all in the Statistical Mechanics literature) it is assumed $\beta < 0$, in particular $\beta = -1$, due to the particular role played by this value in the relation between KMS states and Tomita-Takesaki theory (see Section 4.1 and [Ha92, BR97a]). Moreover, notice that the KMS condition implies that every thermal equilibrium state is invariant, to see that it is enough to take $B = \mathbb{1}$ in (1.3.69).

At first glance, the KMS condition looks a bit dry and abstract. The physical intuition behind this condition is that it selects those states for which the system behaves as a thermal reservoir, according to the Zeroth Law of Thermodynamics. This is better understood by looking at quantum statistical mechanical systems[12]. In particular, in [Se86] the physical content of the KMS condition is seen to be clarified in the three following ways:

1. The KMS condition is equivalent to the local thermodynamical stability. Here, we mean that a state satisfies the local thermodynamical stability if no local modifications of it lead to a reduction of the free energy of the system, see also the original papers [AS77, Se77, Se80] for more details.

2. Given a physical system **E** weakly and locally coupled with another system **S**, the KMS condition characterises those states for which **E** drives **S** to the thermal equilibrium at its own temperature.

3. In the previous setting, the coupling of the system **E**, prepared in a KMS state at inverse temperature β, induces transitions between the eigenstates of **S** that satisfy the *detailed*

[12]Note that getting an intuition in the realm of QFT is hard also because an interacting KMS state has been built only recently in [FL14, Li13], see also Section 2.3. Nevertheless, we will see that the picture we introduce here is compatible with what we will prove concerning the stability of KMS states in Chapter 3.

balance condition. More precisely, calling P_i the occupation probability of the eigenstates ψ_i of $\mathbf{S}$ and W_{kj} the transition rate from the level k to j, then the detailed balance condition states that

$$W_{jk}P_j = W_{kj}P_k,$$

which, given $E_{j/k}$ the energy levels of $\psi_{j/k}$ respectively, implies

$$\frac{W_{jk}}{W_{kj}} = e^{\beta(E_j - E_k)}.$$

This is the content of the celebrated paper [KFGV77].

Out of these conditions we understand that a system in a KMS state is able to resist to local (*i.e.* bounded) perturbations, in this sense interpreting it as thermal equilibrium one is correct. We will discuss this topic thoroughly in Chapter 3, see also [BR97b, Section 5.4.].

Despite the former discussion holds in statistical mechanics, KMS states for free field theories are known to exist since a long time and also a relativistic version of the KMS condition has been studied in [BB94]. Actually, an explicit formula for the (integral kernel of) 2-point function can be derived. It reads as follows

$$\omega_2^\beta(x-y) = \frac{1}{(2\pi)^3}\int \frac{\operatorname{sign}(p_0)\,\delta\left(p^2-m^2\right)}{1-e^{\beta p_0}} e^{\mathrm{i}p(x-y)}\, d^4p.$$

The p_0-integration leads to

$$\omega_2^\beta(x-y) = \frac{1}{(2\pi)^3}\int \left(b_+(\mathbf{k})e^{\mathrm{i}E(\mathbf{k})(x_0-y_0)} + b_-(\mathbf{k})e^{-\mathrm{i}E(\mathbf{k})(x_0-y_0)}\right) e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\frac{d^3\mathbf{k}}{2E(\mathbf{k})}, \tag{1.3.70}$$

where

$$E(\mathbf{k}) \doteq \sqrt{\mathbf{k}^2+m^2}, \qquad b_+(\mathbf{k}) \doteq \frac{1}{1-e^{-\beta E(\mathbf{k})}}, \qquad b_-(\mathbf{k}) \doteq \frac{1}{e^{\beta E(\mathbf{k})}-1} = e^{-\beta E(\mathbf{k})}b_+(\mathbf{k}).$$

To conclude our survey on thermal states, we have just a comment about the necessity of extending the KMS condition, which, as stated in Definition 1.3.11, does not fit directly in the perturbative setting we are going to develop. This adaptation is the so-called *Multiple KMS Condition* and was introduced by Araki in [Ar73], see also [BR97b, Section 5.4.1]. We formulate it for any algebra $\mathscr{A}[\![\hbar]\!]$ of formal power series as follows:

Definition 1.3.12. Let α_t be a one-parameter group of automorphisms of $\mathscr{A}[\![\hbar]\!]$. A state ω^β on $\mathscr{A}[\![\hbar]\!]$ satisfies the multiple KMS condition with respect to α_t with inverse temperature β if the function

$$\mathbb{R}^n \ni (t_1,\dots,t_n) \mapsto \omega^\beta\left(\alpha_{t_1}(A_1)\star\cdots\star\alpha_{t_n}(A_n)\right) \quad \forall\, A_1,\dots,A_n \in \mathscr{A}[\![\hbar]\!]$$

have an analytic prolongation to the strip

$$\mathscr{I}_n(\beta) \doteq \left\{\mathbf{z}\in\mathbb{C}^n \mid 0 < \Im(z_j) - \Im(z_i) < \hbar\beta,\ 1\le i<j\le n\right\},$$

and it is bounded and continuous at the boundary, fulfilling the boundary conditions

$$\omega^\beta\left(\alpha_{t_1}(A_1)\star\cdots\star\alpha_{t_{k-1}}(A_{k-1})\star\alpha_{t_k+\mathrm{i}\hbar\beta}(A_k)\star\cdots\star\alpha_{t_n+\mathrm{i}\hbar\beta}(A_n)\right) = \omega^\beta\left(\alpha_{t_k}(A_k)\star\cdots\star\alpha_{t_n}(A_n)\star\alpha_{t_1}(A_k)\star\cdots\star\alpha_{t_{k-1}}(A_{k-1})\right).$$

The Hadamard property for the vacuum and for the KMS states has been established in [SV00], where a relation between the passivity and the μSC is also analysed. The quasi-freeness instead was already known by [KW91]. We do not dwell on details any longer, demanding to the original papers.

We limit ourselves to say that the vacuum state satisfies the KMS condition with temperature $T = 0$. This can also be seen by explicitly taking the limit $\beta \to \infty$ in the 2-point function expression (1.3.70).

To conclude the section, we want to present two technical results concerning the time-decaying property of the free KMS state ω^β on Minkowski, which will be useful in following. Those two results are given in [DFP18a], based on [BB02].

Proposition 1.3.3. *Consider the 2-point function of the extremal free massive KMS state at inverse temperature β on the Minkowski space-time $\mathbb{M}$ given in* (1.3.70)*. If $y-x$ is a timelike future pointing vector,*

$$\left| D^{(\alpha)} \omega_2^\beta (x; t_y + t, \mathbf{y}) \right| \leq \frac{C_\alpha}{t^{3/2}}, \qquad t > 1, \tag{1.3.71}$$

where $\alpha \in \mathbb{N}^8$ is a multiindex and $D^{(\alpha)}$ indicates the composition of partial derivatives of order α_i along the $i-$th direction in $\mathbb{M}^2$ for various $i \in \{1, \dots, 8\}$.

Proof. A proof of this proposition can be written following Appendix A in [BB02]. Here for completeness we sketch its main steps. We know that ω_2^β is an Hadamard 2-point function, hence, $\omega_2^\beta - \omega_2^\infty$ is smooth. If $y - x$ is a timelike future pointing vector, the points $(t_y + t, \mathbf{y})$ and y are connected by a timelike geodesic for every t, and thus $(x; t_y + t, \mathbf{y})$ is contained neither in the singular support of ω_2^β nor of ω_2^∞, hence the 2-point functions ω_2^β and ω_2^∞ are both described by a smooth function in a neighborhood of $(x; t_y + t, \mathbf{y})$. We recall that the massive vacuum 2-point function (see e.g. [BDF09]) can be written also as

$$\omega_2^\infty (x; t_y + t, \mathbf{y}) = 4\pi \frac{m}{\mathrm{i}\sqrt{(t + t_y - t_x)^2 - |\mathbf{x} - \mathbf{y}|^2}} K_1 \left(\mathrm{i}m \sqrt{(t + t_y - t_x)^2 - |\mathbf{x} - \mathbf{y}|^2} \right)$$

where K_1 is the modified Bessel function of second kind and of index 1. Hence, using the asymptotic form of the modified Bessel function, see [GR07, 8.451 (6).], for large values of t, and at fixed x and y, $|\omega_2^\infty (x; t_y + t, \mathbf{y})| \leq C/t^{3/2}$. Let us consider

$$t^{3/2} \left[\omega_2^\beta - \omega_2^\infty \right] (0; t, \mathbf{x}) = c t^{3/2} \sum_{\sigma \in \{+1, -1\}} \int_m^\infty \left(\sqrt{E^2 - m^2} \right) \frac{\sin \left(\sqrt{E^2 - m^2} |\mathbf{x}| \right)}{\sqrt{E^2 - m^2} |\mathbf{x}|} \frac{1}{e^{\beta E} - 1} e^{\mathrm{i}\sigma E t} dE$$

for $t > |\mathbf{x}|$ and for a suitable constant c. Performing a change of integration variable $w = (E - m)t$ we obtain

$$t^{3/2} \left[\omega_2^\beta - \omega_2^\infty \right] (0; t, \mathbf{x}) = \sum_{\sigma \in \{+1, -1\}} \int_0^\infty \sqrt{w}\, b_\sigma \left(\frac{w}{t} \right) e^{\mathrm{i}\sigma w} dw$$

where b_σ is a suitable bounded function which decays rapidly for large values of its argument. The integral in the right hand side of the previous expression can be proven to be bounded uniformly

in t operating in the following way. First of all we split the integral in two, so to isolate $b_\sigma(0)$:

$$\int_0^\infty \sqrt{w}\, b_\sigma\left(\frac{w}{t}\right) e^{\mathrm{i}\sigma w} dw = \lim_{\epsilon\to 0^+} \int_0^\infty \sqrt{w}\, b_\sigma(0) e^{\mathrm{i}\sigma w-\epsilon w} dw + \lim_{\epsilon\to 0^+} \int_0^\infty \sqrt{w}\left(b_\sigma\left(\frac{w}{t}\right) - b_\sigma(0)\right) e^{\mathrm{i}\sigma w-\epsilon w} dw.$$

The limit $\epsilon \to 0$ of the first term gives a finite result. To prove that the second term is bounded we write $e^{\mathrm{i}\sigma w-\epsilon w} = (\mathrm{i}\sigma-\epsilon)^{-2}\partial_w^2(e^{\mathrm{i}\sigma w-\epsilon w}-1)$ and we integrate by parts two times ending up with

$$\int_0^\infty \sqrt{w}\left(b_\sigma\left(\frac{w}{t}\right) - b_\sigma(0)\right) e^{\mathrm{i}\sigma w-\epsilon w} dw = \int_0^\infty w^{-3/2}\left(e^{\mathrm{i}\sigma w-\epsilon w}-1\right) c_\sigma\left(\frac{w}{t}\right) dw$$

where c_σ is another suitable bounded function. Hence, also this second term is bounded in time by a constant. Thus we can conclude that

$$\left|\left[\omega_2^\beta - \omega_2^\infty\right](x; t_y + t, \mathbf{y})\right| \leq \frac{C}{t^{3/2}}.$$

Combining both estimates we obtain the result in the case $\alpha = 0$.

The proof for the case of a generic α, can be obtained in a similar way. To estimate $D^{(\alpha)}\omega_2^\beta$, we observe that when the derivatives are applied to the factor in front of the Bessel function, the decaying for large t is improved. Furthermore, the recursive relations of Bessel functions and their asymptotic properties imply

$$\frac{d}{dx}K_n(x) = \frac{n}{x}K_n(x) - K_{n+1}(x), \qquad |K_n(y)| \leq \frac{c_n}{\sqrt{|y|}}, \qquad y \gg n.$$

Hence, the decaying rate of $D^{(\alpha)}\omega_2^\beta$ for large t is not worse then that of the case $\alpha = 0$. To estimate the contribution $D^{(\alpha)}\left(\omega_2^\beta - \omega_2^\infty\right)$, we apply the derivatives to $\frac{\sin(\sqrt{E^2-m^2}|\mathbf{x}|)}{\sqrt{E^2-m^2}|\mathbf{x}|}e^{\mathrm{i}\sigma Et}$, and afterwards we proceed in the same way as for the case $\alpha = 0$. Again, the decay in t can not be worse then that of the case $\alpha = 0$. □

Proposition 1.3.4. *Let $A, B \in \mathscr{F}_{\mu c}$. Let ω_2^β the 2-point function* (1.3.70)*. It holds that*

$$\left|\left\langle \omega_2^\beta, \frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)\right\rangle\right| \leq \frac{C}{(|t_1-t_2|+r)^{3/2}}$$

for every t_1, t_2 and for some constants C, r which may depend on A and B.

Proof. The microcausal functionals $A, B \in \mathscr{F}_{\mu c}$ have compact support by definition, so we may find a compact set $\mathbb{K} \subset \mathbb{M}$ containing the supports of both. Hence, the action of time translations is such that $\mathrm{spt}(\alpha_t(A)) \subset \mathbb{K}_t \doteq \{(\tau, \mathbf{x}) \in M | (\tau - t, \mathbf{x}) \in \mathbb{K}\}$, *i.e.* it is contained in the t-translated of $\mathbb{K}$. Since $\mathbb{K}$ is compact, there are no lightlike geodesics intersecting both $\mathbb{K}_{t_1}$ and $\mathbb{K}_{t_2}$ if $|t_1 - t_2| > d$, with d sufficiently large. By the Hadamard properties, the integral kernel of ω_2^β is a smooth function when restricted to $\mathbb{K}_{t_1} \times \mathbb{K}_{t_2}$. Since $\frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)$ is a distribution, by continuity we have that, for every $f \in \mathscr{E}\left(\mathbb{K}_{t_1} \times \mathbb{K}_{t_2}\right)$

$$\left|\left\langle f, \frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)\right\rangle\right| \leq C_1 \sum_{|\alpha|\leq N} \|D^\alpha f\|_\infty$$

where α is a multi-index, while N and C_1 are two fixed constants. Hence, Proposition 1.3.3 implies that

$$\left|\left\langle \omega_2^\beta, \frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)\right\rangle\right| \leq \frac{C_2}{(|t_1-t_2|)^{3/2}} \tag{1.3.72}$$

for every $|t_1-t_2|>d$ and for some constant C_2. For every $|t_1-t_2|\leq d$, the product of the distributions ω_2^β and $\frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)$ is well defined because, ω_2^β is an Hadamard 2-point function and A and B are in $\mathscr{F}_{\mu c}$, thus the Hörmander criterium for multiplication of distributions stated in Proposition 1.2.2 is satisfied. Furthermore, from the support properties of A and B we have that $\omega_2^\beta\cdot\frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)\in\mathscr{E}'(\mathbb{M}^2)$. By continuity we have that

$$\left|\left\langle \omega_2^\beta, \frac{\delta^2}{\delta\phi_1\delta\phi_2}\alpha_{t_1}(A)\otimes\alpha_{t_2}(B)\right\rangle\right| \leq C_3, \tag{1.3.73}$$

for every $|t_1-t_2|\leq d$. Combining (1.3.72) and (1.3.73) we have the result. □

1.3.4 Extension of the algebra $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$

In the previous subsection we explained why the Hadamard condition is suitable for the definition of Wick powers of regular observables. Actually, a combination of the functional formalism and of the Hadamard condition makes the inclusion of Wick polynomials in the algebra of observables possible. The problem in including in the algebra a generic microcausal functional is related to the problem of defining powers of the causal propagators. More precisely, let us consider the $\star$ product of two square monomials $F_i=\int f_i\phi^2\,d\mu_g$, for $i=1,2$: According to equation (1.3.50), at the second order we have a contribution of the form $\langle f_1,\Delta^2 f_2\rangle$, which is ill-defined due to the microlocal properties of Δ, as can be argued by direct computation. Here is the point where the peculiar Hadamard singular structure, determined by the μSC, enters the game.

Since the problem is related to the singularity of the causal propagator, the solution would be to switch to another topologically *-isomorphic algebra endowed with a better-behaved $\star$ product, which will be constructed using the 2-point function of a quasi-free Hadamard state ω, see [BDF09]. This leads to the definition of the following product

$$(F\star_\omega G)(\phi)\doteq(F\cdot G)(\phi)+\sum_{n=1}^{\infty}\frac{\hbar^n}{n!}\left\langle F^{(n)}(\phi),\omega_2^{\otimes n}G^{(n)}(\phi)\right\rangle \qquad \forall F,G\in\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]. \tag{1.3.74}$$

Also this product can be rewritten as

$$F\star_\omega G\equiv\mathbf{m}\circ e^{\Gamma_\omega}(F\otimes G),$$

where $\mathbf{m}$ is defined in (1.3.51) and Γ_ω is given by

$$\Gamma_\omega(F\otimes G)(\phi_1,\phi_2)\doteq\hbar\left\langle F^{(1)}(\phi_1),\omega_2 G^{(1)}(\phi_2)\right\rangle, \tag{1.3.75}$$

and it can be extended to the generic n-tensor product as

$$\Gamma_{\omega,ij}(F_1\otimes\cdots\otimes F_n)\doteq\hbar\left\langle F_i^{(1)},\omega_2 F_j^{(1)}\right\rangle\prod_{\substack{k=1\\k\neq i,j}}^{n}F_k. \tag{1.3.76}$$

The topological *-isomorphism between $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ and the algebra $\mathscr{A}_{\mathrm{reg},\omega}[\![\hbar]\!]$ is explicitly realised by the map $\alpha_{\omega_S} : \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!] \to \mathscr{A}_{\mathrm{reg},\omega}[\![\hbar]\!]$ defined by

$$\big[\alpha_{\omega_S}(F)\big](\phi) \doteq F(\phi) + \sum_{n=1}^{\infty} \frac{\hbar^n}{n!} \Big\langle \omega_S^{\otimes n}, F^{(2n)}(\phi) \Big\rangle, \tag{1.3.77}$$

where $\omega_S \doteq \omega_2 - \frac{\mathrm{i}}{2}\Delta$ is the symmetric part of the 2-point function of ω as per equation (1.3.62). This fact allows to make contact with the discussion about the existence of several equivalent star products for a physical theory which followed Definition 1.3.2.

By the μSC (1.3.64), it is easy to see that the $\star_\omega$ product is less singular then the one generated by the causal propagator. Furthermore, in [HW01, HW02] it is proven that the Hörmander criterium 1.2.2 guarantees that powers of the 2-point function of a generic Hadamard state are well-defined, hence it can be generalised to microcausal or local functionals. This allows for an extension of the $\star_\omega$ product, as follows:

$$F \star_\omega G \equiv \mathbf{m} \circ e^{\Gamma_\omega}(F \otimes G) \qquad \forall F, G \in \mathscr{F}_{\mu\mathrm{c}}[\![\hbar]\!].$$

Finally, the sought extension of the algebra of observables is possible. This is obtained by taking the closure in the Hörmander topology of $\mathscr{F}_{\mu\mathrm{c}}[\![\hbar]\!]$[13], which can be shown to be $\mathscr{F}_{\mu\mathrm{c}}[\![\hbar]\!]$ itself. Hence we have the following definition:

Definition 1.3.13 (Quantum Algebra of Observables)**.** The free, quantum topological *-algebra of off-shell observables for a massive scalar field theory is the data $\mathscr{A}_\omega[\![\hbar]\!] \doteq \big(\mathscr{F}_{\mu\mathrm{c}}[\![\hbar]\!], \star_\omega, ^*\big)$, where $\mathscr{F}_{\mu\mathrm{c}}[\![\hbar]\!]$ is the set of formal power series built over the microcausal functionals (1.2.29), $\star_\omega$ is defined in equation (1.3.74) and * is the complex conjugation.

The suffix ω in the definition of the algebra denotes the fact that the algebra is built out using the product defined with the 2-point function of a Hadamard state ω. Actually, this suggests the fact that the whole construction is state-dependent, so contradicting the whole spirit of algebraic quantisation. To see that this is not the case, we appeal again to the *-isomorphism (1.3.77) and to the fact that $w \doteq \omega_2 - \omega_2'$ is a smooth function for any couple of Hadamard states ω, ω'. Hence, in particular $\alpha_w : \mathscr{A}_{\omega'}[\![\hbar]\!] \to \mathscr{A}_\omega[\![\hbar]\!]$ is a *-isomorphism, which indeed establishes the state-independence of the construction. Notice that the α used here is slightly different from equation (1.3.77): In particular w is a smooth function and it has been tacitly extended to microcausal functionals $\mathscr{F}_{\mu\mathrm{c}}$, nevertheless the action of the map is well-defined and analogous to the one presented in (1.3.77). In what follows we will use α with this new meaning very often.

To make contact with the previous discussion concerning the choice of the star product among an equivalence class of them, we notice that the isomorphism α_w tells us that the products defined with different Hadamard states are in fact equivalent, in the sense of Definition 1.3.2. Hence, the question of what Hadamard function we shall choose arises. The answer can be found thinking about what state we want to use to compute expectation values of (products of) observables. In fact, a direct computation based on the definition of the star product shows that for a quasi-free state ω

$$\omega\big(F_1(\phi) \star_\omega \cdots \star_\omega F_n(\phi)\big) = F_1(\phi) \star_\omega \cdots \star_\omega F_n(\phi)\big|_{\phi=0} \tag{1.3.78}$$

[13] We recall that here we are considering polynomial elements only, see Section 1.2.2

for all $F_1,\dots,F_n \in \mathscr{A}_\omega[\![\hbar]\!]$, where the product $\star_\omega$ is built out of the state ω on which we are taking expectation values. This property provides an heavy simplification in the computations and so it will head us towards a choice of the algebra in the next sections.

In conclusion, we want to stress that the *-isomorphism α_w acts as the identity on linear functionals only. This means that a change in the state induces a different Wick ordering on the observables, which implies a modification of the physical meaning of local observables. A remarkable example of this fact is the phenomenon known as the *thermal mass*. Let us consider the products constructed out of the 2-point functions of the vacuum and of the extremal (α_t,β)-KMS state, defined in equations (1.3.68) and (1.3.70) respectively. Let us consider the ϕ^4 observable

$$F \doteq \int f(x)\phi^4(x)\,dx$$

and let us apply α_w, with $w \doteq \omega_2^\beta - \omega_2^{\text{vac}}$, on it

$$\alpha_w(F) = F + 6\hbar\iint w(x,y)\phi^2(x)f(x)\delta(x,y)\,dx\,dy + 3\hbar^2\iint w^2(x,y)f(x)\delta(x,y)\,dx\,dy,$$

where w has the explicit form:

$$w(x,y) = \frac{1}{(2\pi)^3}\int \frac{\delta(p^2-m^2)}{e^{\beta|p_0|}-1}e^{-ip(x-y)}d^4p$$

Hence we notice that the functional F is modified and, while we can neglect the contribution of order $\hbar^2$ (it is a constant), the one of order $\hbar$ is non-trivial since it is proportional to ϕ^2. This term can be absorbed in the free Lagrangian and it gives rise to the contribution known as the thermal mass. It can be computed explicitly by evaluating $w(x,x)$:

$$w(x,x) = \frac{1}{(2\pi)^3}\int \frac{\delta(p^2-m^2)}{e^{\beta|p_0|}-1}d^4p = \frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3}\frac{1}{e^{\beta E(\mathbf{p})}-1}\frac{d^3\mathbf{p}}{2E(\mathbf{p})},$$

where $E(\mathbf{p}) \doteq \sqrt{\mathbf{p}^2+m^2}$. Switching to polar coordinates ($|\mathbf{p}| \equiv p$) we obtain

$$w(x,x) = \frac{4\pi}{2(2\pi)^3}\int \frac{p^2dp}{E(\mathbf{p})}\frac{1}{e^{\beta E(\mathbf{p})}-1} = 2\frac{1}{4\pi^2\beta^2}\int_{\beta m}^\infty \frac{\sqrt{z^2-(\beta m)^2}}{e^z-1}dz,$$

where we have used the change of variable $z \doteq \sqrt{p^2-(\beta m)^2}$, which leads to the factor 2 because of the appearance of the module in writing p as a function of z. In conclusion, we obtain

$$w(x,x) = \frac{1}{2\pi^2\beta^2}G(\beta m), \qquad G(y) \doteq \int_y^\infty \frac{\sqrt{x^2-y^2}}{e^x-1}dx,$$

where the function G has the property that $G(0) = \pi^2/6$. Applying the isomorphism to the whole action of a massive scalar field, implementing F as interaction potential, it can be shown that this contribution gives a correction to the mass of the theory, which corresponds to the thermal mass

$$\frac{m_\beta^2}{2} = \frac{m}{2} + \frac{\lambda}{4}\frac{\hbar}{2\pi^2\beta^2}G(\beta m).$$

In the case of a massless Klein-Gordon theory, we see that the field acquires a positive mass:

$$m_\beta^2 = \frac{\lambda\hbar}{24\beta^2}.$$

The Haag-Kastler Axioms

For concluding this section we want to discuss briefly the validity of the Haag-Kastler axioms for the free quantum theory. As previously done, we have to redefine the theory in terms of a net of algebras $\{\mathscr{A}_\omega(\mathbb{O}) : \mathbb{O} \subset \mathbb{M} \text{ bounded}\}$, which constitutes no problem at all. Then, the isotony axiom is trivially satisfied, for the same reason that led to this conclusion in the classical theory. The causality descends from the definition of the $\star$ product, which implies that an expression for the commutator like (1.3.55), which involves the causal propagator Δ. So, as for the classical case, the causality is fulfilled due to the support properties of the causal propagator, which vanishes if evaluated on spacelike separated arguments.

A deeper discussion concerns the time-slice axioms. In order to check its validity, one needs to work with the on-shell formalism since it has to do with the dynamics. Considered that, checking the validity of the time-slice axiom is not a trivial task, so we will not tackle this problem here. A proof is given, for instance, in [CF09]. For completeness, we limit ourselves to report here Theorem 2 of this paper, which is its main result concerning the free theory.

Theorem 1.3.2 (Time-Slice Axiom for the Free Theory)**.** *Given Σ_I a neighbourhood of a Cauchy surface $\Sigma \subset \mathbb{M}$, then $\mathscr{A}_\omega(\Sigma_I)$ is isomorphic to the algebra $\mathscr{A}_\omega[\![\hbar]\!]$ built over the whole space-time.*

CHAPTER 2

THE INTERACTING MASSIVE SCALAR FIELD

In the previous chapter we achieved a satisfactory quantisation of the free, real scalar field theory relying on the functional formalism in the algebraic framework, so now we would like to consider the corresponding self-interacting model. Unfortunately, the non-linearity of the equations of motion of interacting theories forbids an application of the techniques we adopted in the previous chapter, that heavily rely on the presence of a causal propagator. The search of a way-out led physicists to use *perturbation theory*. In spite of giving striking results in terms of theoretical predictions, a big clue in this approach is its lack of mathematical rigour, which has been highlighted by several very well-known results, one for all the celebrated Haag's Theorem [Ha55]. Several insights to overcome this impasse were provided by mathematical physicists through the years, ranging from the construction of exactly-solvable models in lower dimensions, to the study and understanding of renormalisation.

It must be said that also the perturbative approach is not free of problems. One of the main difficulties is to cope with the infinities appearing at every order in the series, which correspond to the well-known *ultraviolet and infrared divergencies*. The issue of the ultraviolet behaviour is completely solved in pAQFT via the renormalisation of the time-ordered product, as we will see in Section 2.1. Concerning the infrared regime, in pAQFT at least at algebraic level the issue is solved by showing that it is possible to take the so-called algebraic adiabatic limit. Unfortunately, problems remain at the level of IR-divergencies of interacting states: Their well-posedness and their finiteness has to be discussed case-by-case, studying the so-called *weak adiabatic limit*.

A third problem we would like to mention is the resummation of the perturbative series, which is in fact out of control using either the algebraic approach or other methods. This is actually one of the biggest open questions concerning quantum field theories.

In spite of the importance and of the interest of this subject, we are forced to follow a prag-

matic approach and stick to the main subject of the thesis. For this reason, we will limit ourselves to present the rigorous construction of perturbation theory for a massive scalar field with polynomial self-interaction on Minkowski space-time $\mathbb{M}$. This will be achieved by the so-called Epstein and Glaser *causal perturbation theory* [EG73], adapted to the AQFT framework [BrFr00, BDF09, HW01, HW02]. The success of this method is not limited to its mathematical rigour, which allowed for a well-posed definition of the time-ordered product and for a clear understanding of the renormalisation, but it also has the advantage of being applicable on a general globally hyperbolic background.

This chapter is organised as follows: In the first part we will give insights on the construction of the time-ordered product and its axioms. This includes the definition of the Feynman propagators and of the Epstein-Glaser iterative procedure. Thence, we introduce the S-matrix as time-ordered exponential and we explain how this is related to the quantisation of the Møller morphisms given in (1.2.46) and to the Bogoliubov formula. This will provide a way to construct a Haag-Kastler net of interacting algebras, in particular we will discuss thoroughly the time-slice axiom and the adiabatic limit. In the final part, we turn to study the states for the interacting theory, focusing on the interacting KMS state introduced in [FL14, Li13], which acts a prominent role in this work. In spite of its importance, we will limit ourselves to a simple sketch of the construction due to its length and to its highly technical content.

Since the construction of the KMS state in [FL14] is performed for a real, scalar quantum field on Minkowski space-time only and since all our results are also formulated in this environment, for simplicity we we will stick to this case. Nonetheless, in Section 2.4 we will discuss some possible extensions of the construction, namely the case of a space-time with compact Cauchy surfaces and of a vector boson field.

2.1 The Time-Ordered Products and Renormalisation

The off-shell algebra for the free scalar field is described as the triple $\mathscr{A}_\omega[\![\hbar]\!] = \big(\mathscr{F}_{\mu c}[\![\hbar]\!], \star_\omega, ^*\big)$, where a (harmless) choice of an Hadamard state ω has to be made. In particular, the $\star_\omega$ product is defined as a functional differential operator on the space of functionals as in (1.3.75), hence we would like to define the time-ordered product accordingly. To begin with, in order to avoid regularity problems, we start working with regular functionals $\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]$ only. We will deal with the extension to more singular observables later on.

Heuristically, given two observables $F, G \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!] = \big(\mathscr{F}_{\mathrm{reg}}, \star_\Delta, ^*\big)$, a time-ordered product $\cdot_{T_\Delta}$ should fulfill the following relation

$$F \cdot_{T_\Delta} G = \begin{cases} F \star_\Delta G & \text{if} \quad F \succsim G \\ G \star_\Delta F & \text{if} \quad G \succsim F \end{cases}, \tag{2.1.1}$$

where $F \succsim G$ means that F is in the future of G with respect to a Cauchy surface, *i.e.* there exists a Cauchy surface which separates $\mathrm{spt}(F)$ and $\mathrm{spt}(G)$ in such a way that $\mathrm{spt}(F)$ is in its future and

$\mathrm{spt}(G)$ in its past. A product satisfying this requirement can be realised as follows:

$$\left(F \cdot_{T_\Delta} G\right)(\phi) \doteq (F \cdot G)(\phi) + \sum_{n=1}^{\infty} \frac{\hbar^n}{n!} \left\langle F^{(n)}(\phi), \left(\mathrm{i}\Delta^{\mathrm{D}}\right)^{\otimes n} G^{(n)}(\phi) \right\rangle \qquad \forall F, G \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!], \tag{2.1.2}$$

where $\Delta^{\mathrm{D}} \doteq \frac{1}{2}\left(\Delta^{\mathrm{A}} + \Delta^{\mathrm{R}}\right)$ is the Dirac propagator associated with the Klein-Gordon operator P defined in (1.2.15). Due to the support properties of the advanced and retarded Green functions stated in Definition 1.1.21, the time-ordered product is symmetric, as expected. Notice that this definition is well-posed only if both F and G are regular functionals.

The so-defined product is associative, commutative and isomorphic to the pointwise product by means of the following map:

$$F \cdot_{T_\Delta} G = \mathscr{T}_{\mathrm{reg}}\left(\mathscr{T}_{\mathrm{reg}}^{-1}(F) \cdot \mathscr{T}_{\mathrm{reg}}^{-1}(G)\right); \qquad \mathscr{T}_{\mathrm{reg}} F\left(\phi\right) \doteq F\left(\phi\right) + \sum_{n=1}^{\infty} \frac{\hbar^n}{n!} \left\langle \left(\mathrm{i}\Delta^{\mathrm{D}}\right)^{\otimes n}, F^{(2n)}\left(\phi\right) \right\rangle \quad \forall F \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!].$$

The map $\mathscr{T}_{\mathrm{reg}}$ is often called *time-ordering operator* and it can be interpreted as a map sending the classical algebra to a quantum one, in fact on the quantum regular functionals we have now two different products:

$$\mathscr{T}_{\mathrm{reg}} : \mathscr{A}_{\mathrm{cls,reg}} \to \left(\mathscr{A}_{\mathrm{reg}}[\![\hbar]\!], \star_\Delta, \cdot_T\right).$$

Indeed, this construction is still unsatisfactory since it does not include non-linear functionals, so it excludes the physically interesting interactions. Furthermore, it can be seen that the Dirac operator does not allow to get a well-posed time-ordered product in the general case. The idea is to follow the path taken for the free theory and extend the time-ordered product by considering a different Hadamard bi-distribution instead of the Dirac propagator. The need of preserving the causality leads to the introduction of the *Feynman propagator* $\omega^{\mathrm{F}} \doteq \mathrm{i}\Delta^{\mathrm{A}} + \omega_2$. Choosing a different Hadamard state means defining the time-ordering of Wick polynomials ordered with a different state. This causes in fact no real problems, the ambiguities arising may in fact be cured via renormalisation, because algebras defined with different $\star_\omega$ products are *-isomorphic. In addition, all this is telling us that the time-ordered product and the star one are not mutually associative. A way to keep this directly into account was found in [HW01, HW02] via the introduction of the time-ordering map, as we shall see later.

The extension to non-regular functionals can be done recalling the isomorphism Γ_ω defined in (1.3.75) and applying it to the time-ordering map $\mathscr{T}_{\mathrm{reg}}$, so obtaining the general time-ordering map

$$\mathscr{T} \doteq \alpha_\omega \circ \mathscr{T}_{\mathrm{reg}}; \qquad \mathscr{T} F\left(\phi\right) \doteq F\left(\phi\right) + \sum_{n=1}^{\infty} \frac{\hbar^n}{n!} \left\langle \left(\omega^{\mathrm{F}}\right)^{\otimes n}, F^{(2n)}\left(\phi\right) \right\rangle \quad \forall F \in \mathscr{A}_{\mathrm{reg}}[\![\hbar]\!]. \tag{2.1.3}$$

Notice that this definition still respects the heuristic requirement (2.1.1), as soon as the Feynman propagator is built out of the same Hadamard state used in the construction of the free $\star$ product. This leads to an explicit expression for (the integral kernel of) the Feynman propagator constructed out of a translation invariant Hadamard state ω:

$$\omega^{\mathrm{F}}(x-y) = \theta(x_0 - y_0)\omega_2(x-y) + \theta(y_0 - x_0)\omega_2(y-x), \tag{2.1.4}$$

θ being the Heaviside step function. The Feynman propagator is well-defined thanks to the Hörmander criterium 1.2.2, which applies to the product of θ with the 2-point function of any Hadamard state ω. The same criterium tells us also that the wave-front set of the Feynman propagator is actually "worst" than the Hadamard one, prescribed by the microlocal spectrum condition (1.3.64). It is possible to show that this is given by

$$\mathrm{WF}\left(\omega^{\mathrm{F}}\right) = \left\{(x,k_x;y,k_y) \in \mathrm{T}^*\mathbb{M}\setminus\{0\} \,\middle|\, (x,k_x)\sim(y,-k_y),\, x\neq y,\, k_x \rhd\!\!\!/ \lhd 0 \text{ if } x \in J_{+/-}(y)\right\}$$
$$\cup \left\{(x,k_x;x,-k_x) \in \mathrm{T}^*\mathbb{M} \,\middle|\, x\in\mathbb{M},\, k_x \in \mathrm{T}^*_x\mathbb{M}\setminus\{0\}\right\}, \quad (2.1.5)$$

in particular we see that the wave-front set of ω^{F} at zero is the same as that of the Dirac delta, which means that powers of the Feynman propagators can not be contracted with functional derivatives of local functionals [Ke10]. In particular, the Hörmander criterium can be used to define powers of the Feynman propagator out of the thin diagonal. The extension of this product in the coincidence limit is instead problematic, but nevertheless possible, and it amounts for the introduction of *renormalisation*. Several works have been done concerning this topic and a huge amount of literature has been written about it. A multitude of renormalisation schemes have been developed in the literature, for instance the Pauli-Villars scheme, dimensional regularisation and so on, see [PS95]. In this thesis we will limit ourselves to summarise what has been done in the AQFT framework, focusing on the *causal perturbation theory* of Epstein and Glaser [EG73]. For a complete account see [BDF09, BrFr00, HW01, HW02] and the references therein quoted.

Causal perturbation theory is an iterative procedure that allows for the construction of time-ordered products of local fields up to the thin diagonal of the space-time at every order in perturbation theory. The extension to the full space-time is then performed extending the distribution $(\omega^{\mathrm{F}})^n$ using the ideas of Steinmann scaling limit, see [BrFr00]. This is done at every but fixed perturbative order, and every order is built out of the previous one. The problem in defining the time-ordered product in the whole space-time is the aforementioned irregular behaviour of the powers of the Feynman propagator at the origin. The extension to the full domain is nonetheless not unique, but can be obtained up to renormalisation ambiguities. Hence, we may see the definition of the time-ordered product as a two-fold procedure: As a first step we will construct it by giving axioms for the time-ordering operator $\mathscr{T}$, extending it to the product of n local functionals. In the second step we will sketch how to extend it to the full Minkowski, namely we will perform the renormalisation. Since the main results of this thesis will not depend on the choice of a renormalisation scheme, we will be quick in our analysis, presenting the main ideas and avoiding most of the details. Moreover, we want to stress that all the following analysis may be generalised to a generic globally-hyperbolic space-time.

First of all, we fix the n-th order of the time-ordered product by using a multiple time-ordering map, which is the obvious generalisation of equation (2.1.3) and, whenever it exists, it is given by

$$\mathscr{T}_n\left(\mathscr{T}^{-1}(F_1),\dots,\mathscr{T}^{-1}(F_n)\right) \doteq F_1 \cdot_T \cdots \cdot_T F_n.$$

In particular, we point out that it is well-defined for every $F_1,\dots,F_n \in \mathscr{F}_{\mathrm{loc}}$ with pairwise disjoint supports. Of course, the time-ordering map can not be arbitrary, but it should satisfy certain

physical conditions. These constraints are assumed as axioms that the time-ordered product must fulfill, see [HW01, HW02, EG73]. They read as follows:

(T1) Initial Conditions: Since we have in mind an iterative construction, as a first axiom we have to specify the initial conditions, which will enable us to start the procedure. They are indeed pretty natural, in particular we choose

$$\mathscr{T}_0 \equiv 1, \qquad \mathscr{T}_1 \equiv \mathrm{Id}. \tag{2.1.6}$$

(T2) Causal factorisation: Given $F_1,\dots,F_n \in \mathscr{F}_{\mathrm{loc}}$ such that $F_i \succsim F_j$ for every $i = 1,\dots,k$ and $j = k+1,\dots,n$, we have

$$\mathscr{T}_n(F_1,\dots,F_n) = \mathscr{T}_k(F_1,\dots,F_k) \star_\omega \mathscr{T}_{n-k}(F_{k+1},\dots,F_n). \tag{2.1.7}$$

This requirement is the generalization of the condition (2.1.1).

(T3) Symmetry: For every permutation π of the set $\{1,\dots,n\}$ we require

$$\mathscr{T}_n(F_1,\dots,F_n) = \mathscr{T}_n\left(F_{\pi(1)},\dots,F_{\pi(n)}\right). \tag{2.1.8}$$

(T4) Unitarity: Given a partition $P = \left(P_1,\dots,P_j\right)$ of the set $\{1,\dots,n\}$ into pairwise disjoint subsets, we assume

$$\mathscr{T}_n(F_1,\dots,F_n)^* = \sum_{\mathscr{P}} (-1)^{n+j}\, \mathscr{T}_{|\mathscr{P}_1|}\left(F_{p_{1,1}},\dots,F_{p_{1,|\mathscr{P}_1|}}\right) \star_\omega \cdots \star_\omega \mathscr{T}_{|\mathscr{P}_j|}\left(F_{p_{j,1}},\dots,F_{p_{j,|P_j|}}\right), \tag{2.1.9}$$

where $p_{i,l}$ denotes the l-th element of the partition $\mathscr{P}_j$ with cardinality $\left|\mathscr{P}_j\right|$.

(T5) ϕ-Locality: We ask the time-ordered product, seen as a functional on the configurations space $\mathscr{E}$, to depend on $\phi \in \mathscr{E}$ only via the functional derivatives of the functionals. In particular, we assume the following product rule to be fullfilled:

$$\frac{\delta}{\delta\phi}\mathscr{T}_n(F_1,\dots,F_n) = \sum_{k=1}^{n} \mathscr{T}_n\left(F_1,\dots,\frac{\delta F_k}{\delta\phi},\dots,F_n\right). \tag{2.1.10}$$

(T6) Poincaré-Invariance: Denoted with α_{P} the action of the Poincaré group on $\mathscr{F}_{\mathrm{loc}}$ as per footnote 11, we assume that

$$\alpha_{\mathrm{P}}(\mathscr{T}_n(F_1,\dots,F_n)) = \mathscr{T}_n(\alpha_{\mathrm{P}}(F_1),\dots,\alpha_{\mathrm{P}}(F_n)). \tag{2.1.11}$$

Remark 2.1.1. In our presentation, we are following what is done in [BDF09], which is slightly different with respect to the construction originally performed by Hollands and Wald [HW01, HW02]. In particular, Hollands and Wald did not require any condition on the first order map $\mathscr{T}_1$. This implies that they had to insert the inverse time-ordering in their formulas, so keeping into account the counterterms needed to to fix the renormalisation freedoms. Actually, since $\mathscr{T}_1$ is applied on local functionals only, the condition $\mathscr{T}_1 \neq \mathrm{Id}$ amounts essentially to a different definition of the Wick polynomials, see the quoted literature for further details.

Remark 2.1.2. We stress that the time-ordering map is defined on local functionals only. This is due to the fact that its extension to non-local observables, say generic microcausal functionals, would require the use of non-local renormalisation counterterms.

A family of maps $\mathscr{T}_n$ satisfying those axioms have been proved to exist first in the original paper by Epstein and Glaser [EG73] and, later on, the time-ordered product has been constructed for QFTs on curved backgrounds by Hollands and Wald in [HW02]. As previously anticipated, the construction of these maps is not unique. The obstruction is due to the form of the wave-front set of the Feynman propagator (2.1.5), as it may be argued by the following computation, based on the explicit expression of time-ordered product given in equation (2.1.2), which now is naturally extended on local functionals. For instance, given two quadratic (local) functionals

$$F = \frac{1}{2}\int \phi^2(x) f(x)\, dx, \qquad G = \frac{1}{2}\int \phi^2(y) g(y)\, dy, \qquad \mathrm{spt}(f)\cap \mathrm{spt}(g) = \emptyset,$$

equation (2.1.2) leads to

$$\mathscr{T}_2(F,G)\big(\phi\big) = (F\cdot_T G)\big(\phi\big) = \\ F\big(\phi\big)\cdot G\big(\phi\big) + \hbar \iint \phi(x)\phi(y)\omega^{\mathrm{F}}(x,y) f(x) g(y)\, dx dy + \frac{\hbar^2}{2}\iint \Big[\omega^{\mathrm{F}}(x,y)\Big]^2 f(x) g(y)\, dx dy.$$

The problem in the previous formula is the square of the Feynman propagator: By the form of its wave-front set (2.1.5) we see that, if $x \neq y$ and if $(x,k;y,k')$ belongs to $\mathrm{WF}\big(\omega^{\mathrm{F}}\big)$, then k and $-k'$ are cotangent to a null geodesic connecting x and y. Moreover, k and p are future-pointing if $x \succsim y$ (past-directed otherwise), so both $k+p \neq 0$ and $k'+p' \neq 0$. This implies that the hypotheses of the Hörmander criterium 1.2.2 are met, so the square of the Feynman propagator is well-defined as a distribution on the complement of the thin diagonal $\mathrm{diag}(2)$. On the other hand, if $x \equiv y$ and if $(x,k;x,k') \in \mathrm{WF}(\omega^{\mathrm{F}})$, the only restriction we have is $k = -k'$, hence the Whitney sum of $\mathrm{WF}\big(\omega^{\mathrm{F}}\big)$ with itself intersects the zero section. Therefore we may use Proposition 1.2.2 to define $(\omega^{\mathrm{F}})^2$ on $\mathscr{D}\big(\mathbb{M}^2 \setminus \mathrm{diag}(2)\big)$ only. Hence, the problem of defining the time-ordered product reduces to the problem of the extension of the (powers of the) Feynman propagator to an everywhere-defined distribution. As we anticipated, this issue remains also in the generic n-th order, explaining why the construction of $\mathscr{T}_n$ amounts to the extension of numerical distributions to the thin diagonal $\mathrm{diag}(n) \subset \mathbb{M}^n$. In particular, exploiting the axioms, the construction proceeds recursively, and after having constructed the product at order $n-1$, causal factorisation permits to construct the sought distribution at order n up to the thin diagonal and one is left with the problem of extending that distribution to the thin diagonal.

The problem of extending distribution is nonetheless a non-trivial one and we shall not expect every distribution to be extensible. A possibility to tackle the issue is based on the notion of *Steinmann scaling degree* and on the related *degree of divergence* of a distribution [Ste71].

Definition 2.1.1. Let $U \subseteq \mathbb{R}^n$ be a scaling invariant open subset, which means that $\lambda U \subseteq U$ for all $0 < \lambda \leq 1$, and let $u \in \mathscr{D}'(U)$ be a distribution on U. Let $u_\lambda(x) \doteq u(\lambda x)$ be the scaled distribution.

We define the scaling degree towards 0 of u as

$$\mathrm{sd}(u) \doteq \inf_{\delta\in\mathbb{R}} \left\{ \lim_{\lambda\to 0} \lambda^{\delta} u_{\lambda} = 0 \right\}.$$

We also introduce the degree of divergence of t as

$$\mathrm{div}(u) \doteq \mathrm{sd}(u) - n.$$

Notice that the scaling degree may be infinite. The importance of the scaling degree can be argued from the theorem below, which uses it to classify the distributions which can be extended and, furthermore, it gives information about how ambiguous is the extension.

Theorem 2.1.1. *Let $u_0 \in \mathscr{D}'(\mathbb{R}^n \setminus \{0\})$.*

1. *If $\mathrm{sd}(u_0) < n$, then there exists a unique distribution $u \in \mathscr{D}'(\mathbb{R}^n)$ such that*

$$u(\phi) = u_0(\phi) \qquad \forall\, \phi \in \mathscr{D}(\mathbb{R}^n \setminus \{0\})$$

   with $\mathrm{sd}(u_0) = \mathrm{sd}(u)$;

2. *If $n \leq \mathrm{sd}(u_0) < \infty$ there are several distributions $u \in \mathscr{D}'(\mathbb{R}^n)$ such that*

$$u(\phi) = u_0(\phi) \qquad \forall\, \phi \in \mathscr{D}(\mathbb{R}^n \setminus \{0\})$$

   with $\mathrm{sd}(u_0) = \mathrm{sd}(u)$. Two such distributions u, t differ by derivatives of the δ distribution, more precisely

$$u - t = \mathrm{P}[\partial]\delta,$$

   where P is a polynomial with degree $\deg(\mathrm{P}) \leq \mathrm{sd}(u_0) - n$.

3. *If $\mathrm{sd}(u_0) = \infty$ there exists no distribution $u \in \mathscr{D}'(\mathbb{R}^n)$ extending u_0.*

A proof of this theorem and a complete account on the subject can be found in [BrFr00]. The role of this result in the renormalisation process can be understood by noticing that the scaling degree of the n^{th}-power of the Feynman propagator on the 4-dimensional Minkowski space is $2n$, hence it admits an extension to the whole space-time which is unique up to a $2n$-degree polynomial in the derivatives of the Dirac delta. As expected, the Feynman propagator can be extended uniquely. The ambiguity introduced in item 2. in fact corresponds to what are customarily called the *renormalisation ambiguities*. In particular, in [EG73] it is proved that, given two choices of time-ordering $\{\mathscr{T}_n\}_{n\in\mathbb{N}}$ and $\{\mathscr{T}'_n\}_{n\in\mathbb{N}}$ which coincide up to the order $n-1$, the ambiguities in the definition are fully considered by adding multilinear maps $\mathscr{Z}_n : \mathscr{F}_{\mathrm{loc}}^{\otimes n} \to \mathscr{F}_{\mathrm{loc}}$:

$$\mathscr{T}'_n(F_1,\ldots,F_n) = \mathscr{T}_n(F_1,\ldots,F_n) + \mathscr{Z}_n(F_1,\ldots,F_n).$$

The last theorem guarantees the existence of the extension only, but sadly it tells nothing about how to construct such extensions and how to reduce the freedom in finding the extensions, which is what we explicitly need. In general, this is a hard task and requires rather involved computations. A way to reduce the complexity is the introduction of *Feynman diagrams*, which

are helpful in handling the combinatorics underlying the construction (see [BrFr00, Ke10, Re16] for a complete account on the subject). Nevertheless, we stress that in pAQFT they are not fundamental objects, but they are rather derived, together with the corresponding Feynman rules, from the time-ordered products $\mathscr{T}_n$. Regarding the freedom, in Minkowski it can be reduced to a number of constants assuming translation symmetry. In the case of curved backgrounds the freedom is reduced imposing covariance [HW01].

Actually, for the purposes of this thesis, it is sufficient to know that a time-ordered product may be constructed: Our results will be independent from its choice (and from the corresponding choice of a renormalisation scheme), so we refer to [BrFr00, Fre10, FR15] and to the references therein for further details.

The availability of the time-ordered product, where we are assuming to have all the ambiguities fixed, enables us to define the *formal S-matrix* as its generating functional, namely as a map $S : \mathscr{F}_{\mathrm{loc}} \to \mathscr{F}_{\mu c}[\![\hbar, \lambda]\!]$, $\mathscr{F}_{\mathrm{loc}}$ being the space of local functionals given in Definition 1.2.10, obtained as follows:

$$V_1 \cdot_T \ldots \cdot_T V_n \doteq \frac{1}{\mathrm{i}^n} \frac{\mathrm{d}^n}{\mathrm{d}\lambda_1 \cdots \mathrm{d}\lambda_n}\bigg|_{\lambda_1=\cdots=\lambda_n=0} S\left(\sum_{k=1}^{n} \lambda_k V_k\right) \tag{2.1.12}$$

for all $n \in \mathbb{N}$ and all $V_1, \ldots, V_n \in \mathscr{F}_{\mathrm{loc}}$. In particular, this is explicitly given by the time-ordered exponential

$$S(V) \doteq \exp_{\cdot_T}\left(\frac{\mathrm{i}}{\hbar} V\right) \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \mathscr{T}_n\left(\left(\frac{\mathrm{i}}{\hbar} V\right)^{\otimes n}\right) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\mathrm{i}^n}{\hbar^n} \underbrace{V \cdot_T \cdots \cdot_T V}_{n \text{ times}} \qquad \forall\, V \in \mathscr{F}_{\mathrm{loc}}. \tag{2.1.13}$$

The adjective "formal" comes from the fact that those maps are algebraic analogous of the usual S-matrices defined in scattering theory for Quantum Mechanics, which are unitary operators on the Hilbert space of the theory. In addition, they are constructed as a formal power series, which usually can not be summed. Moreover, the formal S-matrix is built out of an interaction V_g on which a cutoff $g \in \mathscr{D}$ has been inserted to avoid infrared divergencies. What we expect is that, given a representation π of the algebra on a Hilbert space, $\pi\left(S\left(V_g\right)\right)$ tends to the physical S-matrix in the adiabatic limit[1] $g \to 1$. Actually, this convergence has been proven only in very few cases, *e.g.* for the vacuum representation of massive fields, see [EG73]. In our framework, the formal S-matrix has to be understood in the sense of formal power series both in the argument (more specifically, in the coupling constant λ for the case of $S(\lambda V)$) and as a formal power series in $\hbar$[2].

Due to its nature of generating functional of a time-ordered product, we require a list of axioms for the formal S-matrices. These axioms correspond to the ones previously discussed for the $\cdot_T$ product. In particular, different choices of the S-matrix amount to different time-ordered products.

[1] We will discuss this topic thoroughly in the next section.

[2] Recall that this is not really the case in the present thesis, since we are assuming to work with polynomials in $\hbar$ only, as explained in (1.2.32).

(S1) Initial Conditions: Concerning the formal power series in λ, we choose the initial conditions

$$S(0) = \mathbb{1}, \qquad \frac{1}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} S(\lambda V) = V \qquad \forall\, V \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!],$$

while with respect to the one in $\hbar$ we ask

$$S = \mathbb{1} + O(\hbar).$$

(S2) Causal Factorisation: Given $F, G, V \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!]$ with $F \succsim G$, we ask

$$S(F+V+G) = S(F+V) \star_\omega S(V)^{\star_\omega -1} \star_\omega S(V+G).$$

(S3) Unitarity: $S(V)^* = S(V^*)^{\star_\omega -1}$.

(S4) ϕ-Locality: This condition guarantees that the S-matrix depends on the field configurations only through the functional derivatives of the functionals, that is

$$\frac{1}{\mathrm{i}}\frac{\delta}{\delta\phi} S(V) = \mathscr{T}_1\left(\frac{\delta V}{\delta\phi}\right) \cdot_T S(V) \qquad \forall\, V \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!].$$

(S5) Poincaré-Invariance: Given α_{P} the automorphism implementing the Poincaré transformations on the algebra, we require $\alpha_{\mathrm{P}}(S(V)) = S(\alpha_{\mathrm{P}}(V))$ for all $V \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!]$.

Definition 2.1.2 (Formal S-matrix)**.** We call S-matrix any map $S : \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!] \to \mathscr{F}_{\mu\mathrm{c}}[\![\hbar]\!]$ which is analytic in the neighbourhood of the origin and which satisfies the axioms **(S1)**-**(S5)**. Via equation (2.1.12), any formal S-matrix defines a time-ordered product which fullfils the axioms **(T1)**-**(T6)**.

One of the great advantages of working with this axiomatic approach to the construction of time-ordered product is that it enables us to formulate interacting theories in a way which is completely independent of the regularisation scheme. In addition, by the introduction of the *Stückelberg-Petermann renormalisation group*, we are also able to prove that every regularisation scheme is equivalent up to finite renormalisation, see [BDF09, HW03, Stü51, SP53].

Definition 2.1.3. Let $\mathfrak{Z}$ be the set of $Z : \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!] \to \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!]$ analytic in a neighbourhood of the origin which fullfil the following axioms:

(Z1) Initial Conditions: For all $F \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!]$, we require

$$Z(0) = 0, \qquad \frac{1}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}\lambda}\bigg|_{\lambda=0} Z(\lambda F) = F,$$

concerning the power series in the argument, while for the one in $\hbar$ we have

$$Z(F) = F + O(\hbar);$$

(Z2) Additivity: The map Z are additive in the sense of Definition 1.2.9;

(Z3) ϕ-ndependence: For all $F \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!]$, Z is independent of the field configuration ϕ, that is $\frac{\delta}{\delta\phi} Z = 0$, which implies that Z preserves the localisation of the interaction, see [BDF09] for more details;

(Z4) Poincaré-Invariance: $\alpha_{\mathrm{P}}(Z(F)) = Z(\alpha_{\mathrm{P}}(F))$ for all $F \in \mathscr{F}_{\mathrm{loc}}[\![\hbar]\!]$ and all Poincaré transformations α_{P}.

The data $(\mathfrak{Z}, \circ)$, where $\circ$ is the composition, forms a group.

The axioms in the definition of the Stückelberg-Petermann renormalisation group are motivated by the following result, proven in [BDF09], which in fact is the *main theorem of renormalisation*.

Theorem 2.1.2. *Given a formal S-matrix S and $Z \in \mathfrak{Z}$, then $S \circ Z$ is again a formal S-matrix. Furthermore, for any two formal S-matrices S, S' there exists $Z \in \mathfrak{Z}$ such that $S' = S \circ Z$.*

This theorem implies that every regularisation scheme can be used to define the S-matrix, since the use of two different ones amounts to add a map $Z \in \mathfrak{Z}$. As anticipated in the previous chapter, Z does not respect the linear dependence on the cutoff usually present in the interaction potential; this is the reason which motivates *a posteriori* the introduction of the formalism of the generalised actions $\mathfrak{S}$ in Section 1.2.3, see [BDF09] for further details.

2.2 The Algebra of Interacting Observables

Relying on the formalism introduced in the previous section, we want to construct an Haag-Kastler net of *-algebras of interacting observables

$$\{\mathscr{A}_g(\mathcal{O}) : \mathcal{O} \subset \mathbb{M} \text{ bounded}\}$$

for a massive scalar field theory with polynomial self-interaction. This model is described by the interacting Klein-Gordon equation

$$P\phi + \lambda V_g^{(1)}(\phi) = 0, \tag{2.2.14}$$

where P is the Klein-Gordon operator (1.2.15) and $V^{(1)}$ is the first functional derivative of the interaction Lagrangian. This was defined in Example 1.2.2, but for the comfort of the reader we report it here, adapting the notation to the Minkowskian case

$$L_I(\phi) \equiv V_g(\phi) \doteq \int \mathrm{P}[\phi](x) g(x) dx, \tag{2.2.15}$$

where $g \in \mathscr{D}$ and P is a generic polynomial in the field configuration $\phi \in \mathscr{E}$. The presence of the cutoff g is fundamental since it guarantees that the theory we are to develop is both UV and IR finite. Nonetheless, from a physical point of view, the interactions are everywhere defined, hence the insertion of g is a mere mathematical artefact and, eventually, we will have to remove the cutoff, taking the so-called *adiabatic limit* $g \to 1$. This is a highly non-trivial feature of the theory, on which we will spend some time in the following.

The principal tool for introducing the interactions is the formal S-matrix, from which we will construct a *relative S-matrix*, which will be directly involved in the construction of the interacting observables. The first problem is the ambiguity of their definition, which must be fixed via renormalisation in order to obtain unique physical predictions. Of particular importance to this avail are the renormalisable interactions. In the case of a scalar field theory over the 4-dimensional Minkowski the only renormalisable, local interactions are those of the form

$$\mathrm{P}[\phi](x) = \frac{\lambda_1}{3!}\phi^3(x) + \frac{\lambda_2}{4!}\phi^4(x).$$

For those kind of models, the image of the renormalisation group is finite-dimensional, so that only a finite amount of counterterms is needed to fix the time-ordered products. In particular, this means that at every fixed perturbative order, a renormalisable theory is predictive after one fixes a finite number of parameter of the theory, which are generally determined by experiments. This is in accordance to what one finds in the physical literature, see for instance [PS95, Zi02]. In order to build the interacting theory, we will always assume that the time-ordered product is fixed (or at least fixable) at every order n, so that the S-matrices are unambiguously defined and may be taken as the main ingredient in the construction. This implies that our formalism is well-suited also for treating models that are not renormalisable, in the sense of what we have said above. This is due to the fact that we are using formal power series, hence at every fixed order only a finite number of counterterms are required to renormalise. For non-renormalisable interactions, this number gets bigger and bigger as the perturbative order grows.

Another problem related to the construction of the S-matrix concerns its dependence on the Hadamard state ω out of which we have built the star product $\star_\omega$, which enters highly non-trivially in the causal factorisation properties **(T2)** and **(S2)**. To this aim, we will initially define the net for a fixed Hadamard function ω, and later on we will show that this is in fact independent of this choice. This means that the interacting theory is independent of the chosen state[3], as required by the algebraic approach.

The separation between the purely algebraic aspects and the ones concerning the states of the theory has also the advantage of disentangle the UV and IR divergencies often present in interacting QFTs. The UV ones are in fact properly algebraic and they are cured with renormalisation, as we saw in the previous section. The presence of UV infinites in canonical QFT is in fact related to the use of unrenormalised time-ordered products in perturbation theory, see [PS95]. The IR divergencies are more subtle and they have to do with the adiabatic limit, namely the removal of the cutoff g we put on the interaction Lagrangian (2.2.15) as an IR regulator. At algebraic level this amounts to take the so-called algebraic adiabatic limit, which consists in showing that algebras built with interactions with different cut off (possibly not compactly supported) are isomorphic. As we shall see later, the reason for that can be traced back to the causal factorisation property of the S-matrices, see [BrFr00] for a complete account on the subject. The real issue with the adiabatic limit, which is the origin of the infrared divergencies often encountered in the physics literature, enters the game when trying to construct interacting states. It turns out that

[3] Actually, phenomena related to the change of the background state will still be present, likewise it happened for the star product (*e.g.* the thermal mass phenomenon). Again, this may be due to the use of a Feynman propagator which comes from the "wrong" Hadamard state.

they may explicitly depend on the cutoff, hence the problem of the existence of the limit, which in this case is named weak adiabatic limit, has to be addressed case by case. This issue will be addressed more thoroughly in the next section.

The first step towards the definition of a Haag-Kastler net is the definition of the observables for the interacting theory on a bounded region $\mathbb{O} \subset \mathbb{M}$. We consider smooth compactly supported functions $g : \mathbb{M} \to \mathbb{R}$ (we will often use the notation $g \in \mathscr{D}$, as usual in this work) and the formal S-matrices generated by the interaction potentials V_g labelled by $g \in \mathscr{D}$, which, for brevity, we will denote as

$$S(g) \equiv S\left(V_g\right).$$

Thus, we define the local algebras $\mathscr{A}_0(\mathbb{O})[\![\hbar, \lambda]\!]$ as the *-algebras generated by $S(g)$ with $\mathrm{spt}(g) \subset \mathbb{O}$, obtaining a translation covariant Haag-Kastler net. The notation is justified by the fact that, by definition of the S-matrix as a time-ordered exponential (2.1.13), their elements are formal power series both in $\hbar$ and in the coupling constant λ. The Haag-Kastler axioms are in fact satisfied: The isotony is straightforward, the covariance follows from the axiom **(S5)**. To check the locality, we consider two spacelike separated $f, g \in \mathscr{D}$ such that $\mathrm{spt}(f) \cap J_{\pm}(\mathrm{spt}(g)) = \emptyset$. By the causal factorisation property **(S2)** we obtain

$$S(f) \star_\omega S(g) = S(f+g) = S(g) \star_\omega S(f).$$

At this point, we observe that the map $g \mapsto S(g)$ induces a large family of objects satisfying the causal factorisation, which are defined as follows:

Definition 2.2.1 (Relative S-matrix)**.** The relative S-matrix between two local functionals $F, G \in \mathscr{F}_{\mathrm{loc}}$ is defined as

$$S_G(F) \doteq S^{\star_\omega -1}(G) \star_\omega S(G+F). \tag{2.2.16}$$

If F, G are two local functionals smeared with $f, g \in \mathscr{D}$, *e.g.* they are two interaction potentials V_f, V_g respectively, we will denote the relative S-matrix as

$$S_g(f) \doteq S(g)^{\star_\omega -1} \star_\omega S(f+g). \tag{2.2.17}$$

As it will be clear soon, the relative S-matrix corresponds to the retarded observable $S(f)$ under the influence of the interaction Lagrangian V_g, f labelling any observable F. Actually, we start observing that they satisfy the causal factorisation property.

Proposition 2.2.1. *In the framework of Definition 2.2.1, the relative S-matrix fulfills the causal factorisation property* (**S2**)*.*

Proof. Let $f, h, g, g' \in \mathscr{D}$ such that $\mathrm{spt}(f) \cap J_-(\mathrm{spt}(h)) = \emptyset$. Then

$$\begin{aligned} S_g\left(f+g'+h\right) = S(g)^{\star_\omega -1} \star_\omega S\left(f+g+g'+h\right) \overset{\textbf{(S2)}}{=} \\ S(g)^{\star_\omega -1} \star_\omega S(f+g+g') \star_\omega S(g+g')^{\star_\omega -1} \star_\omega S(g+g'+h) = \\ S_g(f+g') \star_\omega S_g(g')^{\star_\omega -1} \star_\omega S(g)^{\star_\omega -1} \star_\omega S(g) \star_\omega S_g(g'+h) = \\ S_g(f+g') \star_\omega S_g(g')^{\star_\omega -1} \star_\omega S_g(g'+h). \quad \square \end{aligned}$$

This property justifies the definition of the Haag-Kastler net $\mathscr{A}_g(\mathcal{O})[\![\hbar,\lambda]\!]$ of interacting theory as the one obtained as inductive limit on the local algebras

$$\mathscr{A}_g(\mathcal{O}) \doteq \left[\{S_g(f):\ \mathrm{spt}(f)\subset\mathcal{O}\}\right], \tag{2.2.18}$$

where the square brackets denote that we are considering the algebra generated by the element in the set.

Of pivotal importance in the construction of the net is the retarded character of the relative S-matrices, which means that $S_g(f)$ depends only on the behaviour of g in the past of $\mathrm{spt}(f)$, more in detail, if $\mathrm{spt}(g-g')\cap J_-(\mathrm{spt}(f))=\emptyset$, then

$$S_g(f) = S(g)^{\star_\omega -1}\star_\omega S\left(g-g'+g'+f\right) = \\ S(g)^{\star_\omega -1}\star_\omega S\left(g-g'+g'\right)\star_\omega S(g')^{\star_\omega -1}\star_\omega S(g'+f) = S_{g'}(f).$$

Furthermore, $S_g(f)$ depends on g outside the future of $\mathrm{spt}(f)$ only via a (formal) unitary transformation independent of f. More precisely, given $\mathrm{spt}(g-g')\cap J_+(\mathrm{spt}(f))=\emptyset$, we have

$$\begin{aligned} S_g(f) = S(g)^{\star_\omega -1}\star_\omega S\left(f+g'+g-g'\right) = \\ S(g)^{\star_\omega -1}\star_\omega S(f+g')\star_\omega S(g')^{\star_\omega -1}\star_\omega S(g'+g-g') = \\ S(g)^{\star_\omega -1}\star_\omega S(g')\star_\omega S(g)^{\star_\omega -1}\star_\omega S(f+g')\star_\omega S_{g'}(g-g') = \\ S_{g'}(g-g')^{\star_\omega -1}\star_\omega S_{g'}(f)\star_\omega S_{g'}(g-g'). \end{aligned}$$

The former results can be summarised in three properties, *i.e.* the *causal factorisation*:

$$S_g(F+G) = S_g(F)\star_\omega S_g(G) \qquad \forall F,G\in\mathscr{F}_{\mathrm{loc}} \text{ s.t. } F\succsim G, \tag{2.2.19}$$

and the *retardation*

$$S_{g+g'}(F) = S_g(F) \qquad \forall F\in\mathscr{F}_{\mathrm{loc}},\ \forall g'\in\mathscr{D} \text{ s.t. } V_{g'}\succsim F. \tag{2.2.20}$$

On the other hand, we have also that

$$S_{g+g'}(F) = U\star_\omega^{-1} S_g(F)\star_\omega U, \qquad U = S_g(g'), \tag{2.2.21}$$

where $V_{g'}\succsim F$. This means that the change of the support of the potential in the past of the observables induces unitary transformation.

These last three properties (2.2.19) and (2.2.20) of the relative S-matrices imply that the algebras $\mathscr{A}_g(\mathcal{O})[\![\hbar,\lambda]\!]$ depends on the interaction only locally up to unitary transformations. This feature is crucial for the development of the theory, since it allows to perform the adiabatic limit $g\to 1$ at the algebraic level (the so-called *algebraic adiabatic limit*) because it implies that the interacting observables are independent by the cutoff g we put on the interaction Lagrangian (2.2.15).

To see this let $G:\mathbb{M}\to\mathbb{R}$ be a smooth function and $\mathcal{O}$ a bounded region. Then we define

$$[G]_{\mathcal{O}} \doteq \{g\in\mathscr{D}:\ g\equiv G \text{ on a neighbourhood of } J_+(\mathcal{O})\cap J_-(\mathcal{O})\}.$$

Hence we consider the maps $S_{G,\mathcal{O}}(f):[G]_{\mathcal{O}}\to\mathscr{A}_G(\mathcal{O})[\![\hbar,\lambda]\!]$ which associate to every $g\in[G]_{\mathcal{O}}$ a relative S-matrix $S_g(f)$, with $\mathrm{spt}(f)\subset\mathcal{O}$, which generates the local algebras $\mathscr{A}_G(\mathcal{O})[\![\hbar,\lambda]\!]$. The

evaluation maps $e_{g,G} : S_{G,\mathbb{O}}(f) \mapsto S_g(f)$ are isomorphisms from $\mathscr{A}_G(\mathbb{O})[\![\hbar,\lambda]\!]$ to $\mathscr{A}_g(\mathbb{O})[\![\hbar,\lambda]\!]$ for all $g \in [G]_{\mathbb{O}}$. At this stage, the local net of algebras is defined through the following embeddings

$$i_{\mathbb{O}_1,\mathbb{O}_2} : \mathscr{A}_G(\mathbb{O}_1)[\![\hbar,\lambda]\!] \to \mathscr{A}_G(\mathbb{O}_2)[\![\hbar,\lambda]\!]; \qquad i_{\mathbb{O}_1,\mathbb{O}_2}\left(S_{G,\mathbb{O}_1}(f)\right) = S_{G,\mathbb{O}_2(f)},$$

for $\mathbb{O}_1 \subset \mathbb{O}_2$ and $f \in \mathscr{D}$ with $\mathrm{spt}(f) \subset \mathbb{O}_2$. Finally, we define the inductive limit $\mathscr{A}_G[\![\hbar,\lambda]\!]$ by means of the final projection $i_{\mathbb{O}} : \mathscr{A}_G(\mathbb{O})[\![\hbar,\lambda]\!] \to \mathscr{A}_G[\![\hbar,\lambda]\!]$ and we set

$$S_G(f) = i_{\mathbb{O}}\left(S_{G,\mathbb{O}}(f)\right).$$

This machinery allows us to change the cutoff on the interaction, making it a non-compactly supported function. Since this is made through isomorphisms of algebras of observables, we argue that the algebraic adiabatic limit can be taken without any problem, leaving the theory well-defined. To conclude the section, we notice that the net is indeed covariant:

Proposition 2.2.2. *Given a translation-invariant smooth function $G : \mathbb{M} \to \mathbb{R}$, then the net of algebras $\mathbb{O} \mapsto \mathscr{A}_G(\mathbb{O})[\![\hbar,\lambda]\!]$ becomes covariant by setting*

$$\alpha_x^G(S_G(f)) \doteq S_G(\alpha_x(f)).$$

Proof. We follow strictly [FR15, Theorem 2]. The goal is to show that α_x^G extends to an isomorphism $\mathscr{A}_G(\mathbb{O})[\![\hbar,\lambda]\!] \to \mathscr{A}_G(\mathbb{O}+x)[\![\hbar,\lambda]\!]$, where $\mathbb{O}+x \doteq \{y \in \mathbb{M} \mid y = z+x,\, z \in \mathbb{O},\, x \in \mathbb{M}\}$. To this avail, consider $\mathbb{O}_1 \supset \mathbb{O} \cup \mathbb{O} - x$ and $g \in [G]_{\mathbb{O}_1}$. Then $g, \alpha_x(g) \in [G]_{\mathbb{O}}$ and there exists $\rho_x^{\pm}$ such that

$$\alpha_x(g) = g + \rho_x^+ + \rho_x^-, \qquad \mathrm{spt}\left(\rho_x^{\pm}\right) \cap J_{\mp}(\mathbb{O}) = \emptyset.$$

Then, by the causal factorisation property, we have that

$$\alpha_x^G(S_G(f)) = e_{g,G}^{-1}\left(U_g^{-1}(x) \star_\omega \alpha_x\left(e_{g,G}(S_{G(f)})\right) \star_\omega U_g(x)\right),$$

where $U_g(x) = S_g\left(\rho_x^-\right)$ as per equation (2.2.21), hence the thesis follows by the isomorphism property of evaluation map $e_{g,G}$ defined above. □

This proposition, together with what we proved earlier, confirms that the net $\mathscr{A}_G[\![\hbar,\lambda]\!]$ satisfies the Haag-Kastler axioms of locality, isotony and covariance. The time-slice axiom deserves a more careful discussion, in fact it deals with the on-shell theory and, up to now, we only worked in the off-shell framework. Furthermore, the time-slice enters heavily also in the construction of the states, so a deeper look into it is required.

Another important aspect concerns the abstract character of the former construction: In spite of being perfectly rigorous, it is in practice impossible to construct the S-matrix exactly. A solution to this issue comes from the perturbative approach, which we have not fully exploited yet. What it is usually done in perturbation theory is an expansion around the free theory. In our language, this corresponds to embed the interacting algebra into the free one using the so-called *Bogoliubov map*, which is nothing but the quantisation of the classical Møller maps (1.2.46) defined for the classical theory.

2.2.1 The Time-Slice Axiom and the Dynamics

The construction we set up in the previous section was done for the off-shell formalism but, if we want to prove the time-slice axiom an on-shell approach is needed. Actually, it is impossible to perform an on-shell version of the interacting theory starting from the algebra $\mathscr{A}_{\mathrm{on}}[\![\hbar]\!]$ because perturbation theory does not respect the quotient used to defined it. Hence the implementation of an interacting version of the time-slice axiom requires something else. The solution was found in [CF09] and it requires to embed the interacting algebra into the free one using the Bogoliubov map. This enables to take advantage of the time-slice axiom known for the free theory, see Theorem 1.3.2 and take the on-shell quotient at that level. The identification of the interacting observables in $\mathscr{A}_G[\![\hbar,\lambda]\!]$ with some free ones in $\mathscr{A}_\omega[\![\hbar,\lambda]\!]$ proceeds following what we did in the classical picture using the Møller morphisms (1.2.46). In particular, the sought quantisation of these maps is obtained by taking the linear part of the relative S-matrix, see [BoSh59].

Definition 2.2.2 (Bogoliubov Map)**.** The linear part of a relative S-matrix is a linear map, named Bogoliubov map, $R_{V_g} : \mathscr{F}_{\mathrm{loc}} \to \mathscr{A}_\omega[\![\hbar]\!]$ defined by

$$R_{V_g}(F) \doteq \frac{\hbar}{\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}\mu}\bigg|_{\mu=0} S\left(V_g\right)^{\star_\omega -1} \star_\omega S\left(V_g + \mu F\right) = S\left(V_g\right)^{\star_\omega -1} \star_\omega \left(S\left(V_g\right) \cdot_T F\right). \tag{2.2.22}$$

The functional $R_{V_g}(F)$ is interpreted as the retarded, interacting observable associated with $F \in \mathscr{A}_\omega[\![\hbar]\!]$ with respect to the interaction V_g. For simplicity of notation, we will omit the suffix g, writing simply $R_V(F)$ instead of $R_{V_g}(F)$. Notice that the Bogoliubov map is well-defined for off-shell observables only. An evidence of the fact that the Bogoliubov map intertwines between interacting and free observables can be obtained considering a linear, on-shell functional F_{Pf}, P being the free Klein-Gordon operator, and applying on it equation (2.2.22). This gives

$$F_{Pf} = R_V\left(F_{Pf}\right) + \lambda R_V\left(V^{(1)}\right),$$

which means that weak solutions of the free equation of motion are sent into weak solutions of the interacting one, or, in other words, this is an off-shell version of the equations of motion. Moreover, this formula expresses clearly the perturbative feature of the theory we are developing; in fact an interacting observable equals a free one plus an interaction Lagrangian-dependent term, as expected.

By definition, causal factorisation property and the retardation proper of the relative S-matrices descend to the interacting observables. Furthermore, one would like to define also an *interacting time-ordered product*: Heuristically, we would expect it to satisfy a relation analogous to the one introduced in equation (2.1.1), namely:

$$R_V(F) \cdot_{T,V} R_V(G) = \begin{cases} R_V(F) \star_\omega R_V(G) & \text{for } F \succsim G \\ R_V(G) \star_\omega R_V(F) & \text{for } G \succsim F \end{cases}, \tag{2.2.23}$$

Then, assuming $F \succsim G$, we can argue that the former relation would correspond to the causal

factorisation:

$$R_V(F \cdot_T G) = -\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}\mu_1 \mathrm{d}\mu_2}\bigg|_{\mu_1=\mu_2=0} S(V_g)^{\star_\omega -1} \star_\omega S\left(V_g + \mu_1 F + \mu_2 G\right) =$$
$$-\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}\mu_1 \mathrm{d}\mu_2}\bigg|_{\mu_1=\mu_2=0} S\left(V_g^{\star_\omega -1} \star_\omega\right) S_g\left(\mu_1 F\right) \star_\omega S_g\left(\mu_2 G\right) = R_V(F) \star_\omega R_V(G) = R_V(F) \cdot_{T,V} R_V(G),$$

where the non-interacting causal factorisation has been used in the second step. Concerning the retardation, given $\mathrm{spt}(g')$ in the future of F, then $R_{V_{g+g'}}(F) = R_{V_g}(F)$. In particular, if $V_g \succsim F$, then $R_{V_g}(F) = F$: This is particularly satisfactory since it implies that, if the interaction is turned on in the future of an observable F, then F is not affected by it, so causality is preserved.

Unfortunately, the Bogoliubov map is not surjective, hence we can not achieve a description of the interacting observables and of the interacting time-ordered product by simply inverting it. In particular, it is impossible to define an interacting product as

$$F \star_V G \doteq R_V^{-1}\big(R_V(F) \star_\omega R_V(G)\big).$$

This product is indeed only well-defined for regular functionals, but, as already noticed, they are not sufficient for a complete description of the scalar field theory. Hence, we will consider as the interacting algebra the *-subalgebra $\mathscr{A}_V[\![\hbar,\lambda]\!] \subseteq \mathscr{A}_\omega[\![\hbar,\lambda]\!]$ generated by the Bogoliubov elements $R_V(F)$ for all $F \in \mathscr{A}_\omega[\![\hbar]\!]$.

At this stage the time-slice axiom enters the game: Together with the causal properties of the S-matrices, it allows to identify the interacting algebra with the free one. This is a key feature of the theory and it will play a prominent role in the following part of this work, hence we are going to deal with it carefully.

The proof of its validity in pAQFT was first found by Chilian and Fredenhagen in [CF09] and it is based on the causal factorisation property **(S2)** (and its descendants for the relative S-matrix and for the Bogoliubov map) and on the initial condition $S(0) = \mathbb{1}$. To start with we present the following technical lemma, which corresponds to Proposition 3 in the appendix of [CF09], where its proof can be found.

Lemma 2.2.1. *Given a globally hyperbolic space-time $\mathbb{M}$, $\mathbb{K} \subset \mathbb{M}$ compact and $\mathbb{P} \subset \mathbb{M}$ past-compact. Then $J_-(\mathbb{K}) \cap \mathbb{P}$ is contained in a compact set.*

Taking a relative S-matrix $S_g(f)$ where g is past compact, the former lemma implies that $J_-(\mathbb{K}) \cap \mathrm{spt}(g)$ for every compact region $\mathbb{K}$ is contained in a relatively compact region $\mathbb{O}$, so there exists $h \in \mathscr{D}$ such that $h \equiv g$ on $J_-(\mathbb{K})$, that is $h \in [G]_{J_-(\mathbb{K})}$, then $S_g(f) = S_h(f)$ for all f such that $\mathrm{spt}(f) \subset \mathbb{K}$. Moreover, as we have already seen, $S_h(f)$ does not depend on the choice of h.

Theorem 2.2.1 (Time-Slice Axiom for the Interacting Net)**.** *Given Σ_I a neighbourhood of a Cauchy surface $\Sigma \subset \mathbb{M}$, then $\mathscr{A}_G(\Sigma_\mathrm{I})[\![\hbar,\lambda]\!]$ is isomorphic to the interacting algebra $\mathscr{A}_G[\![\hbar,\lambda]\!]$ built over the whole Minkowski.*

Before entering the details of the proof, which are rather technical, we would like to give an heuristic explanation of the idea behind it and of its consequences. First of all, we point

out that we will use thoroughly the following facts: The relative S-matrix $S_g(f)$ is well-defined also for past-compact g, satisfies the causal factorisation property as per Proposition 2.2.1 and it trivialises if the interaction is localised in the future of the observables. Furthermore, a change in the cutoff g will cause a modification of the observables which can be proved to be an isomorphism realised by the composition with (formal) unitary operators. The issue here is that the time-slice axiom for the free theory holds on-shell, but the perturbative interacting framework is developed completely off-shell. As we mentioned previously, the reason is due to the fact that the quotient which implements the dynamics in the free theory is not preserved by perturbation theory and by the time-ordering. The on-shellness of the time-slice axiom for the free theory and the off-shell nature of perturbation theory then seem to be in an unsolvable contrast. The way to avoid the issue is to perform the quotient on the free algebra only after the application of the map which embeds the interacting algebra into the free one. It is important to notice that the embedding is the identity in the past of any Cauchy surface Σ which is in the past of the interaction, namely $\mathrm{spt}(V_g) \cap J_+(\Sigma) = \emptyset$.

This observation is of pivotal importance for the subject of this thesis, in Chapter 4 in particular, the identification of the two algebras implies that we can define interacting states at free level. In particular, the state turns out to be insensitive to the additional unitaries needed to identify the two, so it may be equivalently defined on one or on the other. This fact will allow us to define consistently the relative entropy and to compare interacting states obtained with different perturbations which, *a priori* are defined on different interacting algebras, but which after that may be seen as states on the same, free algebra.

Proof. The proof we are going to present follows closely the original one presented in [CF09]. Let us consider a relatively compact region $\mathbb{O}$ and a Cauchy surface Σ, assuming that both are included in the future of a second Cauchy surface Σ_1, namely $\mathbb{O}, \Sigma \subset J_+(\Sigma_1)$. We may then consider g a smooth function supported in $J_+^\circ(\Sigma_1)$ which is equal to one in $\mathbb{O}$ and Σ_ϵ. Given also $\epsilon > 0$, we consider $\Sigma_\epsilon \doteq (-\epsilon, \epsilon) \times \Sigma$ an open neighbourhood of Σ.

We are going to prove that

$$\mathscr{A}_g(\mathbb{O})[\![\hbar, \lambda]\!] \subset \mathscr{A}_g(\Sigma_\epsilon)[\![\hbar, \lambda]\!] \qquad \forall\, \epsilon \in \mathbb{R}.$$

We already know that

1. $\mathscr{A}_g(\mathbb{O})[\![\hbar, \lambda]\!] \subset \mathscr{A}_0(\mathbb{M})[\![\hbar, \lambda]\!]$ by construction;
2. $\mathscr{A}_0(\Sigma_\epsilon)[\![\hbar, \lambda]\!] = \mathscr{A}_0(\mathbb{M})[\![\hbar, \lambda]\!]$ for every ϵ because of the time-slice axiom for the free theory, Theorem 1.3.2.

Hence, in order to conclude the proof we just need to show that $\mathscr{A}_0(\mathbb{M})[\![\hbar, \lambda]\!] \subset \mathscr{A}_g(\Sigma_\epsilon)[\![\hbar, \lambda]\!]$. We recall that $\mathscr{A}_0(\mathbb{O})[\![\hbar, \lambda]\!]$ is the algebra generated by the formal S-matrices $S(g)$, with $\mathrm{spt}(g) \subset \mathbb{O}$, while $\mathscr{A}_g(\mathbb{O})[\![\hbar, \lambda]\!]$ is the algebra generated by the relative S-matrices $S_g(f)$ with $\mathrm{spt}(f) \subset \mathbb{O}$. For simplicity of notation, in the following we will omit to specify that the algebras are made of formal power series. Moreover, we will also avoid to write the $\star_\omega$ product explicitly.

The starting point is showing that we can associate to every formal S-matrix $S(f)$ a relative S-matrix $S_{g,g'}(f) \in \mathscr{A}_g(\Sigma_\epsilon)$, with g, g' properly supported. This association will also generate a surjective endomorphism of $\mathscr{A}_0(\mathbb{M})$ which, in fact, will realise the time-slice axiom. To do so, we will tacitly use the causal factorisation property (**S2**) repeatedly.

Consider $\Sigma_{\epsilon'}$ such that $\mathrm{spt}(f) \subset \Sigma_{\epsilon'}$, with $\epsilon' < \epsilon$ and define g' such that

$$g' \equiv g \text{ on } \Sigma_{\epsilon'}, \qquad \mathrm{spt}(g') \subset \Sigma_\epsilon.$$

This permits to define the following relative S-matrix

$$S_{g,g'}(f) \doteq S_g(-h')^{-1} S_g(-h' + f), \qquad \text{where} \qquad \begin{cases} \mathrm{spt}(f) \subset \mathbb{K}^\circ \\ \mathrm{spt}(h') \subset \Sigma_\epsilon \\ h' \equiv g' \text{ on } J_-(\mathbb{K}) \end{cases},$$

$\mathbb{K}$ being a compact set contained in $\Sigma_{\epsilon'}$ and $\mathbb{K}^\circ$ being the interior of $\mathbb{K}$. $S_{g,g'}(f)$ is independent of the choice of h'. Furthermore, we notice that $S_{g,g'}(f)$ is an element of $\mathscr{A}_g(\Sigma_\epsilon)$. By definition of relative S-matrix (2.2.17) we have

$$S_{g,g'}(f) = S(h - h')^{-1} S(h - h' + f), \qquad \text{where} \qquad \begin{cases} \mathrm{spt}(h') \subset \mathbb{L}^\circ \\ h \equiv g \text{ on } J_-(\mathbb{L}) \end{cases},$$

$\mathbb{L}$ being compact. Then we may choose a partition of unity in such a way that

$$h - h' = h_+ + h_- \qquad \text{where} \qquad \mathrm{spt}(h_\pm) \cap J_\mp(\mathrm{spt}(f)) = \emptyset.$$

Due to the causal factorisation property we have

$$S_{g,g'}(f) = S(h_-) S(f) S(h_-)^{-1}.$$

This formula leads to two important consequences:

- Given $A \in \mathscr{A}_0(\mathbb{K})$[4], with $\mathbb{K} \subset \Sigma_{\epsilon'}$, and h, h' as above, we have

$$S(h_-)^{-1} A S(h_-) \in \mathscr{A}_g(\Sigma_\epsilon).$$

- Taking $\epsilon'' < \epsilon'$ and considering $\mathbb{O}'' \doteq \Sigma_{\epsilon''} \cap J_+(J_-(\mathbb{K}) \cap \Sigma_\epsilon)$, we may use the time-slice axiom for the free theory to obtain

$$S_{h_-}^{-1} A S_{h_-} \in \mathscr{A}_0(\mathbb{O}'').$$

The combination of these two facts implies that the map $S(f) \mapsto S_{g,g'}(f)$, with $\mathrm{spt}(f) \subset \Sigma_{\epsilon'}$, extends to the endomorphism

$$\alpha : \mathscr{A}_0(\mathbb{M}) \to \mathscr{A}_0(\mathbb{M}), \qquad \alpha(\mathscr{A}_0(\mathbb{M})) \subseteq \mathscr{A}_g(\Sigma_\epsilon).$$

This is what we need due to properties (1) and (2) highlighted at the beginning. We know already that α is injective since, for every relatively compact $\mathbb{K}'$ there is an invertible element $U \in \mathscr{A}_0(\mathbb{M})$

[4] To be more precise, we shall take $\mathscr{A}_0(\mathbb{O}')$, with $\mathbb{O}'$ relatively compact with closure $\mathbb{K}$.

such that $\alpha(A) = UAU^{-1}$ for all $A \in \mathscr{A}_0(\mathbb{K}')$.

In order to conclude the proof we need to show that α is surjective, in that case we have that

$$\mathscr{A}_0(\mathbb{M}) = \alpha(\mathscr{A}_0(\mathbb{M})) \subseteq \mathscr{A}_g(\Sigma_\epsilon).$$

To this avail, we consider a partition of unity such that

$$g - g' = g_+ + g_- \qquad \text{where} \qquad \operatorname{spt}(g_\pm) \cap J_\mp(\Sigma_{\epsilon'}) = \emptyset.$$

By definition of α and using the causal factorisation we obtain that

$$\alpha(S(f)) = S_{g_-}(f), \qquad \operatorname{spt}(f) \subset \Sigma_{\epsilon'}.$$

This formula is telling us that an interaction in the past (*i.e.* supported in $\operatorname{spt}(g_-)$) causes an endomorphism of the algebra. Furthermore, we may generate this endomorphism using invertible elements $S(h_-)$, with h_- as above, that is coinciding with g_- in the past of a compact subregion of Σ which is large enough.

Actually, we can do more, we can take a third Cauchy surface Σ_2 in the past of Σ_1 and look at $\mathbb{D} \doteq J_-(\Sigma_1) \cap J_+(\Sigma_2)$, then we choose

$$h_- \equiv g_- \qquad \text{on} \qquad J_+(J_-(\mathbb{K}) \cap \mathbb{D}),$$

for $\mathbb{K}$ compact as above. The time-slice axiom 1.3.2 then implies that $\mathscr{A}_0(\mathbb{K}) \subset \mathscr{A}_0(J_-(\mathbb{K}) \cap \mathbb{D})$, which in turn is generated by elements $S(f)$ with compactly supported f such that $\operatorname{spt}(f) \subset J_-(\mathbb{K}) \cap \mathbb{D}$. In this setting, $\operatorname{spt}(f)$ is in the past of Σ_1, while $\operatorname{spt}(h_-)$ is in its future, so the causal factorisation **(S2)** applies and we found the sought (approximation of) the inverse of α:

$$\alpha^{-1}_{h_-}(S(f)) = S(h_-)S(f)S(h_-)^{-1} = S(h_- + f)S(h_-)^{-1},$$

which in addition is independent of the choice of h_-. This proves the existence of the inverse of α on $\mathscr{A}_0(J_-(\mathbb{K}) \cap \mathbb{D}) \supset \mathscr{A}_0(\mathbb{K})$ for all compacts $\mathbb{K} \subset \Sigma_{\epsilon'}$, and hence everywhere by the time-slice axiom. This concludes the proof. □

Remark 2.2.1. The time-slice axiom and the causal factorisation property have a deep implication. From the previous proof we deduce that the free and the interacting algebra are isomorphic. Anyway, the isomorphism is not a canonical one, in particular the various elements are intertwined by unitaries. Actually, one gets a canonical isomorphism in the case of regular observables, which is given by the Bogoliubov map.

Heuristically, we may argue that the presence of an isomorphism is not that strange, in fact $R_V(F) = F$ if $V \gtrsim F$, so the interacting and the free algebras are really the same in the past of the interaction. The time-slice axiom then allows to restrict the algebra to a neighbourhood of a Cauchy surface, and then propagate the construction to the whole Minkowski. The combination of these two ideas guarantees that the Bogoliubov map is indeed a (non canonical) *-isomorphism, which will be crucial to us since it will make possible the identification of states on the free and

on the interacting algebras. The key point is that states are insensitive to the presence of the unitaries, namely the evaluation on a state "makes the isomorphism canonical". This fact is crucial in the definition of the entropy for perturbative QFT which will be given in Chapter 4.

The last aspect we want to discuss is the role of the covariance, in the sense of Proposition 2.2.2, in the switching from the S-matrices to the Bogoliubov elements. In particular, we define the space-time translations as

$$\alpha_x^{V_g}(R_V(F)) \doteq R_V(\alpha_x(F)) \qquad \forall\, x \in \mathbb{M},\ \forall\, F \in \mathscr{A}_\omega(\mathbb{O})[\![\hbar]\!].$$

Notice that we will usually omit the dependence from the cutoff, writing simply α_x^V instead of $\alpha_x^{V_g}$. If in particular x is a time-coordinate, the former definition generates a one parameter group of isomorphisms of the algebra of interacting observables, given by

$$\alpha_t^V(R_V(F)) \doteq R_V(\alpha_t(F)), \tag{2.2.24}$$

which is interpreted as the *interacting time evolution*, often called also *interacting dynamics*. Anyway, we will return on this subject in the next section, when we will discuss states for the interacting theory.

Connection with the path integral approach

Before proceeding with the study of the states in the interacting theory, we would like to clarify the connection with the mostly used path integral approach to QFT [PS95, Zi02]. In fact, in spite of its lack of mathematical rigour, this approach has revealed to be very successful in furnishing very accurate predictions, thus the agreement between the two would be a good consistency test for pAQFT. We warn the reader that this section is meant to give an interpretation to the whole formalism hitherto developed, so for the sake of clarity we will not take over a mathematically rigorous discussion and we will skip most of the mathematical details.

In the path integral framework usually a Gaussian measure $\mathfrak{D}_F$ on the space of field configurations with covariance ω_F is defined and then the generating functional is introduced as the characteristic function of this measure, namely

$$Z_0(J) \doteq \frac{1}{N_0}\int e^{\mathrm{i}J_f(\psi)}\mathfrak{D}_F(\phi-\psi) \qquad \forall\, f \in \mathscr{D},$$

where N_0 is a normalisation factor, often interpreted as a partition function, which is given by

$$N_0 \doteq \int \mathfrak{D}_F(\phi) \equiv \int e^{\frac{\mathrm{i}}{\hbar}L_0(\phi)}d\phi,$$

while $J_f(\psi)$ is a linear functional, which we denote by J instead of F only to make contact with the notations of the physical literature. Thus, the time ordered-product is defined by the functional derivatives of the generating functional, as follows:

$$\frac{1}{\mathrm{i}^n}\frac{\delta^n}{\delta J_f(x_1)\cdots\delta J_f(x_n)}\bigg|_{f=0} Z_0(\phi;f) = \mathscr{T}_{0,n}\left(\mathrm{Ev}_{x_1}(\phi),\dots,\mathrm{Ev}_{x_n}(\phi)\right),$$

where $\mathrm{Ev}_x(\phi)$ is the evaluation functional defined in (1.3.65). It is easy then to recognise in the previous formula the time-ordered exponential, thus the generating functional corresponds to the formal S-matrix. This definition does not take into account non-linear functionals and interactions, so we have to modify the path integral to take into account an interaction V. This leads to the famous Feynman-Kac formula

$$Z(J) \doteq \frac{1}{N}\int e^{\mathrm{i}J_f(\psi)} e^{-\frac{\mathrm{i}}{\hbar}L_I(\psi)} \mathfrak{D}_F(\phi-\psi) = \frac{1}{N}\int e^{\mathrm{i}J_f(\phi)} e^{\frac{\mathrm{i}}{\hbar}(L_0-L_I)(\phi)} d\phi, \qquad N \doteq \int e^{\frac{\mathrm{i}}{\hbar}(L_0-L_I)(\phi)} d\phi.$$

The insertion of the interaction Lagrangian makes Z correspond to the relative S-matrix in the pAQFT formalism. Hence, taking the first functional derivative amounts to applying the Bogoliubov map, as shown by the following computation

$$\frac{1}{\mathrm{i}}\frac{\delta}{\delta J_f(\phi)}\bigg|_{f=0} Z(J) = \frac{1}{N}\int \phi\, e^{\frac{\mathrm{i}}{\hbar}[L_0-L_I](\phi)} d\phi = \frac{1}{\mathrm{i}}\frac{\delta}{\delta J_f(\phi)} S\left(V + J_f\right)(\phi) = S(V)\cdot_T J_f(\phi),$$

where the normalisation $S(V)^{\star_\omega -1}$ is only apparently missing, since it is just given by the normalisation factor. It must be stressed that, in the usual path integral formulation of QFT, no cutoffs are inserted in the interaction, hence the so-obtained time-ordered product is IR divergent and the renormalisation must be applied later. In addition, the absence of the cutoff implies that the interactions are meant as infinitely extended, so the correspondence with the relative S-matrix is sort of spoiled. More precisely, this has to do with the notion of adiabatic limit. In the path integral approach, usually only the vacuum expectation values are taken into account, which are known to be infra-red finite for the massive free scalar field, so once renormalisation is performed, a finite theory is at hand. In particular, the Gell-Mann and Low formula holds [DF01a]

$$\left\langle \phi(x_1),\dots,\phi(x_n)\right\rangle = \frac{\left\langle \Omega \,\middle|\, \mathscr{T}_n\left(\mathrm{Ev}_{x_1}(\phi),\dots,\mathrm{Ev}_{x_n}(\phi)\right)\Omega\right\rangle}{\langle \Omega\,|\,\Omega\rangle},$$

where the crochet $\left\langle \phi(x_1),\dots,\phi(x_n)\right\rangle$ stands for the n-point correlation functions, $|\Omega\rangle$ is the vector representative of the vacuum state and

$$\left\langle \Omega \,\middle|\, F(\phi)\Omega\right\rangle \doteq \int F(\phi)\, e^{\frac{\mathrm{i}}{\hbar}[L_0-L_I](\phi)} d\phi,$$

for every functional F on the field configurations. In our framework this simply corresponds to the evaluation on the vacuum state on Bogoliubov elements and taking the adiabatic limit at the level of the state:

$$\lim_{g\to 1} \omega_g^{\mathrm{vac}}\left(R_{V_g}(F)\right) = \frac{\omega^{\mathrm{vac}}(S(V)\cdot_T F)}{\omega^{\mathrm{vac}}(S(V))}.$$

Actually, the algebraic viewpoint highlights that the vacuum state is not the only physically meaningful one and that the Gell-Mann and Low formula does not holds for all physical states, see [DF01a]. We will see this explicitly in the case of the interacting KMS state in the next section. But, apart from this consideration, the previous equation shows that the two approaches yield to the same result.

A further difference concerns the role of the Feynman diagrams: In the path integral formulation they are considered as fundamental objects that encode the key features of the model, providing a full physical picture. In pAQFT they loose their privileged role and they are rather

considered as a mere computational tool. They can be derived taking advantage of a diagrammatic interpretation that can be given to the $\star$ product (1.3.74), in particular every term of the summand of the form

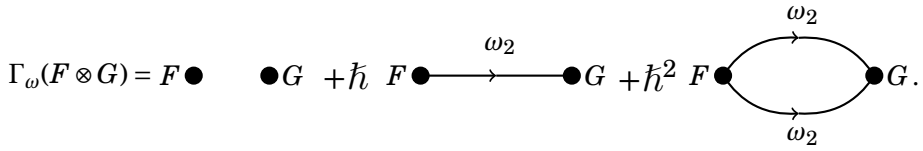
$$\Gamma^{(2)}(F,G) = \left\langle F^{(n)}, \omega_2^{\otimes n} G^{(n)} \right\rangle$$

corresponds to a graph with n lines connecting the vertices given by F, G (recall equation (1.3.76)). In particular every line gives a contribution proportional to ω_2.

Example 2.2.1. In this example we want to consider the diagrammatic expansion led by the star product $\star_\omega$ between two quadratic functionals $F, G \in \mathscr{A}_\omega[\![\hbar]\!]$. Recalling the expression of $\star_\omega$ in terms of the operator Γ_ω, see equation (1.3.75), we can compute

$$\Gamma_\omega(F \otimes G) = F \cdot G + \hbar \left\langle F^{(1)}, \omega_2 G^{(1)} \right\rangle + \hbar^2 \left\langle F^{(2)}, \omega_2^{\otimes 2} G^{(2)} \right\rangle,$$

to which corresponds the diagrammatic expression



Notice that this expression corresponds to a diagrammatic expression in which tadpoles have already been removed.

Since the $\star$ and the $\cdot_T$ products are in fact equal in form, a similar graphic interpretation can be given also to the time-ordered product, where the role of the 2-point function of the state is replaced by the Feynamn propagator ω^{F}. This corresponds to the usual Feynman graphs used in the physical literature, see [Ke10].

2.3 The Interacting KMS State

This subsection consists in a review of the construction of a KMS state for the interacting theory, which was performed for the first time in [FL14] (see also [Li13]). In this work, the authors succeeded in generalising the Araki perturbation theory (see [BR97b]) to Quantum Field Theory, showing that the state obtained this way is not affected by infra-red divergences, even if the adiabatic limit is taken. This construction was developed for a massive Klein-Gordon theory on Minkowksi, and subsequently extended to the massless case for $\lambda\phi^4$ interactions in [DrHaPi16]. This is preceded by some generalities on states for the interacting theories.

2.3.1 States for the Interacting Theory

In this section we face the problem of defining states on the interacting algebra $\mathscr{A}_V[\![\hbar,\lambda]\!]$. We already know how to deal with states over an algebra of formal power series from Section 1.3.3, so this does not constitutes an issue. Hence a state for the interacting theory is a positive, linear and normalised (in the sense of formal power series) functional

$$\omega : \mathscr{A}_G[\![\hbar,\lambda]\!] \to \mathbb{C}[\![\hbar,\lambda]\!].$$

Actually, we have to keep in mind that the full algebra $\mathscr{A}_G[\![\hbar,\lambda]\!]$ is built as an inductive limit via the whole procedure explained in the previous section, hence if we want to define states over it we shall rather define them on the local algebras $\mathscr{A}_G(\mathcal{O})[\![\hbar,\lambda]\!]$. But this creates a huge problem concerning the adiabatic limit $g \to 1$. As we have seen, the causal factorisation property give us a way to change the supports of the functionals and to enlarge it in such a way to enable us to take the limit algebraically. At the level of states this is not that simple. The question of existence of the adiabatic limit at the level of states, usually called *weak adiabatic limit*, has to be discussed case by case and there are very few examples where the issue is solved. Concerning the vacuum case, the weak adiabatic limit is known to exist since [EG73], in the case of KMS states this was the main result of [FL14] for a massive scalar field theory, while for the massless one the construction was done in [DrHaPi16]. Regarding massless particles, some further interesting results have been achieved recently in [Du18].

In general, the situation we have to deal with is the following: The interacting state ω^V is defined on the local algebras $\mathscr{A}_G(\mathcal{O})[\![\hbar,\lambda]\!]$, so we have a sequence $\{\omega_g^V(A_g)\}$ for all $A_g \in \mathscr{A}_G(\mathcal{O})[\![\hbar,\lambda]\!]$ and we have to study the limit $g \to 1$ of this sequence. The first thing we have to do is to define how to explicitly perform the limit in rigorous mathematical terms. The solution to this problem is to take the limit in the sense of van Hove:

Definition 2.3.1 (Def. 2, [FL14])**.** A van Hove sequence is a sequence of compactly supported functions $\{h_n\}_{n\in\mathbb{N}}$ such that $0 \le h_n \le 1$ and

$$h_n(x) = \begin{cases} h_n(x) = 1 & \text{if } |x| < n \\ h_n(x) = 0 & \text{if } |x| > n+1 \end{cases}.$$

A functional ω converges to ℓ in the sense of van Hove if $\lim_{n\to\infty} \omega(h_n) = \ell$ for every van Hove sequence. In this case we write

$$\underset{h\to 1}{\text{vH-lim}}\, \omega(h) = \ell.$$

Once we have defined how to take the limit, we should check wether the limit exists and can be effectively taken. Actually it is easy to argue from the former discussion how the existence of the limit depends on the state and on its *clustering properties*, *i.e.* on the way it decades for large space and time directions. This explains why the existence of the weak adiabatic limit must be discussed case by case. Furthermore, its non-existence is interpreted as the presence of infrared divergencies in the theory.

The hard task is then to find a way to explicitly construct interacting states. A way to do so is taking advantage of the Bogoliubov map and of the identification of the interacting and the free algebra. A possibility is to induce an interacting state by composing a free one with the Bogoliubov map, that is

$$\omega_g^V \doteq \omega \circ R_{V_g}.$$

We have already seen that if we restrict to regular functionals $\mathscr{A}_{\text{reg}}[\![\hbar]\!]$, the Bogoliubov map is indeed an isomorphism which allows us to define an interacting star product $\star_V$. This implies that every state on the free algebra can be pushed forward to the interacting algebra generated by

regular functionals $\mathscr{A}^V_{\mathrm{reg}}$. Moreover, any concern about the adiabatic limit is avoided in this way, since the dependance on the cutoff here is present in the Bogoliubov map only. More precisely, using the time-slice axiom we may restrict ourselves in constructing the interacting state on a neighbourhood of a Cauchy surface Σ_ϵ. Then, for any observable F supported in a region $\mathbb{O}$, the support of its associated Bogoliubov element $R_{V_g}(F)$ is $J_-(\mathbb{O}) \cap \Sigma_\epsilon$, and this is not touched by the adiabatic limit due to the causal factorisation properties (or, in other words, due to the well-definiteness of the algebraic adiabatic limit). Furthermore, this is true for any class of functionals and not only for regular ones.

At the same time, we stress that the Bogoliubov map is not an isomorphism anymore when applied to local functionals, so the induced state ω^V_g can not be transported back to the "true" interacting algebra, but it remains defined on the *-subalgebra $\mathscr{A}^V[\![\hbar,\lambda]\!]$ generated by the Bogoliubov elements (which is identified with the free algebra by the time-slice axiom and the causal factorisation property), which we interpret as the *-algebra of the interacting observables.

Furthermore, we can define the n-point function for the induced state ω^V for local functionals $F_1,\dots,F_n \in \mathscr{F}_{\mathrm{loc}}(\mathbb{O})$ by

$$\omega^V_g\left(F_1 \star_{V_g} \cdots \star_{V_g} F_n\right) \doteq \omega\left(R_{V_g}(F_1) \star_\omega \cdots \star_\omega R_{V_g}(F_n)\right), \tag{2.3.25}$$

and this enables us to define expectation values and, in principle, to achieve predictions. This agrees with other approaches to perturbation theory present in the literature, for examples with the ones using Wightman functions, such as [Ste93]. Actually, not all the interacting states are of the form $\omega \circ R_{V_g}$, and they actually turn to depend on the cutoff in a highly non-trivial fashion: In this case the weak adiabatic limit must be addressed carefully and a well-defined state is not always obtained. This is the case, for example, for the definition of an interacting KMS state: Several attempts has been made of defining it as $\text{vH-lim}_{g\to 1}\,\omega^\beta \circ R_{V_g}$, but all them were affected by IR divergencies, see for instance [Al90, LW87, Ste95]. The correct construction has been achieved only recently in [FL14, Li13] and will be the subject of the next section. What we want to stress here is that equation (2.3.25) defines the interacting states as functionals on $\mathscr{A}^V[\![\hbar,\lambda]\!]$ as well as on the free algebra $\mathscr{A}_\omega[\![\hbar,\lambda]\!]$, and that there is no loss of generality in looking at them as state on the free algebra. This viewpoint will be adopted in Chapter 4 and it will allow us to confront different interacting states in order to define the relative entropy between them.

To conclude, we want to spend some words on the translation-invariance of states defined in the interacting algebras. Actually, as for the free case, most of the interesting states are invariant under the action of time-translations; this is the case also for the interacting KMS one, which is the main subject of this thesis, so a deeper analysis is in order.

As an exemple, we want to discuss the behaviour under the interacting time-translations defined in equation (2.2.24), the case of a generic Poincaré transformation being analogous. We say that an interacting state ω^V is translation-invariant if

$$\left(\alpha^{V_g}\right)^* \circ \omega^V_g \doteq \omega^V_g \circ \alpha^{V_g} = \omega^V_g.$$

What usually happens is that the presence of the cutoff g in the potential breaks the translation-invariance of interacting states induced by the free one. This comes true because, by definition of

the interacting dynamics, the cutoff is not affected by the translation. On the other hand, these states do not maintain the invariance with respect to the free dynamics, which in fact acts on the Bogoliubov elements as

$$\alpha_t\left(R_{V_g}(F)\right) = R_{\alpha_t(V_g)}(\alpha_t(F)) \qquad \forall F \in \mathscr{F}_{\mathrm{loc}}. \tag{2.3.26}$$

2.3.2 The Construction of the Interacting KMS State

In this section we summarise the construction of the interacting KMS state for a massive scalar field theory on Minkowski space-time $\mathbb{M}$ performed in [FL14], see also [Li13], to which we adhere strictly. The massless case for a $\lambda\phi^4$ interaction was addressed in [DrHaPi16] using the principle of perturbative agreement. Here, we will limit ourselves to furnish the main results and quoting the formulas which will be necessary in the following, for the proofs, above all regarding the finiteness in the weak adiabatic limit, we refer to the original paper.

To start with, we fix some notations and conventions. The theory we are considering is described by the Klein-Gordon equation with a polynomial interaction of the form (2.2.15). Moreover, we will make a choice of the $\star_\omega$ product, in particular, from now on, we will work with the one defined out of the free, extremal, quasi-free KMS state ω^β, whose 2-point function is specified in equation (1.3.70). This choice is motivated by the simplification induced by equation (1.3.78). For sake of brevity, from now on we will omit the specification of the state in the star product, that is we will always write simply $\star$ instead of $\star_{\omega^\beta}$. Furthermore, we will also put $\hbar \equiv 1$[5] and we will avoid to specify that we are dealing with algebras of formal power series, in particular we name $\mathscr{A}_{\omega^\beta}$ and $\mathscr{A}^V$ the free algebra endowed with the star product $\star$ and the interacting algebra respectively. From now on, whenever we will refer to the interacting algebra, we will mean the *-subalgebra of the free algebra generated by the Bogoliubov elements.

The strategy is to define an *Hamiltonian formalism* for perturbative Quantum Field Theory similar to the one available in non-relativistic quantum theories. Having it at our disposal, the perturbative construction of an interacting KMS state may be developed by generalising the perturbation theory of Araki, see [Ar73] or [BR97b, Section 5.4.1.] for a review. Unfortunately, the Hamiltonian of an interacting QFT is too singular to use perturbation of self-adjoint operators and, moreover, the Haag's theorem forbids the representation of a ground state of the interacting theory as a vector in the Fock space. Actually, the Hamiltonian formalism requires a factorisation of the space-time into a Cauchy surface and a time axis, and the observables are assigned in terms of initial data on the surface. Again, the local observables are too singular to be restricted on a Cauchy surface. The way-out is then obtained by restricting the theory on a neighbourhood of a Cauchy surface and then to take advantage of the time-slice axiom (Theorem 2.2.1) for identifying the free and the interacting algebra built over the neighbourhood. This allows for a comparison of the free and the interacting dynamics: After the identification they result to be automorphisms group acting on the same algebra, so they differ by a co-cycle which, if a spatial cutoff is present

[5] We stress that we are assuming from the beginning to work with polynomial functionals in the variable $\hbar$, so this choice causes no loss of generality.

on the interaction, is unitary. The infinitesimal generator of the co-cycle is then interpreted as a regularised interaction Hamiltonian density. At this stage, one realises that the so-obtained framework is the same as the one introduced by Araki, so it is enough to repeat the construction, *mutatis mutandis*. The last, and more tricky step, concerns checking that the state defined in this way remains finite after the weak adiabatic limit is taken. A proof of that is given in [FL14] and it goes by direct computation, heavily using the spatial clustering properties of the free KMS state.

Let us give some more details on the construction. Let $\Sigma \subset \mathbb{M}$ be a Cauchy surface and let $\Sigma_\epsilon \doteq \{(t,\mathbf{x}) | -\epsilon < t < \epsilon\}$, with $\epsilon > 0$, be a time-slice. Then, we consider the theory defined over a region $\mathbb{O} \subset \Sigma_\epsilon$. Due to the causal factorisation property, we may change the cutoff g present in the potential V_g without loss of generality and without changing the physics of the system, therefore we consider the modified potential

$$V_{\chi,h}(\phi) \doteq \int \mathrm{P}[\phi](x) h(\mathbf{x}) \chi(t)\, d^3\mathbf{x}\, dt, \tag{2.3.27}$$

where we have choosen g to be the product of a spatial function $h \in \mathscr{D}\left(\mathbb{R}^3\right)$ and of a temporal, past-compact one $\chi \in C^\infty_{pc}(\mathbb{R})$. In particular, the two functions have to be taken such that $0 \leq h, \chi \leq 1$ and

$$h(\mathbf{x}) = 1 \quad \text{if} \quad \mathbf{x} \in \mathbb{O}_S, \qquad \chi(t) = \begin{cases} 1 & \text{if } t > -\epsilon \\ 0 & \text{if } t < -2\epsilon \end{cases}, \tag{2.3.28}$$

where we are denoting the region where the observables are supported as $\mathbb{O} = (-\epsilon, \epsilon) \times \mathbb{O}_S$. Taking the weak adiabatic limit now corresponds to send $h \to 1$ in the sense of van Hove, as per Definition 2.3.1. In the following, we will often omit the suffix χ since in [FL14] it is proved that the whole construction is independent from χ and ϵ.

The first step consists in relating the interacting dynamics α^V_t, introduced in eqn. (2.2.24), to the free one through a co-cycle U_h:

$$\alpha^V_t(A) = U_h(t) \star \alpha_t(A) \star U_h(t)^{-1}. \tag{2.3.29}$$

In [FL14, Theorem 1.] it is computed explicitly as

$$U_h(t) = S_{h\chi}\left(V_{h\rho^-_t}\right), \tag{2.3.30}$$

where $\alpha_t\left(\chi\right) - \chi = \rho^+_t + \rho^-_t$ and $\mathrm{spt}\left(\rho^\pm_t\right) \cap J_\mp(\mathbb{O}) = \emptyset$. Furthermore, it can be shown that $U_h(t)$ satisfies the following co-cycle relation:

Proposition 2.3.1 (Prop. 1. [FL14])**.** *For t,s such that $|t|, |s| < \delta$, the map $t \mapsto U_h(t)$ satisfies the following co-cycle condition:*

$$U_h(t+s) = U_h(t) \star \alpha_t(U_h(s)). \tag{2.3.31}$$

It follows that $t \mapsto U_h(t)$ can be uniquely extended for all $t \in \mathbb{R}$.

This property enables us to obtain an explicit formula for the co-cycle as a formal power series in its generators:

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s} U_h(t) = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} U_h(t+s) = U_h(t) \star \alpha_t\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} U_h(s)\right) \tag{2.3.32}$$

where we have defined

$$K_h \doteq -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} U_h(s).$$

By the definition of U_h (see eqn. (2.3.30)) we obtain

$$K_h = S(V_h)^{\star-1} \star \frac{\mathrm{d}}{\mathrm{d}\mu}\bigg|_{\mu=0} S\left(V_h - \mu \dot{V}_h\right) = -R_{V_h}\left(\dot{V}_h\right), \tag{2.3.33}$$

where we have defined

$$\dot{V}_h \doteq \int \mathrm{P}[\phi](x)\,\dot{\chi}(t)h(\mathbf{x})\,d^3\mathbf{x}\,dt, \tag{2.3.34}$$

where $\dot{\chi}$ stands for the derivative of χ with respect to t. K_h plays the role of the *interacting Hamiltonian*. Very often we will denote with H the *interacting Hamiltonian density*, which is defined by

$$K_h \doteq \int h(\mathbf{x})H(\mathbf{x})\,d^3\mathbf{x}. \tag{2.3.35}$$

From eqn. (2.3.33) and for $t > 0$ we obtain the solution

$$U_h(t) = \mathbb{1} + \sum_{n=1}^{\infty} \mathrm{i}^n \int_{tS_n} \alpha_{t_1}(K_h) \star \cdots \star \alpha_{t_n}(K_h)\,dT_n, \tag{2.3.36}$$

where we have introduced the compact notation

$$\int_{tS_n} dT_n \equiv \int_0^t dt_n \int_0^{t_n} dt_{n-1} \ldots \int_0^{t_2} dt_1 \tag{2.3.37}$$

for the integration over the simplex

$$tS_n \doteq \left\{\mathbf{t} \in \mathbb{R}^n \,|\, 0 \leq t_1 \leq \ldots \leq t_n \leq t\right\}. \tag{2.3.38}$$

Similarly, we can compute the inverse of U_h as[6]:

$$U_h(t)^{\star-1} = \sum_{n=0}^{\infty} (-\mathrm{i})^n \int_{tS_n} \alpha_{t_n}(K_h) \star \cdots \star \alpha_{t_1}(K_h)\,dT_n. \tag{2.3.39}$$

It is also possible to find an explicit expression for the interacting dynamics α_t^V via the following argument:

$$\alpha_t^V(A) - \alpha_t(A) = \left(\alpha_t^V \circ \alpha_{-t} - \mathbb{1}\right)\alpha_t(A) = \left(\mathrm{Ad}_\star(U(t)) - \mathbb{1}\right)\alpha_t(A),$$

where $\mathrm{Ad}_\star(U(t))(A) \doteq U(t) \star A \star U(t)^{\star-1}$ is the adjoint action referred to the star product. Expanding the terms in bracket we get

$$\left(\mathrm{Ad}_\star(U(t)) - \mathbb{1}\right)(A) = \mathrm{i}\int_0^t \frac{\mathrm{d}}{\mathrm{d}s}\mathrm{Ad}_\star(U_h(s))(A)\,ds = \sum_{n=1}^{\infty} \mathrm{i}^n \int_{tS_n} \left[\alpha_{t_1}(K_h), \ldots, \left[\alpha_{t_n}(K_h), A\right]\right] dT_n,$$

where the commutators are computed using the $\star$-product. In conclusion, the former expansion can be rewritten as:

$$\alpha_t^V(A) = \alpha_t(A) + \sum_{n=1}^{\infty} \mathrm{i}^n \int_{tS_n} \left[\alpha_{t_1}(K_h), \ldots, \left[\alpha_{t_n}(K_h), \alpha_t(A)\right]\right] dT_n, \tag{2.3.40}$$

which is exactly the pAQFT analogue of the perturbation expansion defined in Statistical Mechanics. Notice that all the formulas are meant in the sense of formal power series.

The definition of the interacting KMS state is then summarised in the following theorem:

[6] Pay attention to the reverse order of the variables.

Theorem 2.3.1 (Interacting KMS State)**.** *Let ω^β be an extremal KMS state w.r.t. the time evolution α_t. Then, for all $A \in \mathscr{A}^V$, the function $t \mapsto \omega^\beta(A \star U_h(t))$ admits an analytic prolongation to the strip*

$$\mathscr{I}_\beta \doteq \{z \in \mathbb{C} | \, 0 < \Im(z) < \beta\} \quad \forall A \in \mathscr{A}^V \tag{2.3.41}$$

and the linear functional

$$A \mapsto \omega^{\beta,V}(A) \doteq \operatorname*{vH-lim}_{h\to 1} \omega_h^{\beta,V}(A) \equiv \operatorname*{vH-lim}_{h\to 1} \frac{\omega^\beta\left(A \star U_h(\mathrm{i}\beta)\right)}{\omega^\beta(U_h(\mathrm{i}\beta))} \tag{2.3.42}$$

is well-defined as an extremal KMS state on $\mathscr{A}^V$ with respect to the interacting dynamics α_t^V.

Proof. We limit ourselves to the case where the interaction potential is kept of spatial compact support, that is we will not consider the weak adiabatic limit. This issue is solved and explained in [FL14, Li13]. On the contrary, we are interested in reporting the compactly-supported case since it seems to us that some minor mistakes are present in the proof of [FL14, Theorem 2.] and [Li13, Proposition 4.2.2.], which in any case do not affect the validity of their results.

To show that the analytic continuation is well-defined we construct a unitary operator which intertwines the dynamics at different times. This is nothing but

$$U_h(t,s) = U_h^{\star -1}(t) \star U_h(s) = U_h^{\star -1}(t) \star U_h(t+s-t) = \alpha_t(U_h(s-t)) = \alpha_s\left(U_h(t-s)^{\star -1}\right),$$

where we have repeatedly used the co-cycle relation (2.3.31). Now, using eqn. (2.3.39), we have:

$$U_h(t,s) = \sum_{n=0}^{\infty} (-\mathrm{i}(t-s))^n \int_{S_n} \alpha_{s+u_n(t-s)}(K_h) \star \cdots \star \alpha_{s+u_1(t-s)}(K_h)\, dU_n,$$

where dU_n is the measure on the simplex for the variables u_j as per equation (2.3.37). With this new tool at our disposal we can discuss the analytic extension, in particular we will study the prolongation of the function $G(t,s) \doteq \omega^\beta\left(A \star \alpha_t^V(B) \star U_h(s)\right)$, which amounts to the numerator in the definition of $\omega^{\beta,V}$. For simplifying the notations we will omit the $\star$ symbol for the product and the suffix h:

$$G(t,s) = \omega^\beta\left(AU(t)\alpha_t(B)U(t)^{-1}U(s)\right) = \omega^\beta(AU(t)\alpha_t(B)U(t,s)).$$

We can also expand $G(t,s)$ as a power series in K, obtaining[7]:

$$G(t,s) = \sum_{n=0}^{\infty} \sum_{k=0}^{n} (\mathrm{i}t)^{n-k} (\mathrm{i}(s-t))^k \times \\ \times \int_{S_{n-k}} dU_n \int_{S_k} dV_n\, \omega^\beta\left(A\alpha_{u_1 t}(K)\dots\alpha_{u_{n-k}t}(K)\alpha_t(B)\alpha_{s+v_k(t-s)}(K)\dots\alpha_{s+v_1(t-s)}(K)\right).$$

Recalling the domain of analyticity of the free KMS state, expressed in Definition 1.3.11, we can infer that the analytic extension is well-posed in the following domain

$$\mathscr{I}_\beta^{n+2} = \left\{(z_1,\dots,z_{n+n}) \in \mathbb{C}^{n+2} \,|\, 0 < \Im(z_2) < \cdots < \Im(z_{n+2}) < \beta, \Im(z_1) = 0\right\},$$

[7] In this expression [FL14] inverted the order of the integration variables.

where $\Im(z_1) = 0$ since A has not to be extended. But notice that the order of the time-translations of the variables inside ω^β is, by construction, the correct one, that is:

$$0 < u_1\Im(t) < \cdots < u_{n-k}\Im(t) < \Im(t) < \Im(s) + v_1\Im(t-s) < \cdots < \Im(s) + v_k\Im(t-s) < \beta$$

since $\Im(s)+v_i\Im(t-s) = \Im(t)+\Im(s)(1-v_i) > \Im(t)$ for all i and $v_i > v_j$ for all $i > j$. This fact implies that $G(t,s)$ can be analytically continued into the symplex $\mathscr{I}^2_\beta$ in such a way that it remains bounded on its boundaries, fulfilling the KMS property. In particular, the function $t \mapsto G(t,\mathrm{i}\beta)$ admits an extension for $0 < \Im(t) < \beta$ for all $A,B \in \mathscr{A}^V$ and, thanks to the KMS property of ω^β:

$$G(\mathrm{i}\beta,\mathrm{i}\beta) = \omega^\beta\left(A\,\alpha^V_{\mathrm{i}\beta}(B)U(\mathrm{i}\beta)\right) = \omega^\beta\left(AU(\mathrm{i}\beta)\alpha_{\mathrm{i}\beta}(B)\right) = \omega^\beta\left(BAU(\mathrm{i}\beta)\right).$$

The next step is the proof of the formal positivity of $\omega^{\beta,V}$ in $\hbar$ and in λ. To this avail, denote $\gamma \doteq \beta/2$, then:

$$A \mapsto \omega^\beta\left(A^*AU(\mathrm{i}\beta)\right) = \omega^\beta\left(A^*AU(\mathrm{i}\gamma)\alpha_{\mathrm{i}\gamma}\left(U(\mathrm{i}\gamma)\right)\right) = \omega^\beta\left(U(\mathrm{i}\gamma)^*A^*AU(\mathrm{i}\gamma)\right) = \omega^\beta\left(B^*B\right),$$

where $U(\mathrm{i}\gamma)^* = \alpha_{-\mathrm{i}\gamma}\left(U(\mathrm{i}\gamma)\right)$ and $B = AU(\mathrm{i}\gamma)$. The positivity in $\hbar$ follows from the positivity of ω^β, while, concerning λ, $\omega^{\beta,V}$ is positive since B^*B is a square of formal power series in λ. The normalisation is obtained by dividing by $\omega^\beta\left(U(\mathrm{i}\beta)\right)$. This concludes the proof. □

To conclude, we report a formula which will be of great importance in the following, in which the interacting KMS state is expressed in terms of the connected functions (1.3.57):

$$\omega^{\beta,V}(A) = \sum_{n=0}^{\infty}(-1)^n \int_{\beta S_n} \omega^{\beta,c}\left(A\bigotimes_{k=1}^{n}\alpha_{\mathrm{i}u_k}(K)\right)dU_n. \tag{2.3.43}$$

Moreover, it is possible to show that

$$\log\left(\omega^\beta\left(U(\mathrm{i}\beta)\right)\right) = \sum_{n=1}^{\infty}(-1)^n \int_{\beta S_n} \omega^{\beta,c}\left(\alpha_{\mathrm{i}u_1}(K)\otimes\cdots\otimes\alpha_{\mathrm{i}u_n}(K)\right)dU_n \tag{2.3.44}$$

is well-posed and finite in the adiabatic limit, see [Li13, Proposition 4.4.2.] for the proof.

2.4 Generalisations of the Construction of $\omega^{\beta,V}$

We have seen in the previous section that the interacting KMS state introduced by Fredenhagen and Lindner in [FL14, Li13] has been built for a real, massive scalar field on Minkowski spacetime only: To conclude this chapter we would like to give some insights in possible generalisations of the construction. The main concern about the study of other models regard the well-posedness of the adiabatic limit. The proof given in the original paper is based on the clustering properties in spatial directions of the free KMS state ω^β, which have explicitly been shown in [FL14, Theorem 4.] taking advantage of the form of the 2-point function ω^β_2, see equation (1.3.70). Actually, the shape of the 2-point function and, consequently, also the validity of the spatial clustering varies considering different fields or different backgrounds, so the finiteness of the adiabatic limit is not granted in general.

We would like to stress the fact that the only obstruction to the extension of the construction lie in the weak adiabatic limit. The perturbative theory developed so far is in fact applicable to every globally hyperbolic space-time, so no ultraviolet divergencies occur. Moreover, also algebraic adiabatic limit may be taken harmlessly. Of course, we can not expect the construction to be valid on every globally hyperbolic space-time, but only on static ones because otherwise there will be no natural notion of (free) KMS state because of the lack of a unique time-direction. Hence, as long as the cutoff is present, the Araki construction holds for any kind of field in any static space-time. So, extending the construction really means to study the spatial decay of the 2-point function of the free KMS case by case. In this section we would like to say some words about this problem in some models.

As previously mentioned, something about the extension of the construction has been already made by Drago, Hack and Pinamonti, who managed to treat the massless case for a $\lambda\phi^4$ interaction by a clever use of the principle of perturbative agreement, which allowed to take back the massless situation to the massive one. We refer to the original paper [DrHaPi16] for the full construction.

Nonetheless, other possible generalisations may be thought. Here we want to discuss a couple of them, which are quite immediate and natural, *i.e.* a massive Klein-Gordon field on a static space-time with compact Cauchy surfaces, like the Einstein universe, or the extension to a boson vector model.

2.4.1 Scalar field on static space-times with compact Cauchy surfaces

We would like to sketch here the construction of the interacting KMS state for a static space-time $\mathbb{M}$ with compact Cauchy surfaces Σ. The prototypical example is the Einstein static universe, which is of the form $M = \mathbb{R}\times\Sigma$, where $\Sigma = \mathbb{S}^3$, the 3-sphere. Assuming to have built the interacting algebra $\mathscr{A}^V$ for the scalar field over this background (see [BrFr00, FR12, HW01, HW02] for the treatment of interacting theories on curved manifolds), we may develop the Fredenhagen and Lindner construction as displayed at the end of the previous section, obtaining a state of the form

$$\omega_h^{\beta,V}(A) \doteq \frac{\omega^\beta\left(A\star U_h(\mathrm{i}\beta)\right)}{\omega^\beta\left(U_h(\mathrm{i}\beta)\right)},$$

for all $A\in\mathscr{A}^V(\mathbb{M})$, where the $\star$ product is defined using the 2-point function of the free KMS state ω^β. Here we are considering an interaction potential V_g of the form (2.2.15), where we used the causal factorisation to split the cutoff g in a product $\chi(t)h(\mathbf{x})$ as we did in equation (2.3.28).

The goal is taking the weak adiabatic limit, namely to send $h\to 1$ in the sense of van Hove, see Definition 2.3.1. In this case the compactness of the Cauchy surface, on which the cutoff function h is defined and which has to be covered with balls in the van Hove limit, should make the adiabatic limit well-defined, that is finite. More precisely, we can take advantage of the expansion of $\omega_h^{\beta,V}$ in terms of the connected functions (2.3.43), which holds also out of the adiabatic limit, obtaining

$$\omega_h^{\beta,V}(A) = \sum_{n=1}^{\infty}(-1)^n\int_{\beta S_n}\omega^{\beta,c}\left(A\otimes\alpha_{\mathrm{i}u_1}(K_h)\otimes\cdots\otimes\alpha_{\mathrm{i}u_n}(K_h)\right)dU_n \qquad \forall\, A\in\mathscr{A}^V.$$

Recalling equation (2.3.35) and Definition 2.3.1 we may expand the previous equation as

$$\omega_h^{\beta,V}(A) = \sum_{n=1}^{\infty}(-1)^n \int_{\beta S_n} dU_n \int_{B_m} d^3\mathbf{x}_1 \dots \int_{B_m} d^3\mathbf{x}_n \times \\ \times \omega^{\beta,c}\left(A \otimes \alpha_{iu_1}(h_m(\mathbf{x}_1)H(\mathbf{x}_1)) \otimes \cdots \otimes \alpha_{iu_n}(h_m(\mathbf{x}_n)H(\mathbf{x}_n))\right),$$

where h_m is given in Definition 2.3.1, this formula being valid for all $A \in \mathscr{A}^V$. Eventually, we have to consider the limit $m \to \infty$. In this limit the balls B_m cover all the Cauchy surface Σ, which is compact, and the functions h_m equal 1 everywhere, namely we have

$$\underset{h\to 1}{\text{vH-lim}}\,\omega_h^{\beta,V}(A) = \sum_{n=1}^{\infty}(-1)^n \int_{\beta S_n} dU_n \int_{\Sigma} d^3\mathbf{x}_1 \dots \int_{\Sigma} d^3\mathbf{x}_n\, \omega^{\beta,c}\left(A \otimes \alpha_{iu_1}(H(\mathbf{x}_1)) \otimes \cdots \otimes \alpha_{iu_n}(H(\mathbf{x}_n))\right).$$

This integral is now finite because it involves the integration on a compact set, so the interacting KMS state $\omega^{\beta,V} \doteq \text{vH-lim}_{h\to 1}\omega_h^{\beta,V}$ is well-defined.

2.4.2 The vector boson model on Minkowski space-time

Another direct generalisation of the scalar case consists in the vector boson model, sketched in Example 1.1.2. In this theory, whose description may be found in [KMM17], the field configurations are described as functions $\boldsymbol{\varphi} \in \mathscr{E}(\mathbb{M}, \mathbb{R}^d)$, which we may write as vectors of the form

$$\boldsymbol{\varphi}(x) = \begin{pmatrix} \phi_1(x) \\ \vdots \\ \phi_d(x) \end{pmatrix}, \qquad \phi_1, \dots, \phi_d \in \mathscr{E}.$$

Componentwise, a boson vector field reduces to a real scalar one. Moreover, every component commutes with the others. The observables are then defined as functionals $\boldsymbol{F} : \mathscr{E}(\mathbb{M}, \mathbb{R}^d) \to \mathbb{C}$, for example a linear functional will have the form

$$\mathbf{F}_{\mathbf{f}}(\boldsymbol{\varphi}) = \sum_{k=1}^{d} F_{f_k}(\phi_k), \qquad F_{f_1}, \dots, F_{f_d} \in \mathscr{A}_\omega,$$

where $\mathbf{f} = (f_1, \dots, f_d)$ with $f_j \in \mathscr{D}(\mathbb{M}, \mathbb{C})$ for all j. A general non-linear functional is not of this form, in particular it may mix the components of the field configuration $\boldsymbol{\varphi}$. Since our aim here is just to present some ideas about the generalisation of the construction of [FL14], we prefer to avoid the non-linear case, so considering regular functionals only. In particular, the quantum algebra of regular functionals, which we denote as $\mathscr{A}_\Delta$, is obtained by endowing the space of functionals with the following $\star_\Delta$ product:

$$\mathbf{F} \star_\Delta \mathbf{G} \doteq \mathbf{m} \circ e^{\boldsymbol{\Gamma}}(\mathbf{F} \otimes \mathbf{G}), \qquad \boldsymbol{\Gamma} \doteq \sum_{j=1}^{d} \Gamma_\Delta^{(j)}$$

where $\Gamma_\Delta^{(j)}$ is the functional differential operator implementing the star product for the scalar field given in equation (1.3.75), where the functional derivatives computed with respect to the variable ϕ_j. Moreover, notice that the causal propagator applied to commuting functions is zero, so it annihilates all the non-diagonal terms.

Concerning states, they are defined as usual as positive, normalised linear functionals $\boldsymbol{\omega}$. In general, we do not expect a state to make the correlations vanishing, but an analysis of the 2-point function of the free, extremal KMS $\boldsymbol{\omega^{\beta}}$ on linear functionals shows that actually it is of this form, hence its action on a product of two linear functionals gives

$$\boldsymbol{\omega^{\beta}}(\mathbf{F_f} \star_{\Delta} \mathbf{F_g}) = \sum_{k=1}^{d} \omega^{\beta}\left(F_{f_k} \star_{\Delta} F_{g_k}\right).$$

The idea then is that it is possible to repeat the perturbative construction of the state, defining the interacting KMS state as

$$\boldsymbol{\omega^{\beta,V}} \doteq \underset{h\to 1}{\text{vH-lim}}\, \boldsymbol{\omega_h^{\beta,V}},$$

with obvious meaning of the terms. The well-posedness of the van Hove limit follows applying the proof in [FL14] component by component.

An outline of the Dirac Field

An interesting case which deserves some attention is the Dirac field on Minkowski space-time. Up to now nothing has been said about this case, nevertheless we expect the interacting KMS state to be well-defined in this case. The reason for that is that the expression of the 2-point function for this model shares the same decaying properties of the one for the Klein-Gordon field, see [DaHaPi11]. Nonetheless, as sketched in Example 1.1.2, the formulation of the Dirac field has to be carefully discussed because of the presence of the spin structure. Furthermore also the description of the interacting theory has to be treated in detail. It must be said that we do not see any particular issue concerning the extension and adaptation of the formalism to the treatment of the Dirac field, but actually a full treatment of the problem is not available yet, and actually we leave it to a future investigation.

CHAPTER 3

STABILITY OF INTERACTING KMS STATES

The interacting KMS state $\omega^{\beta,V}$ defined in [FL14] is something new in the perturbative Quantum Field Theory literature, so its properties are yet to be discovered and studied. The present chapter represents a first step in this direction. Since the idea behind the construction of the state is the generalisation of Araki's perturbation theory, we found fruitful to proceed along the same path and take over our analysis generalising known results in Statistical Mechanics to QFT.

In Section 1.3.3 we characterised the KMS states as those ones that are able to resist to bounded perturbations of the dynamics. This is usually referred to as the *stability* of the state. Heuristically, the idea is that if we evolve the free KMS ω^β using the interacting dynamics obtained with a bounded perturbation, in the large-time limit we expect it to converge to the equilibrium state for the interacting system. Similarly, evolving $\omega^{\beta,V}$ with the free dynamics, we expect to reach the free KMS state in the limit. This last phenomenon is usually called *return to equilibrium*. We emphasise that in pAQFT it does not really make sense to talk about "bounded" perturbations, since the observables (and consequently the interaction potentials) are typically unbounded. Moreover, no norms are at disposal. Rather, the role of boundedness will be replaced by the presence of the cutoff, namely if V is in $\mathscr{F}_{\mathrm{loc}}$ or not. We will see explicitly that the adiabatic and the large-time limits do not commute, in particular stability and return of equilibrium hold if the large-time limit is taken in advance, while they fail if we revert their order.

As a matter of fact, the proof of the stability in concrete Statistical Mechanics models is a very hard task, which resulted in a success in very few cases only since it typically amounts to verify some ergodicity of the system, hence the achievement of this result in pAQFT is a pretty remarkable fact.

To start with, and also in order to make our goal clear, in Section 3.1 we will introduce some generalities about stability and return to equilibrium in Quantum Statistical Mechanics, which will serve as a guide for the analysis of the field theoretical case. In the next two sections we

will address the QFT case, first without the adiabatic limit and next by taking it into account, showing that the two sought properties hold true in the first case, while they fail in the other one. As an outcome of the failure of the return to equilibrium, we define a non-equilibrium steady state (NESS) for the free theory. This is the subject of Section 3.4.

Apart from the first section, this chapter is based on [DFP18a], from which most of the proofs are taken and in which the results have first appeared.

3.1 Stability in Quantum Statistical Mechanics

Let us consider a W^*- (or C^*-)dynamical system $(\mathscr{M}, \tau_t)$ as given in Definition 1, and let us suppose that the infinitesimal generator of τ_t is given by

$$\delta(A) \doteq \mathrm{i}[H_0, A] \qquad \forall A \in \mathscr{M},$$

where the self-adjoint operator $H_0 \in \mathscr{M}$ is the Hamiltonian of the system. Notice that δ is a bounded, symmetric derivation in $\mathscr{M}$. Given a bounded, self-adjoint $P \in \mathscr{M}$, we can define a bounded derivation δ_P with domain $\mathrm{Dom}(\delta_P) = \mathscr{M}$ given by $\delta_P(A) \doteq \mathrm{i}[P, A]$ for all $A \in \mathscr{M}$. Then $\delta + \delta_P = \mathrm{i}[H, A]$, with $H \doteq H_0 + P$ generates a one parameter group of *-automorphisms τ_t^P of $\mathscr{M}$. This dynamics is interpreted as the interacting dynamics and it is given as a Dyson series, in total analogy to the one in equation (2.3.40). Furthermore, it is related to the free one by a co-cycle relation as in (2.3.29). In [Ar73], Araki proved that the construction of τ_t^P is well-posed[1] and that it is always possible to find a state $\omega^{\beta,P}$ which satisfies the KMS condition 1.3.11 at the inverse temperature β with respect to the time-evolution τ_t^P, which is defined in analogy with Theorem 2.3.1, see also [BR97b, Section 5.4.1.] for a review. The state $\omega^{\beta,P}$ is defined as a perturbation of the free, extremal (τ_t, β)-KMS state ω^β. Notice that, contrary to the QFT case, here every series converges in the relevant topology on the algebra $\mathscr{M}$, hence this leads to the definition of a second dynamical system over $\mathscr{M}$, which is given by $(\mathscr{M}, \tau_t^P)$ with an equilibrium state $\omega^{\beta,P}$. This is naturally interpreted as describing an interacting physical system. It can be shown that $\omega^{\beta,P}$ is an extremal (τ_t^P, β)-KMS state for the dynamical system $(\mathscr{M}, \tau_t^P)$.

Moreover, this interacting system is obtained as a perturbation of the free one, hence it is reasonable to ask the question about how the original system is able to resist to the perturbation or, in other words, if the perturbed dynamics drives the system from the free thermal equilibrium to the interacting one. This properties are called *stability* and *return to equilibrium* and are mathematically formulated as follows:

Definition 3.1.1. In the former setting, we define the stability property as

$$\lim_{t \to \pm\infty} \omega^\beta(\tau_t^P(A)) = \omega^{\beta,P}(A) \qquad \forall A \in \mathscr{M} \tag{3.1.1}$$

and the return to equilibrium as

$$\lim_{t \to \pm\infty} \omega^{\beta,P}(\tau_t(A)) = \omega^\beta(A) \qquad \forall A \in \mathscr{M}. \tag{3.1.2}$$

[1] The construction actually holds also for unbounded δ and the existence of of the interacting KMS is granted by the existence of the free, extremal KMS state.

Remark 3.1.1. In Statistical Mechanics these two conditions are in fact equivalent: Due to the norm convergence of the perturbative series, the two situations are totally symmetric since we could have started from the dynamical system $(\mathscr{M},\tau_t^P,\omega^{\beta,P})$ and get to $(\mathscr{M},\tau_t,\omega^\beta)$ by applying the perturbation $-P$. Actually, this will not be the case in QFT, hence we preferred to keep the previous terminology fixed for sake of clarity.

The validity of stability and return to equilibrium is a very important aspect concerning the analysis of thermal equilibrium of a physical system and, due to its generality, we can not expect every state to be stable, but rather we should imagine that some further assumptions must be put on the system, for example some form of ergodicity may be asked. Moreover, we have already (heuristically) seen in Section 1.3.3 how stability is connected with the characterisation of the thermal equilibrium. Due to its importance, stability and its relations with equilibrium and with the KMS condition have been thoroughly studied in Statistical Mechanics in the 70's, see for example [BKR78, HKTP74, HTP77, Ro73] and [BR97b, Section 5.4.] for a review. Here we want to present and discuss the main results on this subject, so to make clear what we are going to generalise to perturbative QFT and why we decided to address this problem.

First, we notice that the Araki's construction of the perturbed KMS state can be understood as "time-independent" or "kinematic" form of stability, in the sense that the two equilibrium states are linked at every order by the expansion. On the other hand, what we introduced in Definition 3.1.1 is usually referred to as "time-dependent" stability since it aims to characterise the perturbed equilibrium as obtained from the interacting evolution of the free one (and vice-versa concerning the return to equilibrium), see [Ro73]. This is the reason why this approach is often referred to as the dynamical one. The time-dependent stability is less complete, but it is also more interesting and emphasises different physical properties of the system, for instance it plays a crucial role in the interpretation of the KMS condition as a characteristic of equilibrium.

Let us now go into more details and consider the problem of return to equilibrium, as it is customary in the literature. In [Ro73], see also [BR97b], it is pointed out that for the return to equilibrium $\omega \doteq \lim_{t\to\infty}\omega^{\beta,V}\circ\tau_t$ to happen, the extremality of the initial state $\omega^{\beta,V}$ and some ergodicity on the system $(\mathscr{M},\tau_t)$ are necessary. In particular, this leads to require some dispersion property on the dynamical group τ_t. The necessary assumptions are given by the following theorem.

Theorem 3.1.1 ([Ro73], Theorem 2.)**.** *Let $(\mathscr{M},\tau_t)$ be a C^*-dynamical system and let τ_t^P be the group of automorphisms obtained by perturbing τ_t with a self-adjoint $P\in\mathscr{M}$. Furthermore, let $\omega^{\beta,P}$ be a (τ_t^P,β)-KMS state and ω be a weak*-limit point of $\omega^{\beta,P}\circ\tau_t$ for large times t. If $(\mathscr{M},\tau_t)$ is norm-asymptotically Abelian, that is if*

$$\lim_{t\to\infty}\|[A,\tau_t(B)]\| = 0 \qquad \forall\, A,B\in\mathscr{M},$$

then ω is a (τ_t,β)-KMS state.

This result characterises the assumptions to be asked on the system, but it tells nothing about the existence of the limit state ω: Actually, if there exists a unique free KMS ω^β, this theorem

states that the return to equilibrium holds, but in general there might be more than one limit point, thus the limit may not exist in general. The existence and uniqueness of the limit is granted if we combine the two approaches, appealing to the time-independent perturbation theory, which, guarantees the extremality of both ω^β and $\omega^{\beta,P}$.

If we want to obtain the existence and to get rid of the extremality assumption on $\omega^{\beta,P}$ we need to introduce a stronger ergodicity, taking advantage of the mean ergodic theorem.

Definition 3.1.2 (L^1-Asymptotic Abelianess)**.** A C^*-dynamical system $(\mathscr{M},\tau_t)$ is called $L^1(\mathscr{M}_0)$-asymptotic Abelian if

$$\int_{\mathbb{R}} \|[A,\tau_t(B)]\|\,dt < +\infty$$

for all A,B in a norm-dense *-subalgebra $\mathscr{M}_0$.

The reason for introducing precisely this condition is that it allows to define the Møller morphisms as norm limits of $\tau^P_{-t}\circ\tau_t$ for $t\to\pm\infty$, as we shall see in the following proposition.

Proposition 3.1.1 ([BR97b], Proposition 5.4.10.)**.** *Let $(\mathscr{M},\tau_t)$ be an $L^1(\mathscr{M})$-asymptotic Abelian C^*-dynamical system and let $P\in\mathscr{M}$ self-adjoint. Then the limits*

$$\gamma_\pm(A) \doteq \lim_{t\to\pm\infty} \tau^P_{-t}\circ\tau_t(A) \qquad \forall\, A\in\mathscr{M}$$

exist in norm and are called Møller morphisms. Moreover, they are norm-preserving *-morphisms of $\mathscr{M}$ which intertwine the two time-evolutions, that is

$$\gamma_\pm\circ\tau_t = \tau^P_t\circ\gamma_\pm.$$

If $\mathscr{M}$ is unital, then the adjoints $\gamma^*_\pm$ are affine transformations of the set of states into itself fulfilling the following properties:

1. *$\gamma^*_\pm$ map τ^P_t-invariant (extremal) states into τ_t-invariant (extremal) ones;*
2. *$\gamma^*_\pm$ map (τ^P_t,β)-KMS states into (τ_t,β)-KMS states for all $\beta\in\overline{\mathbb{R}}\setminus\{0\}$;*
3. *If $\beta\in\mathbb{R}\setminus\{0\}$, then $\gamma_+\equiv\gamma_-$ if restricted to the (τ^P,β)-KMS states.*

The maps $\gamma_\pm$ are in fact analogous of the Møller maps defined in equation (1.2.46), which send free solutions into interacting ones. By (2), the existence of the Møller morphisms guarantees the stability, in this sense the previous proposition states that if a system is L^1-Abelian, than return to equilibrium occurs. Another important aspect concerning the Møller morphisms is their invertibility: This is not granted *a priori*, in particular their ranges may be strict *-subalgebras of $\mathscr{M}$. Actually, we will not dwell any longer on the properties of $\gamma_\pm$, for a thorough discussion we refer to the original paper of Robinson [Ro73].

Hitherto, we provided a characterisation of the time-dependent stability which is satisfactory and rigorous. Unfortunately, it is rather difficult to verify the L^1-Abelianess in concrete models, so to check if stability holds. In particular, this condition can not be transposed in perturbative QFT because of the lack of a norm. What we can do is to characterise the stability perturbatively,

in such a way to establish also the compatibility of the time-dependent formalism with the time-independent one. Loosely speaking, we can expand the two sides in equation (3.1.1) in power series using the expansions (2.3.43) and (2.3.40) and check the convergence of the large time-limit order by order. Actually, in order to have the compatibility, we want ω^β to be extremal and to behave well in the large-time behaviour, that is we have to ask it to satisfy the *strong clustering condition*:

Definition 3.1.3 (Strong Clustering Condition)**.** Let ω^β be a (τ_t,β)-KMS state over a C^*- or W^*-dynamical system $(\mathscr{M},\tau_t)$ with $\beta\in\mathbb{R}$. We say that ω^β is strongly clustering if

$$\lim_{t\to\pm\infty}\omega^\beta(A\tau_t(B))=\omega^\beta(A)\omega^\beta(B)\qquad\forall A,B\in\mathscr{M}. \tag{3.1.3}$$

Heuristically, this condition means that any two observables separated in time become uncorrelated in the large-time limit. This condition is crucial for the proof of the following result, see [BKR78, Theorem 2.]:

Theorem 3.1.2. *Let ω^β be the extremal (τ_t,β)-KMS state over a C^*- or W^*-dynamical system $(\mathscr{M},\tau_t)$ and let us assume that it satisfies the strong clustering condition. Then it follows that*

$$\lim_{T\to\pm\infty}\int_0^T\omega^\beta([A,\tau_t(B)])\,dt=\mathrm{i}\int_0^\beta\omega^{\beta,c}(A,\tau_{\mathrm{i}u}(B))\,du\qquad\forall A,B\in\mathscr{M},$$

and hence

$$\lim_{T\to\infty}\int_{-T}^T\omega^\beta([A,\tau_t(B)])\,dt=0\qquad\forall A,B\in\mathscr{M}. \tag{3.1.4}$$

This theorem shows the compatibility of time-dependent and time-independent stability at first order. This result directly generalises to pAQFT if the adiabatic limit is not taken into account, see Theorem 3.2.1 in the next section and the relative proof (which is basically the same given in [BKR78]). In Statistical Mechanics, this theorem is telling us something more, in particular it is possible to show that the condition (3.1.4) together with some ergodicity property is equivalent to the KMS condition for $\beta\in\overline{\mathbb{R}}$, see [BR97b, Section 5.4.2.] and references therein quoted for further details.

The prove of the previous theorem extends also at the n-th perturbative order:

Proposition 3.1.2. *Let ω^β be the extremal (τ_t,β)-KMS state over a C^*- or W^*-dynamical system $(\mathscr{M},\tau_t)$ and let us assume that it satisfies the strong clustering condition. Then, for all $A,B\in\mathscr{M}$,*

$$\lim_{T_1\to\pm\infty}\cdots\lim_{T_n\to\pm\infty}\int_0^{T_1}dt_1\cdots\int_0^{T_n}dt_n\,\omega^\beta\big([\tau_{t_n}(B),\cdots[\tau_{t_1}(B),A]]\big)=$$
$$(-\mathrm{i})^n\int_0^\beta du_1\int_0^{u_1}du_2\cdots\int_0^{u_{n-1}}du_n\,\omega^{\beta,c}\big(A\otimes\tau_{\mathrm{i}u_n}(B)\otimes\cdots\otimes\tau_{\mathrm{i}u_1}(B)\big).$$

Remark 3.1.2. The proof of this proposition is given in [BKR78]. It must be stressed that this result does not amount for the stability of the state, as meant in Definition 3.1.1. In fact, here the large-time limits are taken order by order and, in the proof, exchanges in the order of the limits are present, justified with the norm-convergence of the series. What it is actually proven then is a term-by-term agreement of the two expansions of the two members in equation (3.1.1).

Indeed, this is reasonable since, as previously explained, ergodicity of the system is crucial, moreover it is known by the explicit study of models that the clustering condition *per se* does not imply stability. On the other hand, the way of arguing used in the proofs of Theorem 3.1.2 and Proposition 3.1.2 is the only one which generalises to pAQFT, where both the members of equation (3.1.1) are expressed as formal power series, so, in this framework, equality at every perturbative order is what we look for (see Section 1.3.1 for details on the convergence in the sense of formal power series).

As a matter of fact, also in our treatment of the field theoretical framework we will see that strong clustering alone is not enough for generalising the proof of Proposition 3.1.2, in particular we will need to introduce (and verify) a clustering property of the free state with respect to the interacting dynamics.

3.2 Stability for Compactly-Supported Perturbations

We would like to study the stability of the KMS state of the free theory under perturbations described by the potential V_h in (2.3.27). We will work with the algebra $\mathscr{A}_{\omega^\beta}$, which is the free, off-shell quantum algebra of microcausal functionals as per Definition 1.3.13 generated with the star product $\star$ obtained using the 2-point function of ω^β, the extremal and quasi-free (α_t, β)-KMS state of the free theory. Here α_t is the time evolution given by the Minkowski time-translation (1.3.67) and $\beta \in \mathbb{R}$ is the inverse temperature. As a quasi-free state, it is completely determined by its 2-point function (1.3.70), which we report here for the comfort of the reader

$$\omega_2^\beta(x-y) = \frac{1}{(2\pi)^3}\int \frac{d^3\mathbf{k}}{2E(\mathbf{k})}\left(b_+(\mathbf{k})e^{\mathrm{i}E(\mathbf{k})(x_0-y_0)} + b_-(\mathbf{k})e^{-\mathrm{i}E(\mathbf{k})(x_0-y_0)}\right)e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})},$$

with, $E_\mathbf{k} = \sqrt{\mathbf{k}^2+m^2}$ and $b_+(\mathbf{k}) = (1-e^{-E_\mathbf{k}\beta})^{-1}$, $b_-(\mathbf{k}) = e^{-\beta E_\mathbf{k}} b_+(\mathbf{k})$.

As pointed out in Section 1.3.3, ω^β induces a state on the interacting algebra $\mathscr{A}^V$ which we recall is generated by the elements of $\mathscr{A}_{\omega^\beta}$ obtained applying the Bogoliubov map (2.2.22) to local fields.

The goal of this and of the next sections is to check if the free, extremal KMS state ω^β satisfies the stability and the return to equilibrium as per Definition 3.1.1. As anticipated in Section 3.1, we will study the problem starting from the results of [BKR78] (cf. Theorem 3.1.2 and Proposition 3.1.2) and transposing them in perturbative quantum field theories. Nonetheless, we must be carefull since the elements of $\mathscr{A}^V$ are known as formal power series only, hence we can not rely on the results involving norm convergences. In particular, we stress that all the limits and expressions that will appear in the following should be meant in the sense of formal power series.

A first difference appearing with the Statistical Mechanics case is the presence of the adiabatic limit $h \to 1$. A typical situation in Statistical Mechanics is that one studies a system in a box, and then takes the thermodynamic limit[2], expanding the box. Actually, what one finds is a quasi-periodic behaviour in time, hence typically the existence of the large-time limit for a system in a

[2] In Statistical Mechanics, what we usually call "adiabatic limit" corresponds to what is actually referred to as "thermodynamic limit", which, loosely speaking, is the infinite volume limit of a finite-dimensional system. Heuristically,

box does not exist, so no doubts on the order of the limits arise: The thermodynamic limit has to be taken in advance.

The situation in pAQFT is completely different, hence it is interesting to consider both cases. In this section we will address the case where the adiabatic limit is not considered, from time to time we will refer to this by talking about bounded perturbations. The setting we will use is the same introduced in Section 2.3.2 where the potential V_h is defined in equation (2.3.27) and it is smeared by a spatial function $h \in \mathscr{D}(\mathbb{R}^3)$ which is equal to 1 on $\mathbb{O}$ and with a past compact temporal function χ such that $\chi \equiv 1$ on $J_+(\mathbb{O})$. The precise definitions of the cutoffs is given in equation (2.3.28). In order to keep track of this, we will add a suffix h to all the relevant quantities, *e.g.* we will write V_h for the interaction potential, $U_h(t)$ for the co-cycle, K_h for its generator and so on. For simplicity, we will not specify the dependence on h in the symbols we used to denote the interacting algebra, the Bogoliubov map and the interacting dynamics, for which we will write $\mathscr{A}^V$, $R_V(\cdot)$ and α^V_t respectively. Furthermore, we will often denote with A, B the generic elements in $\mathscr{A}^V$, meaning that they are given as linear combinations of products of Bogoliubov elements of the form

$$R_V(F_1) \star \cdots \star R_V(F_n) \qquad \forall F_1, \ldots, F_n(\mathbb{O}) \in \mathscr{F}_{\mu c},\ \forall n \in \mathbb{N}.$$

Following [BKR78], we first show that ω^β satisfies a clustering condition, which is a crucial assumption in the proof of Theorem 3.1.2. We have actually the following proposition:

Proposition 3.2.1 (Clustering condition for α_t)**.** *Consider two interacting observables $A, B \in \mathscr{A}^V(\mathbb{O})$, where the algebra is constructed using interacting potential is V_h defined in* (2.3.27)*. Then*

$$\lim_{t\to\infty} \omega^\beta(A \star \alpha_t(B)) = \omega^\beta(A)\omega^\beta(B)$$

in the sense of formal power series in the coupling constant.

Proof. We notice that since V_h is of compact support, the product $R_V(F_1) \star \cdots \star R_V(F_n)$ is of compact support too. Actually, $\mathrm{spt}(R_V(F_i)) \subset J_+(\mathrm{spt} V_h) \cap J_-(\mathrm{spt} F_i)$ which is a compact set if V_h is of spatial compact support and if $F_i \in \mathscr{A}_{\omega^\beta}(\mathbb{O})$. Hence, the supports of both A and B are compact, so we suppose, as we may, that both of them are contained in a compact set $\mathbb{K}$. From (1.3.74) and thanks to the invariance of ω^β under α_t, we have

$$\omega^\beta(A \star \alpha_t(B)) - \omega^\beta(A)\omega^\beta(B) = \sum_{n=1}^{\infty} \frac{1}{n!} \left\langle A^{(n)}, \left(\omega_2^\beta\right)^{\otimes n} \alpha_t(B)^{(n)} \right\rangle. \tag{3.2.5}$$

Notice that the distributional support of $A^{(n)}$ is contained in $\mathbb{K}^n$ while that of $(\alpha_t(B))^{(n)}$ is contained in $\mathbb{K}_t^n$ where $\mathbb{K}_t$ is $\mathbb{K}$ translated in time t, namely

$$\mathbb{K}_t := \{(\tau, \mathbf{x}) \in \mathbb{M} | (\tau - t, \mathbf{x}) \in \mathbb{K}\}.$$

Whenever t is sufficiently large there are no null geodesics which intersect at the same time $\mathbb{K}$ and $\mathbb{K}_t$. For this reason, and because (x, y) are contained in the singular support of ω_2^β only if

the statistical mechanical adiabatic limit corresponds to a large-time limit in which the time variation is particularly slow. Actually, this notion will never appear in the present work and the only adiabatic limit involved is the QFT one.

x, y are joined by a null geodesic, the integral kernel of $\left(\omega_2^\beta\right)^{\otimes n}$ restricted to $(\mathbb{K}\times\mathbb{K}_t)^n$ is smooth for sufficiently large t. Hence, the limit of (3.2.5) for large times is governed by the decaying properties of the 2-point function $\omega_2^\beta(x,y)$ when $x-y$ is a large timelike vector. More precisely, we know from Proposition 1.3.3 that

$$\left|D^{(\alpha)}\omega_2^\beta(x;t_y+t,\mathbf{y})\right| \leq \frac{C_\alpha}{t^{3/2}} \tag{3.2.6}$$

where $\alpha\in\mathbb{N}^8$ is a multi index and $D^{(\alpha)}$ indicates partial derivatives of order $|\alpha|=\sum_{i=1}^n \alpha_i$ along the directions determined by α and C_α are some positive constants. Furthermore,

$$\left\langle A^{(n)}, \left(\omega_2^\beta\right)^{\otimes n} \alpha_t(B)^{(n)}\right\rangle = A^{(n)}\otimes B^{(n)}(\Lambda_{\mathbb{K}^{2n}}\omega_t^{\beta n})$$

where ω_t^β equals ω_2^β with the second entry translated by $-t$ along the selected Minkowski time. Here $\Lambda_{\mathbb{K}^{2n}}$ is a compactly supported function in M^{2n} which is equal to 1 on $\mathbb{K}^{2n}$, notice that the precise form of the function does not enter in the final result because of the support of $A^{(n)}\otimes B^{(n)}$. Furthermore, as discussed above, for large values of t, $\Lambda_{\mathbb{K}^{2n}}\left(\omega_t^\beta\right)^{\otimes n}$ is smooth. The distributions $A^{(n)}\otimes B^{(n)}$ are of compact support, hence, by continuity we have that

$$\left|\left\langle A^{(n)}, \left(\omega_2^\beta\right)^{\otimes n} \alpha_t(B)^{(n)}\right\rangle\right| \leq C_n \sum_{|\alpha|<K_n} \left\|D^{(\alpha)}\Lambda_{\mathbb{K}^{2n}}\left(\omega_t^\beta\right)^{\otimes n}\right\|_\infty,$$

where C_n and K_n are fixed constants. Thanks to (3.2.6), the right hand side of the previous inequality vanishes in the limit $t\to\infty$. Hence, we have the result because, the sum over n in (3.2.5) converges to 0 in the sense of formal power series. □

The clustering condition established in Proposition 3.2.1 permits to show that the interacting KMS $\omega^{\beta,V}$ evolved with the free evolution converges pointwise in $\mathscr{A}^V$ to the free KMS state. Actually,

$$\lim_{T\to\infty}\omega_h^{\beta,V}(\alpha_T(A)) = \lim_{T\to\infty}\frac{\omega^\beta\left(\alpha_T(A)\star U_h(\mathrm{i}\beta)\right)}{\omega^\beta\left(U_h(\mathrm{i}\beta)\right)} = \omega^\beta(A) \tag{3.2.7}$$

where the limit is taken in the sense of formal power series in the coupling constant λ. Furthermore, in the first equality we used the definition (2.3.42) and in the second one the result of Proposition 3.2.1 extended to U_h. As discussed in the introduction, the condition (3.2.7) is very close to one of the stability conditions analysed in [HHW67, Ro73, BKR78], see (3.1.1). However, for our purposes, we would like to prove that the free KMS state evolved with the interacting dynamics tends to the interacting KMS state constructed in [Li13, FL14], i.e. the limit stated in (3.1.2). In any case, the clustering condition obtained in Proposition 3.2.1 allows to have stability up to first order in V_h. Actually we have the following theorem, whose proof can be given in close analogy to the proof of Theorem 3.1.2.

Theorem 3.2.1 (First order stability)**.** *Let ω^β be the extremal KMS state with respect to the evolution α_t at inverse temperature β of the free theory. Then, considering a perturbation V_h as per equation* (2.3.27)*, return to equilibrium* (3.1.2) *holds at first order, i.e.*

$$\lim_{T\to\infty}\mathrm{i}\int_0^T dt\,\omega^\beta([\alpha_t(K_h),\alpha_T(A)]) = -\int_0^\beta du\,\omega^{\beta,c}(A\otimes\alpha_{\mathrm{i}u}(K_h)), \tag{3.2.8}$$

where A is an element of $\mathscr{A}^V(\mathbb{O})$ and K_h is as in (2.3.33)*.*

Before discussing the proof, we notice that, the right hand side of (3.2.8) is the first order contributions in K_h of (2.3.43) while the left hand side is that of ω^β composed with α_t^V in (2.3.40). Since K_h is itself a formal power series in the coupling constant λ, where the order zero vanishes, the proposition implies the stability up to first order in the sense of perturbation theory.

Proof. The proof can be performed in close analogy to the proof of Theorem 2 in [BKR78] once the clustering condition stated in Proposition 3.2.1 is established. Let us start noticing that

$$\begin{aligned} \mathrm{i}\int_0^T dt\,\omega^\beta([\alpha_t(K_h),\alpha_T(A)]) &= \mathrm{i}\int_0^T dt\,\omega^\beta([\alpha_{-t}(K_h),A]) \\ &= \mathrm{i}\int_0^T dt\left(\omega^\beta\left(A\star\alpha_{-t+\mathrm{i}\beta}(K_h)\right)-\omega^\beta(A\star\alpha_{-t}(K_h))\right) \\ &= \int_0^\beta du\left(\omega^\beta(A\star\alpha_{-T+\mathrm{i}u}(K_h))-\omega^\beta(A\star\alpha_{\mathrm{i}u}(K_h))\right), \end{aligned} \tag{3.2.9}$$

where the last equality holds because of the divergence theorem. Actually, thanks to the KMS condition satisfied by ω^β, the function $F(z)\doteq\omega^\beta(A\star\alpha_z(K_h))$ is analytic in the strip $\Im(z)\in[0,\beta]$. Hence $\partial_{\bar z}F(z)=0$, thus the integral of $F(z)$ over a closed oriented curve in the domain of analyticity vanishes. From the clustering condition stated in Propostion 3.2.1 we have that

$$\lim_{T\to\infty}\int_0^\beta du\,\omega^\beta(A\star\alpha_{-T+\mathrm{i}u}(K_h))=\int_0^\beta du\,\omega^\beta(A)\omega^\beta(K_h)=\beta\omega^\beta(A)\omega^\beta(K_h) \tag{3.2.10}$$

hence, using it in (3.2.9) and recalling the definition (1.3.57), we conclude that the limit (3.2.8) holds. □

The clustering condition established in Proposition 3.2.1 does not suffice to prove return to equilibrium to all orders in K_h. Actually, at higher orders, due to the presence of the $\star-$product of various time translated generators, the clustering condition cannot be used to factorise their expectation values. To solve this issue we found convenient to take advantage of the clustering property of the free equilibrium state ω^β with respect to the interacting time-evolution α_t^V, as stated by the following proposition.

Proposition 3.2.2 (Clustering condition for α_t^V)**.** *The following clustering condition*

$$\lim_{t\to\pm\infty}\left[\omega^\beta(A\star\alpha_t^V(B))-\omega^\beta(A)\,\omega^\beta(\alpha_t^V(B))\right]=0\qquad\forall\,A,B\in\mathscr{A}^V(\mathbb{O})$$

holds in the sense of formal power series in the coupling constant whenever the perturbation Lagrangian V_h has compact spatial support. The result still holds also when $A=U_h(\mathrm{i}\beta)\star A'$, with $A'\in\mathscr{A}^V(\mathbb{O})$.

Proof. The definition of the connected functions (1.3.57) implies that the statement of the proposition holds if, at every order of perturbation, the connected function

$$\omega^{\beta,c}\left(A\otimes\alpha_t^V(B)\right)=\omega^\beta\left(A\star\alpha_t^V(B)\right)-\omega^\beta(A)\omega^\beta\left(\alpha_t^V(B)\right)$$

vanishes for large or negative values of t. Let us thus expand α_t^V as in (2.3.40). Hence,

$$\omega^{\beta,c}\left(A\otimes\alpha_t^V(B)\right)=\sum_{n=0}^\infty\mathrm{i}^n\int_{tS_n}\omega^{\beta,c}\left(A\otimes[\alpha_{t_1}(K_h),[\dots[\alpha_{t_n}(K_h),\alpha_t(B)]\dots]]\right)dT_n.$$

The element $n = 0$ in the sum vanishes in the limit of large t thanks to the clustering condition respect to α_t given in Proposition 3.2.1. We show now that the $n-$th element of the previous sum tends to zero for $t \to \infty$ in the sense of formal power series in the coupling constant. To this avail, we notice that

$$[\alpha_{t_1}(K_h),[\dots,[\alpha_{t_n}(K_h),B]\dots]]$$

is a sum of connected components. In order to prove it notice that

$$[A,B] = A \star B - B \star A = \mathbf{m} \circ \left(e^{\Gamma_{12}} - e^{\Gamma_{21}}\right) A \otimes B,$$

where Γ_{ij} is the functional differential operator defined in equation (1.3.76) computed using the 2-point function ω_2^β. For simplicity of notation we have suppressed the ω. Since

$$\omega^{\beta,c}(A \otimes B) = \mathbf{m} \circ \left(e^{\Gamma_{12}} - 1\right) A \otimes B \big|_{(\phi_1,\phi_2)=0},$$

we conclude that $\omega^{\beta,c}(A \otimes [\alpha_{t_1}(K_h),[\dots[\alpha_{t_n}(K_h),B]\dots]])$ is a weighted sum over the set $\mathcal{G}^{o,c}_{n+2}$ of connected oriented graphs with $n+2$ vertices. Every oriented line joining two vertices indicates the presence of a 2-point function. Furthermore, a single graph $G \in \mathcal{G}^{o,c}_{n+2}$ can not contain lines with opposite orientations joining the same two vertices. The orientation is necessary because the 2-point function is not symmetric and because of the presence of subsequent commutators. Examples of graphs are given in the following pictures.

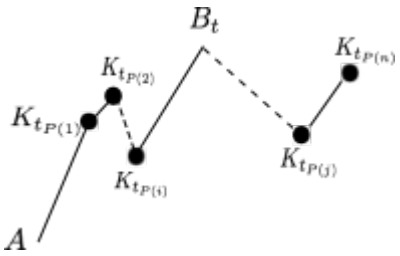


Figure 3.1

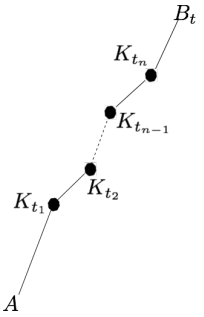


Figure 3.2

We will start discussing the case where the graph G is of the form given in Figure 3.2, which is simple since the time are in crescent order and the end point is B_t, which is the point which will be eventually sent to infinity.

Indicating by c_G the weight of the single graph G, we have that

$$\omega^{\beta,c}\left(A \otimes [\alpha_{t_1}(K_h),[\dots[\alpha_{t_n}(K_h),\alpha_t(B)]\dots]]\right) = \sum_{G \in \mathcal{G}^{o,c}_{n+2}} c_G \int_{tS_n} F_G(t_1,\dots,t_n)\, dT_n,$$

where we used the notation of equations (2.3.37) and (2.3.38) for the integration over the simplex and where

$$F_G(t_1,\dots,t_n) \doteq \mathbf{m} \circ \prod_{l \in E(G)} \Gamma_{s(l)r(l)} \left(A \otimes \alpha_{t_1}(K_h) \otimes \dots \otimes \alpha_{t_n}(K_h) \otimes \alpha_t(B)\right) \Big|_{(\phi_1,\dots\phi_{n+2})=0},$$

$E(G)$ being the set of the lines of G, $s(l), r(l) \in \{0,\dots,n+1\}$ indicating the source and the range of the line l respectively.

Since V_h is of compact spatial support, K_h, A and B are in $\mathscr{F}_{\mu c}$, then a repeated application of Proposition 1.3.4 leads to

$$|F_G(t_1,\dots,t_n)| \leq C_1 \prod_{l\in E(G)} \frac{1}{\left(\left|t_{s(l)}-t_{r(l)}\right|+d\right)^{3/2}} \leq \frac{C_2}{\left(|t_1+d|\,|t_2-t_1+d|\,|t_3-t_2+d|\cdots|t_n-t_{n-1}+d|\,|t-t_n+d|\right)^{-3/2}} \tag{3.2.11}$$

for some constants d, C_1 and C_2. In the last inequality we used the fact that the graph G is connected and that the times $(t_1,\dots,t_n)\in tS_n$. Thus, the integral of F_G over the simplex can be performed and it vanishes in the limit $t\to\infty$ because of the previous inequality.

The general case, namely a graph similar to the one presented in Figure 3.1 (where the subscript P denotes any permutation of the set $\{1,\dots,n\}$) can be treated analogously by noticing the following facts: First of all, we observe that the fact that the times by which every vertex is translated are not in crescent order is harmless because it is the addition of a line going backwards in time in the graph of Figure 3.2 amounts just to the addition of a multiplicative term bounded in the large-time limit. This can be seen from equation (3.2.11). This also contributes that the part of graphs at the right of B_t is a multiplicative term bounded in the limit $t\to\infty$, as can be argued from equation (3.2.11). Hence, the study of graph in Figure 3.1 can be reduced to the analysis of the one in Figure 3.2. □

The previous proposition can be used to show the validity of a (sort of) Gell-Mann and Low factorisation formula for $\omega^{\beta,V}$ with respect to ω^{β}, so permitting to get an interpretation similar to the one achieved at the end of Section 2.2, where we dealt with the comparison with the traditional literature. Nonetheless, we stressed that, in order to have a proper dictionary between the two formulations of QFT, the adiabatic limit must be considered. In this sense, we will see that the failure of the return to equilibrium property in the adiabatic limit $h\to 1$ implies that this sort of Gell-Mann and Low formula is not preserved in the non-spacelike compact case. This will be made explicit in the next section, *cf.* Proposition 3.3.2.

Owing to the clustering condition established in Proposition 3.2.2 we can show that the free KMS state is stable.

Theorem 3.2.2 (Stability)**.** *Let ω^{β} be the extremal KMS state with respect to the evolution α_t at inverse temperature β of the free theory. Then the state is stable under perturbations described by an interaction Lagrangian V_h of spatially compact support. Namely*

$$\lim_{T\to\infty} \omega^{\beta}\left(\alpha_T^V(A)\right) = \omega^{\beta,V}(A) \qquad \forall\, A\in\mathscr{A}^V(\mathcal{O}). \tag{3.2.12}$$

Proof. For simplicity, in this proof, we shall write $U(t)\equiv U_h(t)$, see (2.3.36) for its definition, and we shall not write explicitly the $\star$-product. First we notice that, as a consequence of the co-cycle relation (2.3.31), we have that

$$\mathbb{1} = U(t-t) = U(t)\,\alpha_t(U(-t)) \Rightarrow U(-t)^{-1} = \alpha_{-t}(U(-t)). \tag{3.2.13}$$

Then, together with the time-translation invariance of ω^β, this equation implies

$$\omega^\beta\left(\alpha_t^V(A)\right) = \omega^\beta\left(\alpha_{-t}\alpha_t^V(A)\right) = \omega^\beta\left(U(-t)^{-1}AU(-t)\right) = \omega^\beta\left(U(-t)\alpha_{i\beta}\left(U(-t)^{-1}\right)\alpha_{i\beta}(A)\right), \quad (3.2.14)$$

where in the last equality we have used the KMS condition. Next, we use again the co-cycle condition (2.3.31) and relation (3.2.13) for manipulating $\alpha_{i\beta}\left(U(-t)^{-1}\right)$:

$$\alpha_{i\beta}\left(U(-t)^{-1}\right) = \alpha_{-t}\left(\alpha_{i\beta}(U(t))\right) = \alpha_{-t}\left(U(i\beta)^{-1}\right)\alpha_{-t}\left(U(t+i\beta)\right) = \alpha_{-t}\left(U(i\beta)^{-1}\right)\alpha_{-t}(U(t))U(i\beta) = \alpha_{-t}\left(U(i\beta)^{-1}\right)U(-t)^{-1}U(i\beta).$$

Inserting this equation and using again equation (2.3.29) we obtain

$$\omega^\beta\left(\alpha_T^V(A)\right) = \omega^\beta\left(U(-t)\alpha_{-t}(U(i\beta)^{-1})U(-t)^{-1}U(i\beta)\alpha_{i\beta}(A)\right) = \omega^\beta\left(\alpha_{-t}^V\left(U(i\beta)^{-1}\right)U(i\beta)\alpha_{i\beta}(A)\right).$$

Then, we can take the large time limit $t \to \infty$: The clustering condition obtained in Proposition 3.2.2 implies that

$$\lim_{t\to\infty}\omega^\beta(\alpha_t^V(A)) = \omega^\beta\left(U(i\beta)\alpha_{i\beta}(A)\right)\lim_{t\to\infty}\left[\omega^\beta\left(\alpha_{-t}^V\left(U(i\beta)^{-1}\right)\right)\right].$$

Notice that $\alpha_{-t}^V(\mathbb{1}) = \mathbb{1}$, the state ω^β is normalised, and $\omega^\beta(U(i\beta))$ is finite to all orders in perturbation theory, hence the limit $t \to \infty$ of $\omega^\beta\left(\alpha_{-t}^V\left(U(i\beta)^{-1}\right)\right)$ converges in the sense of perturbation theory to $\omega^\beta\left(U(i\beta)\right)^{-1}$, which is the normalisation factor of $\omega^\beta\left(U(i\beta)\alpha_{i\beta}A\right)$. The application of the KMS condition in the numerator gives the result. □

3.3 Instabilities in the adiabatic limit

In the previous section we have established that KMS states for field theories are stable under spatially compact local perturbations. We will now address the case where the perturbation is constant in space, namely when the adiabatic limit is considered. As in the previous section, we consider a massive theory on a Minkowski space-time $\mathbb{M}$ perturbed with an interaction Lagrangian V_h of the form prescribed in (2.3.27). The test functions h and χ have been defined in (2.3.28). The adiabatic limit corresponds to send $h \to 1$ on all the space-time. Technically speaking, this limit is taken in the sense of van Hove, as per Definition 2.3.1. As a general rule, we will omit the suffix h in the relevant quantities only when the adiabatic limit is considered, for instance we will denote with K the infinitesimal generator in the adiabatic limit vH-$\lim_{h\to 1} K_h$.

The strategy for tackling the problem is similar to the one adopted in the previous section, even though we will see that the arguments used to prove Theorem 3.2.1 or Theorem 3.2.2 fail after having taken the adiabatic limit, hence return to equilibrium (3.1.2) does not hold in this case.

In order to enhance the chances of having at least the convergence we shall consider an ergodic mean of the free KMS state perturbed by V, which is usually introduced to tame the possible oscillations for large times occurring at first orders in perturbation theory. Actually, we study the *ergodic mean* of $\omega^\beta \circ \alpha_\tau^V$

$$\omega_T^{V,+}(A) \doteq \underset{h\to 1}{\text{vH-lim}}\,\frac{1}{T}\int_0^T \omega^\beta(\alpha_\tau^V(A))d\tau \quad (3.3.15)$$

and eventually we will consider the limit $T \to \infty$. We shall see that the clustering condition fails when the adiabatic limit is considered and this failure cannot be repaired by the ergodic mean.

Proposition 3.3.1. *Suppose that* $\frac{\delta^2 V_h}{\delta^2 \phi}\Big|_{\phi=0} \neq 0$. *If the adiabatic limit (*$h \to 1$*) is considered, the clustering condition fails at first order in perturbation theory also when the ergodic mean is considered, i.e.*

$$\lim_{T\to\infty} \underset{h\to 1}{\text{vH-lim}} \left(\frac{1}{T} \int_0^T dt\, \omega^\beta(A \star \alpha_t(K_h)) - \omega^\beta(A)\omega^\beta(K_h) \right) \neq 0$$

for $A = R_V(F_f) \star R_V(F_g)$ *where* F_f *and* F_g *are linear functionals as per Definition 1.2.13 smeared by* $f, g \in \mathscr{D}$ *and* K_h *is as in* (2.3.33).

Proof. Let us consider the case where $V_h = \frac{1}{2}\int h\chi\phi^2 d\mu$, more complicated potentials can be treated analogously. By direct computation, we get

$$\omega^\beta(R_V(F_f) \star R_V(F_g) \star \alpha_t(K_h)) - \omega^\beta(R_V(F_f) \star R_V(F_g))\omega^\beta(K) = \\ \lambda \int \omega_2^\beta(f,y)\omega_2^\beta(g,y)\dot{\chi}_-(y^0+t)h(\mathbf{y})dy^0 d^3\mathbf{y} + O(\lambda^2)$$

where $y = (y^0, \mathbf{y})$ and $\dot{\chi}_-$ is given in (2.3.33). Furthermore, $\omega_2^\beta(f,y) \doteq \langle \omega_2^\beta, f \otimes \delta_y \rangle$ is given in terms of δ_y, the Dirac delta function centered in y, and it is a smooth function thanks to the Hadamard property. Using the exponential decay for large spatial separations of the 2-point functions ω_2^β given in (1.3.70) we have

$$\lim_{h\to 1} \int \omega_2^\beta(f,y)\omega_2^\beta(g,y)\dot{\chi}_-(y^0+t)h(\mathbf{y})dy^0 d^3\mathbf{y} = \int \omega_2^\beta(f,y)\omega_2^\beta(g,y)\dot{\chi}_-(y^0+t)dy^0 d^3\mathbf{y} \doteq \langle F_t, f\otimes g\rangle.$$

We shall now study the form of the distribution F_t. In particular, (1.3.70) implies that

$$F_t(x_1,x_2) = \frac{1}{(2\pi)^6} \int d^3\mathbf{y} dy^0 \dot{\chi}_-(y^0+t) \\ \times \prod_{j=1}^2 \int \left(b_+(\mathbf{k}_j) \frac{e^{iE(\mathbf{k}_j)(x_j^0 - y^0)}}{2E(\mathbf{k}_j)} + b_-(\mathbf{k}_j) \frac{e^{-iE(\mathbf{k}_j)(x_j^0-y^0)}}{2E(\mathbf{k}_j)} \right) e^{-i\mathbf{k}_j(\mathbf{x}_j - \mathbf{y})} d^3\mathbf{k}_j.$$

The integral in $d\mathbf{y}$ gives a delta contribution which forces $\mathbf{k}_1 + \mathbf{k}_2 = 0$. In the product between the various modes there is an y_0-independent contribution which remains unaffected by the t-translation:

$$b_+(\mathbf{k})b_-(\mathbf{k}) \left(\frac{e^{iE(\mathbf{k})(x_1^0 - x_2^0)}}{4E(\mathbf{k})^2} + \frac{e^{-iE(\mathbf{k})(x_1^0-x_2^0)}}{4E(\mathbf{k})^2} \right) = \frac{1}{2E(\mathbf{k})^2} b_+(\mathbf{k})b_-(\mathbf{k}) \cos(E(\mathbf{k})(x_1^0 - x_2^0)).$$

The other contributions are proportional to oscillatory phases $\sim e^{iE(\mathbf{k})t}$ and disappear in the limit of large times thanks to the Riemann-Lebesgue Lemma. Note that this is guaranteed only in presence of the time average. Summing up we find

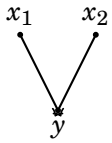
$$w(x_1,x_2) \doteq \lim_{T\to+\infty} \frac{1}{T} \int_0^T dt \int dy \dot{\chi}_-(y^0+t)\omega^\beta(x_1,y)\omega^\beta(x_2,y) \\ = \frac{1}{(2\pi)^3} \int \frac{1}{2E(\mathbf{k})^2} b_+(\mathbf{k})b_-(\mathbf{k}) \cos\left(E(\mathbf{k})(x_1^0 - x_2^0)\right) e^{i\mathbf{k}(\mathbf{x}_1 - \mathbf{x}_2)} d^3\mathbf{k}, \quad (3.3.16)$$

where in the last equality we were able to perform the integral of y^0 thanks to the form of $\dot{\chi}_-(y^0+t)$ given in (2.3.33). Hence, at first order in perturbation theory,

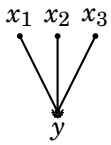
$$\lim_{T\to\infty}\lim_{h\to 1}\frac{1}{T}\int dt\Big(\omega^\beta(R_V(F_f)\star R_V(F_g)\star\alpha_t(K))-\omega^\beta(R_V(F_f)\star R_V(F_g))\omega^\beta(K)\Big)=\lambda w(f,g)+O(\lambda^2).$$

which is in general non-vanishing, thus concluding the proof. □

Example 3.3.1. The proof of the previous proposition can be directly applied in particular to the case of a $\lambda\phi^4$ theory evaluated in a massive KMS state. Actually, in that case, when the $\star_{\omega^\beta}$ product is used to describe the product of the theory, the interacting potential acquires the known contribution called thermal mass, as shown at the end of Section 1.3.4. More in detail, taking advantage of the graphic representation of the star product, we see that the distribution $\omega^\beta(x_1,y)\omega^\beta(x_2,y)$, which enters in the proof of Proposition 3.3.1, can be graphically depicted in the following way

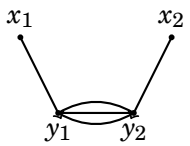


The essential point in the proof of the previous proposition is that, after the spatial integration over the whole **y**-space, a non-vanishing contribution constant in y^0 remains. Hence, the time average over back-in-time translations $y^0\to y^0-t$ does not vanish. Operating in a similar way, one sees that when more lines are attached to the point y, like in



$$=\omega^\beta(x_1,y)\omega^\beta(x_2,y)\omega^\beta(x_3,y),$$

the corresponding contributions vanish essentially because of the Riemann-Lebesgue Lemma. Coming back to the elements which give non-vanishing contributions we observe that even if the vertex y is substituted by two points joined by some internal propagators, due to the momentum conservation, its ergodic mean in the large time limit is again non-vanishing. As an example we could consider the contribution



to a $\lambda\phi^4$ theory with vanishing thermal mass.

The large time limit of $\omega_T^{V,+}$ given in (3.3.15) is even more problematic than this. Actually, in the expansion at higher orders in K, there are new contributions which do not converge even if the ergodic mean is considered. We shall see an explicit example in the following proposition

Proposition 3.3.2. *Consider a quadratic interaction Lagrangian in the adiabatic limit ($h \to 1$). Consider the quadratic field $A = \int_{\mathbb{M}} f\phi^2 d^4x$ where $f \in \mathscr{D}$ and $\int dt f(t,\mathbf{x}) = 0$ for every $\mathbf{x}$. The contribution*

$$Q_T^{(n)}(A) = \frac{1}{T}\int_0^T dt_{n+1}\int_0^{t_{n+1}} dt_n \ldots \int_0^{t_2} dt_1\, \omega^\beta([\alpha_{t_1}(K),\ldots,[\alpha_{t_n}(K),\alpha_{t_{n+1}}(A)]]\ldots])$$

to the ergodic mean $\omega_T^{V,+}(A)$ in (3.3.15) *does not converge for all $n \geq 3$ in the sense of perturbation theory for large T, if the adiabatic limit is taken in advance.*

Proof. We can compute $Q_T^{(n)}(A)$ with a graph expansion as in the proof of Proposition 3.2.2. Here, we discuss the main points which permits to prove the proposition. Only connected oriented graphs are present in the graph expansion of $Q_T^{(n)}(A)$.

$$Q_T^{(n)}(A) = \sum_{G\in\mathscr{G}_{n+1}^{o,c}} \frac{c_G}{T}\int_{TS_{n+1}} dT_n\, \mathbf{m}\circ\left(\prod_{l\in E(G)}\Gamma_{s(l)r(l)}\big(\alpha_{t_1}(K)\otimes\cdots\otimes\alpha_{t_n}(K)\otimes\alpha_{t_{n+1}}(A)\big)\right)\Big|_{(\phi_1,\ldots\phi_{n+1})=0}$$
$$\doteq \frac{1}{T}\int_{TS_{n+1}} F_{n+1}(t_1,\ldots,t_{n+1})\,dT_n,$$

where c_G is a numerical factor which may be vanishing and we have used the notation (2.3.37). Furthermore, Γ_{ij} and $\mathbf{m}$ are defined as in (1.3.76), $E(G)$ is the set of the lines of the graph G and $s(l), r(l) \in \{1,\ldots,n+1\}$ indicate the source and the range of the line l respectively. We notice that, by definition, K is at least linear in the coupling constant λ, *i.e.* $\lambda K = \lambda H + O(\lambda^2)$, hence the lowest order in perturbation theory for $Q_T^{(n)}(A)$ has to be n. Thence, only oriented connected graphs with $n+1$ vertices and $n+1$ lines contribute to $Q_T^{(n)}(A)$. Therefore, every vertex is either the source or the range of exactly two lines. Actually, at order n in perturbation theory,

$$F_{n+1}^{(n)}(t_1,\ldots,t_{n+1}) = \frac{1}{2}\mathbf{m}\circ(\Gamma_{12}^2-\Gamma_{21}^2)\big(\alpha_{t_1}(H)\otimes B_n(t_2,\ldots,t_{n+1})\big)$$

where, for all $n \geq 2$

$$B_n(t_1,\ldots,t_n) \doteq \mathbf{m}\circ(\Gamma_{12}-\Gamma_{21})\big(\alpha_{t_2}(H)\otimes B_{n-1}(t_2,\ldots,t_n)\big), \qquad B_1(t) \doteq \alpha_t(A).$$

Notice that, for every n, B_n are quadratic fields. Furthermore,

$$\Gamma_{12}-\Gamma_{21} = \left\langle \mathrm{i}\Delta, \frac{\delta^2}{\delta\varphi_1\delta\varphi_2}\right\rangle,$$

where $\Delta(x,y) = \mathrm{i}\omega_2^\beta(y,x) - \mathrm{i}\omega_2^\beta(x,y)$ is the causal propagator. Since $\Delta(x,y)$ vanishes for spacelike-separated points (x,y) and since $\frac{\delta H_h}{\delta\phi(x)}$, with H_h defined in (2.3.33), is timelike compact uniformly in h and $\frac{\delta A}{\delta\phi(x)}$ is compact, we have that $B_n(t_1,\ldots,t_n)$ is compactly supported at fixed $t_1,\ldots,t_n$ for every n. Hence, $B_n \in \mathscr{A}_{\omega^\beta}$ even if the adiabatic limit $h \to 1$ is considered. For a similar reason the adiabatic limit can be easily taken also in $F_{n+1}^{(n)}$. Actually, $\omega_2^\beta(x,y)\omega_2^\beta(x,z) - \omega_2^\beta(y,x)\omega_2^\beta(z,x)$, which appears in the expansion of $\big(\Gamma_{12}^2-\Gamma_{21}^2\big)$, vanishes if both $x-y$ and $x-z$ are spacelike vectors. Notice that, once the spatial Fourier transform is taken, using the form of the 2-point function (1.3.70), $F_{n+1}^{(n)}(t_1,\ldots,t_{n+1})$ can be computed directly.

In order to analyse the integral of $F^{(n)}_{n+1}$ over the simplex TS_{n+1}, we further decompose it as a sum over the copies of disjoint subsets of $\{1,\dots,n+1\}$

$$F^{(n)}_{n+1}(t_1,\dots,t_{n+1}) = \sum_{\substack{I,J\subset\{1,\dots,n+1\}\\ I\cap J=\emptyset}} \int \left(e^{2\mathrm{i}E(\mathbf{p})(\sum_{i\in I}t_i-\sum_{j\in J}t_j)}\widehat{\Phi}^+_{I,J}(\mathbf{p}) + e^{-2\mathrm{i}E(\mathbf{p})(\sum_{i\in I}t_i-\sum_{j\in J}t_j)}\widehat{\Phi}^-_{I,J}(\mathbf{p})\right) d^3\mathbf{p},$$

where $\widehat{\Phi}^{\pm}_{I,J}(\mathbf{p})$ are suitable functions which are rapidly decreasing for large spatial momentum $\mathbf{p}$.

Notice that the largest contribution in $Q^{(n)}_T(A)$ is obtained when $|I|$ and $|J|$ are small. By direct inspection we notice that when either I and J are empty sets, both $\Phi^{\pm}_{I,J}$ vanish. When both I and J contain only one element, due to the form of A, the only non-vanishing contribution in the sum is when $I=\{t_1\}$ and $J=\{t_{n+1}\}$ or when $I=\{t_{n+1}\}$ and $J=\{t_1\}$. Hence, the most divergent contribution for large times T to $Q^{(n)}_T(A)$ is given by

$$F^{(n)}_{n+1}(t_1,\dots,t_{n+1}) = \\ C_n\int_{\mathbb{R}^3}(b_+(\mathbf{p})+b_-(\mathbf{p}))\left(\frac{e^{\mathrm{i}2E(\mathbf{p})(t_1-t_{n+1})}}{E(\mathbf{p})^{n+1}}\widehat{\Phi}^+(\mathbf{p}) + (-1)^n\frac{e^{-\mathrm{i}2E(\mathbf{p})(t_1-t_{n+1})}}{E(\mathbf{p})^{n+1}}\widehat{\Phi}^-(\mathbf{p})\right)d^3\mathbf{p}+R,$$

where C_n is a numerical factor and $\widehat{\Phi}_+(\mathbf{p}) = \widehat{\chi}_-(-E(\mathbf{p}))\widehat{f}(E(\mathbf{p}),\mathbf{p})$ and $\widehat{\Phi}_-(\mathbf{p}) = \widehat{\chi}_-(E(\mathbf{p}))\widehat{f}(-E(\mathbf{p}),\mathbf{p})$.

The integral over the simplex TS_{n+1} can be computed before the integration over $\mathbf{p}$ and it gives an oscillating function whose amplitude grows as T^n times $e^{\pm\mathrm{i}E(\mathbf{p})T}$. The integration over $\mathbf{p}$ contributes again with an oscillating function whose amplitude decays as $1/T^{3/2}$. Combining these two terms we obtain that the amplitude of $Q^{(n)}_T(A)$ grows as $T^{n-3/2-1}$, hence for all $n\geq 3$ $Q^{(n)}_T(A)$ does not converge for large T. □

These kind of infrared divergences can be traced back to the difficulties present in the analysis of the existence of adiabatic limit [Al90, LW87]. In the literature it is claimed that, they can be tamed by partial resummations of the perturbative series. However, these kind of resummations are beyond perturbation theory.

In any case, the previous analysis leads us to conclude that, at least perturbatively, the stability does not hold if the potential has unbounded support. This may be heuristically interpreted in the spirit of what we pointed out in Section 1.3.3 concerning the KMS states: If the potential is defined everywhere, the perturbation becomes "too strong" for the system, which is not able to resist any longer. A statistical mechanical analogue would be the situation where an infinite reservoir is coupled to an infinite system, and so it is changed by the backreaction. Actually, we stress that this analogy must be taken carefully since, in our situation, we are dealing with a self-interaction, which makes the physical picture more sophisticated.

3.4 A non-equilibrium steady state for the free field theory

In the previous section we have seen in Proposition 3.3.1 that the clustering condition does not hold in the adiabatic limit. This implies a failure of the stability which, loosely speaking, can be tracked back to the fact that the expansion of the interacting time-evolutions α^V_t, which is given in equation (2.3.40), involves an integration over the simplex TS_n, that becomes infinite in the large time limit, so making all the terms blowing up. On the other hand, the situation involving

the return to equilibrium is different: Despite we can not expect this to hold due to the failure of the clustering and to the need of the ergodic mean, there may be hope to have something finite in the limit. In particular, we expect that, when the ergodic mean of a state converges to another state, these new state is a *non-equilibrium steady state* [Ru00]. This expectation are motivated also by the construction of Fredenhagen and Linder, which tells us that the interacting KMS state $\omega^{\beta,V}$ is well-defined in the adiabatic limit, hence we would expect that also its composition with the free dynamics remains such.

NESS's are interesting objects which have been thoroughly studied above all in Statistical Mechanics, for example [JP02, JP02b, Ru00, SL77], and, more recently, also in free QFT [BeDo15, BeDo16, DLSB15, HL16, HV18]. A typical situation when such states arise is the following: Consider two infinite reservoirs at different temperatures which interact with a small system. Let us assume that the reservoirs do not interact directly, but only through the small system, so that we can assume that they evolve freely. Typically, it happens that the small system eventually reach an equilibrium temperature, but it never reaches the thermal equilibrium because of the presence of heat fluxes, which are constant in time, so making the state stationary. Such situations is studied in full generality in [JP02] and computation of NESS's has been done in several models of this kind, for instance in spin chains, Fermi gases and also in classical Markov chains. In the free QFT framework, the two reservoirs are typically realised by assigning two KMS states on the algebras built on two separated regions of the space-time (*e.g.* in the positive and negative halves of Minkowski).

Concerning interacting (perturbative) QFT, to our knowledge a NESS has been introduced for the first time in [DFP18a], a second proposal (still not completely accomplished) has been made very recently in [HV18], again using the idea of the two reservoirs. Actually, the state of [DFP18a], which we will define in this section, escapes the former picture of the two reservoirs since it is constructed as a by-product of the failure of the return of equilibrium, considering a self-interaction. This atypical structure motivated us to investigate the nature of this state in more depth, leading us to introduce and study relative entropy and entropy production in pAQFT, see [DFP18b] and the following Chapter 4.

In order to construct an example of a non-equilibrium steady state, we revert the point of view and we analyse the ergodic mean of $\omega^{\beta,V}$ with respect to the free time evolution α_t

$$\omega^+(A) \doteq \lim_{T\to\infty} \operatorname*{vH-lim}_{h\to 1} \frac{1}{T}\int_0^T \omega^{\beta,V}(\alpha_t(A))\,dt \qquad \forall\, A \in \mathscr{A}_{\omega^\beta}, \tag{3.4.17}$$

which is seen as a state (defined as a formal power series) for the unperturbed theory.

Theorem 3.4.1. *The functional ω^+ defined in the sense of formal power series in* (3.4.17)*, is a state for the free algebra $\mathscr{A}_{\omega^\beta}$. Furthermore, ω^+ is invariant under the free evolution α_t.*

Proof. $\omega^{\beta,V}$ defined in (2.3.43) is a linear functional over the free algebra given in the sense of formal power series. Furthermore, it is normalized by construction. It is also positive again in the sense of formal power series. It is thus a state over the free algebra. $\omega^{\beta,V}\circ\alpha_t$ is a state because

it is the composition of a state with an automorphism of the algebra. The properties of being positive, normalized and linear are preserved by the ergodic mean of functionals.

In order to prove that the limit $T \to \infty$ exists for every A, we study

$$\omega^{\beta,V}(A) = \omega^{\beta}(A) + \sum_{n=1}^{\infty} (-1)^n \int_{\beta S_n} \omega^{\beta,c}\left(A \otimes \alpha_{\mathrm{i}u_1}(K) \otimes \cdots \otimes \alpha_{\mathrm{i}u_n}(K)\right) dU_n, \tag{3.4.18}$$

where we have used the compact notation for the integration over the simplex introduced in (2.3.37). In [FL14] (see also Appendix C in [DrHaPi16]) it is shown that the state in the adiabatic limit can be obtained in the following way

$$\omega^{\beta,V}(A) = \omega^{\beta}(A) + \sum_{n=1}^{\infty} \int_{\beta S_n} dU_n \int_{\mathbb{R}^3} d^3\mathbf{x}_1 \ldots \int_{\mathbb{R}^3} d^3\mathbf{x}_n \, \omega^{\beta,c}\left(A \otimes \alpha_{\mathrm{i}u_1,\mathbf{x}_1}(R) \otimes \cdots \otimes \alpha_{\mathrm{i}u_n,\mathbf{x}_n}(R)\right), \tag{3.4.19}$$

where $R \doteq -R_V\left(H(\dot{\chi}^- \delta_0)\right)$ in the limit $h \to 1$, δ_0 is the Dirac delta function centered in the origin of $\mathbb{R}^3$ and H is the interacting Hamiltonian density given in (2.3.35). We are thus interested in

$$\omega^{\beta,V}(\alpha_T(A)) = \omega^{\beta}(\alpha_T(A)) + \sum_{n=1}^{\infty} \int_{\beta S_n} dU_n \int_{\mathbb{R}^3} d^3\mathbf{x}_1 \ldots \int_{\mathbb{R}^3} d^3\mathbf{x}_n \, \omega^{\beta,c}\left(\alpha_T(A) \otimes \alpha_{\mathrm{i}u_1,\mathbf{x}_1}(R) \otimes \cdots \otimes \alpha_{\mathrm{i}u_n,\mathbf{x}_n}(R)\right) \tag{3.4.20}$$

for large values of T. Hence, let us study how the following function, related to the integrand of (3.4.20), depends on T

$$F_n(u_0 - \mathrm{i}T, \mathbf{x}_0; u_1, \mathbf{x}_1; \ldots; u_n, \mathbf{x}_n) \doteq \omega^{\beta,c}(\alpha_{\mathrm{i}u_0+T}(A) \otimes \alpha_{\mathrm{i}u_1,\mathbf{x}_1}(A_1) \otimes \cdots \otimes \alpha_{\mathrm{i}u_n,\mathbf{x}_n}(A_n)).$$

In the first part of the subsequent analysis, we follow the proof of Theorem 4 in [FL14]. For completeness, we shall just recall the main steps. Due to the integration domain in (3.4.18) we are interested in the case where $\mathbf{x}_0 = 0$ and

$$0 = u_0 < u_1 < \cdots < u_n < \beta. \tag{3.4.21}$$

Furthermore, without losing generality, we might restrict our attention to the case where $u_{j+1} - u_j \leq \frac{\beta}{2}$ for every j. Actually, if for some $m < n$, $u_{m+1} - u_m > \beta/2$, (3.4.21) implies that $u_j - u_0 < \beta/2$ for every $j \leq m$ and $\beta - u_j < \beta/2$ for $j \geq m+1$. By the KMS condition 1.3.11 we have that

$$\begin{aligned}
&\omega^{\beta,c}(\alpha_{\mathrm{i}u_0+T}(A) \otimes \alpha_{\mathrm{i}u_1,\mathbf{x}_1}(A_1) \otimes \cdots \otimes \alpha_{\mathrm{i}u_n,\mathbf{x}_n}(A_n)) \\
&\quad = \omega^{\beta,c}(\alpha_{\mathrm{i}u_{m+1},\mathbf{x}_{m+1}}(A_{m+1}) \otimes \cdots \otimes \alpha_{\mathrm{i}u_n,\mathbf{x}_n}(A_n) \otimes \alpha_{\mathrm{i}\beta+\mathrm{i}u_0+T}(A) \otimes \cdots \otimes \alpha_{\mathrm{i}\beta+\mathrm{i}u_m,\mathbf{x}_m}(A_m)) \\
&\qquad \doteq F'_n(u_{m+1}, \mathbf{x}_{m+1}; \ldots; u_n, \mathbf{x}_n; u_0 + \beta - \mathrm{i}T, \mathbf{x}_0; u_1 + \beta, \mathbf{x}_1; \ldots; u_m + \beta, \mathbf{x}_m).
\end{aligned}$$

The argument of the new function F'_n have the desired property, actually $u_{m+1} < \cdots < u_n < \beta + u_0 < \cdots < \beta + u_m$ and $\beta + u_m - u_{m+1} < \beta/2$, hence, indicating by $\tilde{u}_i$ the new arguments of F'_n we have that $\tilde{u}_j - \tilde{u}_i < \beta/2$ for every $i < j$.

By definition of connected functions, *cf.* equation (1.3.57), it descends that F_n can be decomposed as a sum over $\mathscr{G}^c_{n+1}$, the set of connected graphs with $n+1$ vertices:

$$F_n(u_0-\mathrm{i}T,\mathbf{x}_0;u_1,\mathbf{x}_1;\dots;u_n,\mathbf{x}_n)=$$
$$\sum_{G\in\mathscr{G}^c_{n+1}}\prod_{i<j}\left(\frac{\Gamma_{ij}^{l_{ij}}}{l_{ij}!}\right)\left(\alpha_{\mathrm{i}u_0+T,\mathbf{x}_0}(A)\otimes\alpha_{\mathrm{i}u_1,\mathbf{x}_1}(A_1)\otimes\cdots\otimes\alpha_{\mathrm{i}u_n,\mathbf{x}_n}(A_n)\right)\Big|_{(\phi_0,\dots,\phi_n)=0}$$
$$\doteq\sum_{G\in\mathscr{G}^c_{n+1}}\frac{1}{\mathrm{Symm}(G)}F_{n,G}(u_0-\mathrm{i}T,\mathbf{x}_0;u_1,\mathbf{x}_1;\dots;u_n,\mathbf{x}_n)$$

where l_{ij} denotes the number of lines joining the vertices i and j in G and $\mathrm{Symm}(G)$ is a suitable numerical factor. In the proof of Theorem 4 in [FL14], $F_{n,G}$ is then expanded as

$$F_{n,G}(u_0,\mathbf{x}_0;u_1,\mathbf{x}_1;\dots;u_n,\mathbf{x}_n)=\int\prod_{l\in\mathbf{E}(G)}\frac{e^{\mathrm{i}\mathbf{p}_l(\mathbf{x}_{s(l)}-\mathbf{x}_{r(l)})}(\lambda_+(p_l)+\lambda_-(p_l))}{2E(l)(1-e^{-\beta E(l)})}\hat{\Psi}(-P,P)dP \tag{3.4.22}$$

where $\mathbf{E}(G)$ is the set of lines of the graph G, $s(l)$ and $r(l)$ are respectively the indexes of the source and the range of the points joined by the line l.

$$\Psi(X,Y)=\prod_{l\in\mathbf{E}(G)}\frac{\delta^2}{\delta\phi_{s(l)}(x_l)\delta\phi_{r(l)}(y_l)}(A_0\otimes\cdots\otimes A_n)\Big|_{(\phi_0,\dots,\phi_n)=0}$$

where X and Y are shorthands for $(x_1,\dots,x_k)$ and $(y_1,\dots,y_k)$ respectively and k indicates the number of lines in $\mathbf{E}(G)$. $\hat{\Psi}(-P,P)$ is the Fourier transform of $\Psi(X,Y)$ and again $P=(p_1,\dots,p_k)$. Moreover, the positive and negative frequency part in Γ_{ij} are denoted by

$$\lambda_+(p_l)=e^{-E(l)(u_{r(l)}-u_{s(l)})}\delta(p_l^0-E(l)),\qquad\lambda_-(p_l)=e^{E(l)(u_{r(l)}-u_{s(l)}-\beta)}\delta(p_l^0+E(l)), \tag{3.4.23}$$

with $E(l)=\sqrt{\mathbf{p}_l^2+m^2}$. The sum over the positive and negative frequency parts present in (3.4.22) can be further expanded as follows

$$F_{n,G}(u_0,\mathbf{x}_0;u_1,\mathbf{x}_1;\dots;u_n,\mathbf{x}_n)=$$
$$\sum_{\{\mathbf{E}_+,\mathbf{E}_-\}\in\mathscr{P}_2(\mathbf{E}(G))}\int\prod_{l_+\in\mathbf{E}_+}\frac{e^{\mathrm{i}\mathbf{p}_{l_+}(\mathbf{x}_{s(l_+)}-\mathbf{x}_{r(l_+)})}\lambda_+(p_{l_+})}{2E(l_+)(1-e^{-\beta E(l_+)})}\prod_{l_-\in\mathbf{E}_-}\frac{e^{\mathrm{i}\mathbf{p}_{l_-}(\mathbf{x}_{s(l_-)}-\mathbf{x}_{r(l_-)})}\lambda_-(p_{l_-})}{2E(l_-)(1-e^{-\beta E(l_-)})}\hat{\Psi}(-P,P)dP, \tag{3.4.24}$$

where $\mathscr{P}_2(\mathbf{E}(G))$ is the set of all possible partitions of $\mathbf{E}(G)$ into two disjoint subsets $\mathbf{E}(G)=\mathbf{E}_+\cup\mathbf{E}_-$ (which can be empty), one for the positive and one for the negative part. Notice that for every $l\in\mathbf{E}(G)$, $u_{r(l)}-u_{s(l)}\leq\beta/2$, hence, the argument of the exponential in $\lambda_-(p_{l_-})$ is always bigger than $-\beta/2E(l_-)$, that is

$$e^{E(l_-)(u_{r(l)}-u_{s(l)}-\beta)}\leq e^{-\frac{\beta}{2}E(l_-)}.$$

The function $\hat{\Psi}(-P,P)$ is the Fourier transform of a compactly supported distribution, hence, it is an entire analytic function which grows at most polynomially in every direction $(-P,P)$, hence

$$\hat{\Phi}(P)\doteq\prod_{l_-\in E_-}e^{E(l_-)(u_{r(l_-)}-u_{s(l_-)}-\beta)}\hat{\Psi}(-P,P)$$

is rapidly decreasing in every direction containing negative frequencies (at least one $p_{l_-}\in P$ has $p^0_{l_-}<0$). Furthermore, by Proposition 8 in [FL14], $\hat{\Psi}(-P,P)$ is of rapid decrease in the directions P contained in $(V^+)^k$ the $k-$fold product of the forward light cone.

Finally, since the δ functions in (3.4.23) forces p_j and p_k to be respectively on the positive and negative mass shell for all $j \in \mathbf{E}_+$ and all $k \in \mathbf{E}_-$, we have that

$$\widehat{\Phi}_m(\mathbf{P}) \doteq \prod_{l_- \in \mathbf{E}_-} e^{E(l_-)(u_{r(l_-)} - u_{s(l_-)} - \beta)} \widehat{\Psi}(-P,P)\Big|_{p_j^0 = \pm E(j), \forall j \in \mathbf{E}_\pm}$$

is of rapid decrease in every spatial momenta $\mathbf{P}$. In particular, this implies that, every integrand in (3.4.24) is absolutely integrable. Furthermore, the spatial integrals in (3.4.19) can be performed to obtain

$$\begin{aligned}
&\int_{\mathbb{R}^3} d^3\mathbf{x}_1 \ldots \int_{\mathbb{R}^3} d^3\mathbf{x}_n \, F_{n,G}(u_0 - \mathrm{i}T, 0; u_1, \mathbf{x}_1; \ldots; u_n, \mathbf{x}_n) \\
&\quad = \sum_{\{\mathbf{E}_+, \mathbf{E}_-\} \in \mathscr{P}_2(\mathbf{E}(G))} \int \prod_{l_+ \in \mathbf{E}_+} \frac{e^{-E(l_+)(u_{r(l_+)} - u_{s(l_+)})}}{2E(l_+)(1 - e^{-\beta E(l_+)})} \prod_{l_- \in \mathbf{E}_-} \frac{e^{E(l_-)(u_{r(l_-)} - u_{s(l_-)} - \beta)}}{2E(l_-)(1 - e^{-\beta E(l_-)})} \hat{\Psi}(-P,P)\Big|_{\substack{p_j^0 = \pm E(j), \\ \forall j \in \mathbf{E}_\pm}} \\
&\qquad \times \prod_{i \in \{1,\ldots,n\}} \delta\left(\sum_{\substack{l \in \mathbf{E}(G) \\ s(l) = i}} \mathbf{p}_l - \sum_{\substack{l \in \mathbf{E}(G) \\ r(l) = i}} \mathbf{p}_l \right) \prod_{\substack{e_+ \in \mathbf{E}_+ \\ s(e_+) = 0}} e^{-\mathrm{i}TE(e_+)} \prod_{\substack{e_- \in \mathbf{E}_- \\ s(e_-) = 0}} e^{\mathrm{i}TE(e_-)} d\mathbf{P}.
\end{aligned}$$

The delta functions over the linear combinations of various p_l enforces the spatial momentum conservation at all but one entry of the tensor product. Since G is a connected graph with $n+1$ vertices, the number of lines, k in G, is always larger or equal to n. The integration over $\mathbf{P}$ is thus an integration over $k-$spatial momenta. The products of n delta functions over some linear combination of various $\mathbf{p}_l$ is thus a well defined distribution provided the n linear combinations $\mathbf{c}_i \doteq \sum_{l \in \mathbf{E}(G), s(l) = i} \mathbf{p}_l - \sum_{l \in \mathbf{E}(G), r(l) = i} \mathbf{p}_l$ with $i \in \{1, \ldots, n\}$ are independent in a neighborhood of the support of the delta functions. The latter condition is again ensured by the fact that the graph G is connected. This fact can be proved checking the maximality of the rank of the $3n \times 3k$ matrix formally defined as $J_{n,k} \doteq \left\{ \frac{\partial \mathbf{c}_i}{\partial \mathbf{p}_l} \right\}_{i \in \{1,\ldots,n\}; l \in \{1,\ldots,k\}}$. For graphs of $n+1$ points with n lines this can be proven by induction on the number of points n. Let G_n be such a graph, then there is always at least one point labeled by $i \neq 0$ which is reached by only one line. If we remove that point and that line from the graph G_n we obtain another connected graph G_{n-1} of n points with $n-1$ lines. The corresponding matrices $J_{n-1,n-1}$ and $J_{n,n}$ are such that $\det J_{n,n} = \pm J_{n-1,n-1}$. Since $\det J_{1,1} = \pm 1$, this finishes the proof in that case. Finally, if k, the number of lines in the connected graph G with $n+1$ points, is larger than n, it is always possible to find a connected subgraph G'_n which has exactly n lines. In this case $J_{n,n}$ is just a submatrix of $J_{n,k}$ and the maximality of the rank of $J_{n,k}$ is ensured by that of $J_{n,n}$.

Furthermore, the ergodic mean of the previous expression gives

$$\begin{aligned}
&\lim_{T \to \infty} \frac{1}{T} \int_0^T d\tau \int_{\mathbb{R}^3} d^3\mathbf{x}_1 \ldots \int_{\mathbb{R}^3} d^3\mathbf{x}_n \, F_{n,G}(u_0 - \mathrm{i}\tau, 0; u_1, \mathbf{x}_1; \ldots; u_n, \mathbf{x}_n) = \\
&\quad \lim_{T \to \infty} \sum_{\{\mathbf{E}_+, \mathbf{E}_-\} \in \mathscr{P}_2(\mathbf{E}(G))} \int \prod_{l_+ \in \mathbf{E}_+} \frac{e^{-E(l_+)(u_{r(l_+)} - u_{s(l_+)})}}{2E(l_+)(1 - e^{-\beta E(l_+)})} \prod_{l_- \in \mathbf{E}_-} \frac{e^{E(l_-)(u_{r(l_-)} - u_{s(l_-)} - \beta)}}{2E(l_-)(1 - e^{-\beta E(l_-)})} \hat{\Psi}(-P,P)\Big|_{\substack{p_j^0 = \pm E(j), \\ \forall j \in \mathbf{E}_\pm}} \\
&\qquad \times \prod_{i \in \{1,\ldots,n\}} \delta\left(\sum_{\substack{l \in \mathbf{E}(G) \\ s(l) = i}} \mathbf{p}_l - \sum_{\substack{l \in \mathbf{E}(G) \\ r(l) = i}} \mathbf{p}_l \right) \frac{1 - e^{\mathrm{i}T\left(\sum_{\substack{e_- \in \mathbf{E}_- \\ s(e_-) = 0}} E(e_-) - \sum_{\substack{e_+ \in \mathbf{E}_+ \\ s(e_+) = 0}} E(e_+) \right)}}{\mathrm{i}T\left(\sum_{\substack{e_- \in \mathbf{E}_- \\ s(e_-) = 0}} E(e_-) - \sum_{\substack{e_+ \in \mathbf{E}_+ \\ s(e_+) = 0}} E(e_+) \right)} d\mathbf{P}
\end{aligned}$$

Notice that, $(1-e^{i\alpha T})/(\alpha T)$ is bounded by a constant uniformly in α and T. Hence, after applying the delta functions, the limit $T\to\infty$ can be taken before the integral over the remaining momenta. This limit vanishes unless $\sum_{e_-\in\mathbf{E}_-,s(e_-)=0}E(e_-)-\sum_{e_+\in\mathbf{E}_+,s(e_+)=0}E(e_+)=0$ on a set of non-zero measure over the remaining momenta, if any. In the latter case it furnishes a finite result. Due to absolute convergence, the ergodic mean and the corresponding limit for $T\to\infty$ of (3.4.20) can be taken before the integral over $(u_1,\dots,u_n)\in\beta S_n$. Hence we have the result. □

The final expression we got at the last step of the previous proof may be non-vanishing: This implies that ω^+ is in general different from ω^β. This is another indirect evidence of the failure of the clustering condition under the adiabatic limit established in Proposition 3.3.1. Actually, the failure of the clustering property for unbounded potentials shows that the state $\omega^+\neq\omega^\beta$. In any case, since ω^+ is stationary with respect to α_t, it is worthy to check explicitly that it does not satisfy the KMS condition with respect to the free dynamics.

Theorem 3.4.2. *ω^+ does not satisfy the KMS condition with respect to α_t.*

Proof. The idea here is to compare ω^+ with ω^β, which satisfies the KMS condition with respect to α_t by definition. In particular, let us test the KMS condition on the difference

$$w(A)\doteq\omega^\beta(A)-\omega^+(A)=\omega^\beta(A)-\lim_{T\to\infty}\frac{1}{T}\int_0^T\omega^{\beta,V}(\alpha_\tau(A))d\tau.$$

Recalling (2.3.43) and (2.3.40), we notice that the contribution of order 0 in λ in the previous expression vanishes, furthermore, by computations similar to the ones performed in the proof of Theorem 3.2.2, we obtain

$$w(A)=\lim_{T\to\infty}\frac{1}{T}\int_0^T d\tau\int_0^\beta du\,\omega^{\beta,c}(A\otimes\alpha_{iu-\tau}(K))+O(\lambda^2)$$

Hence, we have that $w(A)$ is related to the failure of averaged clustering condition given in Proposition 3.3.1. Let us now specialize to the specific case where $A=R_V(F_f)\star R_V(F_g)$ and V is a quadratic potential. Operating as in the proof of Proposition 3.3.1, we have that

$$w(R_V(F_f)\star R_V(F_g))=w(f,g)+O(\lambda^2),$$

where $w(f,g)$ has the form already given in (3.3.16). The translation α_{iu} present in $w(A)$ has no effect at first order in perturbation theory. The function $t\mapsto w(f,g_t)$ does not satisfy the KMS property, as can be argued by looking at the integral kernel of w, which has the form

$$w(x_1,x_2)=\beta\int\frac{1}{4E(\mathbf{k})^2}\frac{\cos(E(\mathbf{k})(x_1^0-x_2^0))}{(\cosh(\beta E(\mathbf{k}))-1)}e^{i\mathbf{k}(\mathbf{x}_1-\mathbf{x}_2)}d^3\mathbf{k}.$$

By direct inspection, we see that the map $t\mapsto w(f,g_t)$ can be analytically continued to the strip $\Im(t)\in[0,\beta]$, however,

$$w(x_1,x_2+i\beta e)-w(x_2,x_1)=$$
$$\beta\int\frac{1}{4E(\mathbf{k})^2}\left[\cos\big(E(\mathbf{k})(x_1^0-x_2^0)\big)+i\sin\big(E(\mathbf{k})(x_1^0-x_2^0)\big)\tanh\left(\frac{\beta E(\mathbf{k})}{2}\right)\right]e^{i\mathbf{k}(\mathbf{x}_1-\mathbf{x}_2)}d^3\mathbf{k}$$

where we have introduced the four-vector $e=(1,0,0,0)$. Hence, the KMS condition for ω^+ does not hold. □

Notice that, when V describes a perturbation of the mass square m^2 to $m^2+\delta m^2$, namely when V is quadratic in the field and no field derivatives are present, the state ω^+ can be constructed exactly. In this case, the mode decomposition of the 2-point function associated with $\omega^{\beta,V}$, looks like (1.3.70), furthermore, we have that the action of α_t and the corresponding time-averaged used in the definition of ω^+ in (3.4.17), transforms the modes $e^{\mathrm{i}E(\mathbf{k})t}$ of the $m^2+\delta m^2$ theory in the modes of the corresponding free theory of mass m. This procedure does not alter the form of the Bose factor b_+, which is the Bose factor at square mass $m^2+\delta m^2$. It is thus clear that ω^+ cannot be a KMS state. For a thorough analysis of the quadratic case we demand to [Dr17].

In the general case, even if the state ω^+ we have obtained is invariant under time translations it is not a KMS state, hence, it can be seen as a NESS for a massive scalar field theory, according to [Ru00]. To analyse the thermodynamical properties of NESS in the context of C^*-dynamical system, the notion of entropy production was introduced by Ojima et al. [OHI88, Oj89, Oj91] and by Jakšić and Pillet [JP01, JP02]. A direct generalisation of this concept to the present case seems not to be possible due to the presence of infrared divergences. Despite this fact, we expect that when spatial densities are considered some of the known results can be recovered. The study of relative entropy and entropy production will be the subject of the following chapter.

CHAPTER 4

RELATIVE ENTROPY AND ENTROPY PRODUCTION

Entropy is one of most important and discussed physical quantities, which plays a key role in the description of various systems, ranging from classical thermodynamics to black holes, passing from quantum information and statistical mechanics. Nonetheless, its role and a satisfactory definition is missing concerning interacting quantum field theory. One of the reason is possibly the non-satisfactory description of states at non-zero temperature, which implies a lack of understanding of the picture of QFT at thermal equilibrium. Actually, the work of Fredenhagen and Lindner [FL14] completely changed this picture giving a rigorous definition of the interacting state $\omega^{\beta,V}$, which also paved the way for the direct generalisation of results known in quantum statistical mechanics. Despite a direct connection between the construction of [FL14] and the other constructions, likewise the Schwinger-Keldysh formalism or the expansions over Matsubara frequencies [LW87, LeB00] is not yet available, it is definitely worthy to start looking at a definition of relative entropy and entropy production. In addiction, such investigation is justified by the possibility of studying the non-equilibrium state ω^{+}, so hoping to find some insights in non-equilibrium aspects of perturbative QFT, which, as a matter of fact, is a very rarely explored field, in spite of its interest.

The strategy will be the usual one, that is translating results present in statistical mechanics to the realm of QFT. In particular, our building blocks are the Araki's definition of relative entropy [Ar76, Ar77] and the formalism of entropy production and non-equilibrium statistical mechanics developed by Jakšić and Pillet, see [JP01, JP02, JP02b], where similar question to ours are asked regard NESS's. Due to the algebraic framework used in those work, we will see that the generalisation is pretty direct and natural, even though less structures are available in pAQFT, above all the lack of modular theory. This implies that the definitions that we are able to provide are less general and of limited application. In particular, we can not expect to characterise relative entropy and entropy production for every state. This is tracked back to the difficulties of defining

states on interacting theories.

The chapter is divided as follows: Section 4.1 is devoted to give a picture of the definition of relative entropy and entropy production in Quantum Statistical Mechanics, giving a sketch about the results we generalised. In order to make it accessible, we also present some needed results about Tomita-Takesaki modular theory. Section 4.2 contains the definition of relative entropy in the framework of pAQFT for states constructed with compactly supported potentials, together with the proof of some of its characterising properties. The problem of the adiabatic limit is addressed in Section 4.3, where it is shown that the relative entropy per unit volume is well-defined. The last section deals with the definition of entropy production and of entropy production density. Furthermore, it also contains some results about it, whose application allows for the proof of the thermodynamical triviality of the non-equilibrium steady state (NESS) obtained at the end of the previous chapter.

This chapter is based on results obtained in [DFP18b], from which most of the proofs and results are taken.

4.1 Relative Entropy and Entropy Production in Quantum Statistical Mechanics

In this section we would like to sketch a picture concerning the notion and the definition of entropy in the realm of Quantum Statistical Mechanics, which is our starting point for the generalisation of these ideas to perturbative QFT. We can not even hope to give a complete and self-consistent treatment about this subject, books may be written on this subject, and actually some had been, see for instance [OP93] for a broad introduction to the subject, oriented also to applications to quantum information. For an overview over the classical case, we suggest the recent lecture notes by Jaǩsić [Ja18].

The definition of entropy, or rather of relative entropy, for a general infinite-dimensional system[1] has been an open problem for long time and it has been solved only in the late 70's. Various solutions have been presented, which in the end turned out to be equivalent: In [Kos86], Kosaki gave a definition based on a variational formula, which is actually very useful in the proofs of various facts, such as monotonicity of relative entropy. Another proposal came from Araki [Ar76, Ar77], where relative entropy is defined by using the relative modular operator. Other definitions came up later on, one for all the work of Donald [Don90], who managed to give an even more general definition. Anyway, we do not want to dwell on this, demanding an interested reader to the quoted literature and reference therein. Instead, we want to focus on the work of Araki, which actually provides a suitable setting for a generalisation to perturbative Quantum Field Theory. To do so, we start by giving some generalities about Tomita-Takesaki modular theory, which are necessary to understand the definition of relative entropy first given in [Ar76].

[1] Actually, for an infinite system, one expects the entropy to be infinite and, in general, ill-defined. A solution is to compute the entropy with respect to a fixed reference state, *i.e.* considering a relative entropy.

4.1.1 A Short Trip into von Neumann Algebras and Modular Theory

Haag in [Ha92, Section V.2.], describes Tomita-Takesaki theory as "a beautiful example of "prestabilized harmony" between physics and mathematics". In our humble opinion, this famous quote is perfectly consistent, and one of the goal of this section is to try to explain why this is so and why Tomita-Takesaki theory is in fact one of the most important achievements of Mathematical Physics. As a matter of fact, the implications and the outcomes of modular theory are manifold, both in the realms of physics and mathematics (and of their overlap). Just to quote some, the classification of factors in von Neumann algebras by Connes [Co73], the definition of non-commutative L^p spaces [AM82], the applications to 2-dimensional CFT, the Unruh effect and, last but not least, the definition of the relative entropy of Araki, which in fact is the main subject of this section.

In Section 1.3.3 we defined the KMS states and we characterised them as the ones describing the thermal equilibrium of the system under investigation. In particular, the equilibrium depends on the dynamics of the system: Referring to the setting of the previous chapter, ω^β is KMS respect to α_t but not respect to α_t^V. Hence, a question naturally arises: Given a state ω, is it possible to find a time-evolution under which it is of thermal equilibrium? Under certain conditions the answer is positive and it is provided by modular theory.

Furthermore, modular theory allows also to give a characterisation of the self-dual positive cone: For a classical system, given an Hausdorff space X, it is well-known that normal states correspond to probability measures via Riesz Theorem. Then, the GNS construction gives the Hilbert space $\mathscr{H}_\mu \equiv L^2(X,\mu)$, μ being the measure, and the algebra is represented as $\pi_\mu(\mathscr{M}) = L^\infty(X,\mu)$, acting via multiplication. The predual $\mathscr{M}_*$ then is naturally identified with $L^1(X,\mu)$, thus a positive functional $\mu \in \mathscr{M}_*$ can be seen as a square root of a unique positive function in L^2, namely there is a unique correspondence between $\mathscr{M}_*^+$, the state space, and $L^2_+(X,\mu) \subset \mathscr{H}_\mu$, the positive elements in the Hilbert space. Then we notice that L^2_+ is a self-dual closed convex cone, where self-duality implies that $\mu(fg) \geq 0$ for all $f \in L^2_+(X,\mu)$ holds if and only if $g \in L^2_+(X,\mu)$ too. Actually, a characterisation of such cone is not trivial in the quantum case, something more can be said if the state is tracial, but we do not dwell on that. For some considerations about it and a more detailed explanation of what we are going to say we refer, for instance, to [BR97a, JOPP12, Ta02, Sak98]. In particular, this section is mainly based on [BR97a].

We start fixing a von Neumann algebra $\mathscr{M}$, which we will always assume to be infinite-dimensional, unless otherwise stated. We call $\mathscr{M}_*$ its pre-dual. We will also always assume the algebra to be concrete, that is we consider it as a subspace of $\mathscr{B}(\mathscr{H})$ for a certain Hilbert space $\mathscr{H}$. In fact, we will mostly think of $\mathscr{M}$ as represented via the GNS construction via a state ω, or as the enveloping algebra of the GNS representation of a given C^*-algebra. The states we will deal with are assumed to be normal and faithful for simplicity, even though some results may be obtained in more generality. Furthermore, we assume $\mathscr{M}$ to be σ-finite, in the sense of the following definition.

Definition 4.1.1. A von Neumann algebra $\mathscr{M}$ is σ-finite if all collections of mutually orthogonal projections have at most a countable cardinality.

This assumption is not very restrictive since it can be shown that every von Neumann algebra on a separable Hilbert space is σ-finite. The converse is instead not true. Actually, most of the following theory has been derived without the assumption of σ-finiteness using weights, but we do not strive for such a generality, which will make the situation more complicated, hence we will always assume $\mathscr{M}$ to be σ-finite. Actually, the σ-finiteness condition as presented above is a bit awkward and it is not clear why it is really useful. It would be rather nice to have a more concrete characterisation. To do so, we first define cyclicity and separability for a von Neumann algebra

Definition 4.1.2. Let $\mathscr{M}$ a von Neumann algebra on a Hilbert space $\mathscr{H}$ and let $\mathscr{K}$ be a subset of $\mathscr{H}$. We say that $\mathscr{K}$ is separating for $\mathscr{M}$ if, for all $A \in \mathscr{M}$, $A\psi = 0$ implies $A = 0$ for all $\psi \in \mathscr{K}$. $\mathscr{K}$ is cyclic for $\mathscr{M}$ if $[\mathscr{M}\mathscr{K}] = \mathscr{K}$, where $[\mathscr{M}\mathscr{K}]$ denotes the linear span of the set $\mathscr{M}\mathscr{K}$.

It can be proven that $\mathscr{K}$ is cyclic for $\mathscr{M}$ if and only if it is separating for its commutant $\mathscr{M}'$. We are ready now to give the desired characterisation of σ-finite von Neumann algebras. The proof of this and of the aforementioned results can be found in [BR97b, Section 2.5.1].

Proposition 4.1.1 (Characterisation of σ-finite von Neumann algebras)**.** *Given a von Neumann algebra $\mathscr{M}$ over the Hilbert space $\mathscr{H}$, the following statements are equivalent:*

1. *$\mathscr{M}$ is σ-finite;*
2. *There exists a countable subset of $\mathscr{H}$ which is separating for $\mathscr{M}$;*
3. *There exists a faithful normal state on $\mathscr{M}$;*
4. *$\mathscr{M}$ is isomorphic with a von Neumann algebra $\pi(\mathscr{M})$ which admits a separating and cyclic vector.*

By the former proposition, a σ-finite $\mathscr{M}$ has a separating and cyclic vector Ω, so the map $\mathscr{M} \ni A \mapsto A\Omega \in \mathscr{H}$ establishes a one-to-one correspondence between $\mathscr{M}$ and a dense subset $[\mathscr{M}\Omega] \subseteq \mathscr{H}$. This means that it is possible to transfer algebraic properties of the algebra on $[\mathscr{M}\Omega]$. Furthermore this guarantees that the assumption of having a faithful, normal state is meaningful.

In order to characterise the positive cone for $\mathscr{M}$, we must study the operator which implements the conjugation operator on the Hilbert space. The reason for doing so is that a positive element in $\mathscr{M}$ is given by A^*A, hence we must consider something of the form $\{A^*A\Omega \,|\, A \in \mathscr{M}\}$. Actually this would be naïve, since the so-obtained cone would not satisfy self-duality[2]:

$$\left\langle A^*A\Omega \middle| B^*B\Omega \right\rangle = \omega\left(A^*AB^*B\right) \neq \omega\left((AB)^*AB\right).$$

In particular, we want to study the anti-linear operator

$$S_0 : [\mathscr{M}\Omega] \to [\mathscr{M}\Omega]; \qquad S_0(A\Omega) \doteq A^*\Omega \quad \forall A \in \mathscr{M}.$$

[2] In the Abelian case or if ω is a trace it is easy to see that self-duality would apply.

It will be also convenient to introduce an "inversion" to the conjugation S_0, which, for reason which should be clear in the following, must be defined on the subspace of $\mathscr{H}$ generated by commutant $\mathscr{M}'$:

$$F_0 : [\mathscr{M}'\Omega] \to [\mathscr{M}'\Omega]; \qquad F_0 A'\Omega \doteq (A')^*\Omega \quad \forall A' \in \mathscr{M}'.$$

By their definitions and to the assumption of σ-finiteness of $\mathscr{M}$, it follows that S_0 and F_0 are densely defined, hence closable, and that

$$S_0^* = \overline{F}_0, \quad F_0^* = \overline{S}_0, \tag{4.1.1}$$

where the bar stands for the closure. Furthermore, for all $\psi \in \mathrm{Dom}\left(\overline{S}_0\right)$, there exists a closed operator Q on $\mathscr{H}$ which is affiliated[3] with $\mathscr{M}$ and it is such that

$$Q\Omega = \psi, \quad Q^*\Omega = \overline{S}_0\psi,$$

and analogously for F_0.

Definition 4.1.3. Let us call $S \doteq \overline{S}_0$ and $F \doteq \overline{F}_0$. We denote with Δ the unique, positive, self-adjoint operator and J the unique, anti-unitary operator occurring in the polar decomposition of S, which are given by

$$S = J\Delta^{\frac{1}{2}}.$$

Δ is called modular operator associated to the couple $\{\mathscr{M}, \Omega\}$ and J is called the modular conjugation.

Some important properties of the modular operator and of the modular conjugation are:

$$\Delta = FS \qquad \Delta^{-1} = SF \qquad S = J\Delta^{\frac{1}{2}} \qquad F = J\Delta^{-\frac{1}{2}}$$
$$J = J^* \qquad J^2 = \mathbb{1} \qquad \Delta^{-\frac{1}{2}} = J\Delta^{\frac{1}{2}}J.$$

We can say that the modular operator reflects, in some sense, the non-tracial behaviour of ω. In fact, if ω were a trace, we would obtain $\Delta \equiv \mathbb{1}$. The proper features of non-commutativity are better understood by looking at some of the structural properties of Δ. An insight can be reached by the following discussion.

Given $A \in \mathscr{M}$, consider the operator SAS: Then, for all $B, C \in \mathscr{M}$ we have:

$$(SAS)BC\Omega = SAC^*B^*\Omega = BCA^*\Omega, \qquad B(SAS)C\Omega = BSAC^*\Omega = BCA^*\Omega$$

which imply that SAS is affiliated with $\mathscr{M}'$. Supposing Δ to be bounded, we can define its inverse as $\Delta^{-1} = J\Delta J$ (S, F are bounded), hence, by the above relations, we get

$$S\mathscr{M}S \subseteq \mathscr{M}' \quad F\mathscr{M}'F \subseteq \mathscr{M},$$

that is

$$\Delta^{-1}\mathscr{M}\Delta = \Delta^{\frac{1}{2}}JJ\Delta^{\frac{1}{2}}\mathscr{M}\Delta^{-\frac{1}{2}}JJ\Delta^{-\frac{1}{2}} = FS\mathscr{M}SF \subseteq F\mathscr{M}'F \subseteq \mathscr{M},$$

[3] A closed operator A on $\mathscr{H}$ is affiliated with $\mathscr{M}$ ($A\eta\mathscr{M}$) if $\mathscr{M}'\,\mathrm{Dom}(A) \subseteq \mathrm{Dom}(A)$ and $AA' \supseteq A'A$ for all $A' \in \mathscr{M}'$

by iterating ($n = 0, 1, 2, \ldots$) we obtain

$$\Delta^n \mathscr{M} \Delta^{-n} \subseteq \mathscr{M}.$$

Let us now consider the analytic continuation $n \mapsto z \in \mathbb{C}$, in particular let us take the following analytic function:

$$f(z) = \|\Delta\|^{-2z} \left\langle \phi \,\middle|\, \left[\Delta^z A \Delta^{-z}, A'\right] \psi \right\rangle.$$

Using $\left\|\Delta^{-1}\right\| = \|J\Delta J\| \, \|\Delta\|$ we have (for $\Re(z) \geq 0$)

$$|f(z)| = O\left(\|\Delta\|^{-2\Re(z)} \left(\|\Delta\|^{|\Re(z)|} \right)^2 \right) = O(1),$$

so, by Carlson Theorem, $f(z) \equiv 0$, hence $\Delta^z \mathscr{M} \Delta^{-z} \subseteq \mathscr{M}'' = \mathscr{M}$ for all $z \in \mathbb{C}$. But since $\Delta^z (\Delta^{-z} \mathscr{M} \Delta^z) \Delta^{-z} \subseteq \Delta^z \mathscr{M} \Delta^{-z}$, we obtain:

$$\Delta^z \mathscr{M} \Delta^{-z} = \mathscr{M}.$$

With the same reasoning as above we also obtain

$$J \mathscr{M} J = J \Delta^{\frac{1}{2}} \mathscr{M} \Delta^{-\frac{1}{2}} J = S \mathscr{M} S \subseteq \mathscr{M}'.$$

A similar relation holds for $\mathscr{M}'$ considering F, thus we have

$$J \mathscr{M} J = \mathscr{M}'.$$

The computations above constitute the proof of the celebrated *Tomita-Takesaki Theorem* in the case of bounded modular operator Δ. In the general case it reads as follows:

Theorem 4.1.1 (Tomita-Takesaki)**.** *Let $\mathscr{M}$ be a von Neumann algebra with cyclic and separating vector Ω and let Δ and J be respectively the modular operator and the modular conjugation associated to it. Then it follows that:*

$$J \mathscr{M} J = \mathscr{M}' \qquad \Delta^{\mathrm{i}t} \mathscr{M} \Delta^{-\mathrm{i}t} = \mathscr{M} \quad \forall\, t \in \mathbb{R}. \tag{4.1.2}$$

The proof of this general case is much more involved and we do not report it here, demanding, for example, to [BR97b, Section 2.5.2.]. The Tomita-Takesaki Theorem allows us to define a key tool in von Neumann algebras theory:

Definition 4.1.4 (Modular Automorphisms Group)**.** Let ω be a faithful state on a von Neumann algebra $\mathscr{M}$ and let $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ be the corresponding cyclic representation. By the Tomita-Takesaki Theorem there exists a σ-weakly continuous one-parameter group of *-automorphisms of $\mathscr{M}$ defined by

$$t \mapsto \sigma_t^\omega; \qquad \sigma_t^\omega(A) \doteq \pi_\omega^{-1}\left(\Delta^{\mathrm{i}t} \pi_\omega(A) \Delta^{-\mathrm{i}t}\right),$$

which is called the modular automorphisms group associated to $(\mathscr{M}, \omega)$.

The modular conjugation is really important in this framework, in fact

$$\left\langle \Delta^{\frac{1}{2}} \pi_\omega(A)\Omega_\omega \,\middle|\, \Delta^{\frac{1}{2}} \pi_\omega(B)\Omega_\omega \right\rangle = \left\langle J\pi_\omega(A^*)\Omega_\omega \,\middle|\, J\pi_\omega(B^*)\Omega_\omega \right\rangle = \left\langle \pi_\omega(A^*)\Omega_\omega \,\middle|\, \pi_\omega(B^*)\Omega_\omega \right\rangle,$$

then, taking $t = \frac{-i\beta}{2}$ for a certain $\beta > 0$, the modular group becomes

$$\omega\left(\sigma^{\omega}_{-i\beta/2}(A)\,\sigma^{\omega}_{i\beta/2}(B)\right) = \omega(BA),$$

which is nothing by a rephrasing of the KMS condition given in Definition 1.3.11. Hence, this is telling us that every faithful, normal state is a thermal equilibrium one with respect to its modular group. Notice that in the "mathematical" literature the usual choice is $\beta = -1$. In this thesis we adopt the "physical" convention and we will always take β positive, since to us it corresponds to an inverse temperature.

Let us now come back to the problem of the positive cone. We have seen that the conjugation is implemented by the operator

$$j : \mathscr{M} \to \mathscr{M}'; \qquad j(A) \doteq JAJ,$$

which *a posteriori* explains why we defined F_0 to act on the commutant. This put us in position to define the *natural positive cone* $\mathscr{H}^+_\omega \subset \mathscr{H}_\omega$ for the couple $(\mathscr{M}, \omega)$ as

$$\mathscr{H}^+_\omega \doteq \{A\, j(A)\Omega \,|\, A \in \mathscr{M}\}.$$

This is the sought non-commutative analogous of the space L^2_+ previously discussed. We have some first properties, which are recollected in [BR97a, Proposition 2.5.26], where it is also possible to find the proof.

Proposition 4.1.2. *The closed cone $\mathscr{H}^+_\omega \subset \mathscr{H}_\omega$ shares the following properties*

1. $\mathscr{H}^+_\omega = \overline{\Delta^{\frac{1}{4}}[\mathscr{M}^+\Omega]}$, *so it is a convex cone. Here $\mathscr{M}^+$ denotes the positive part of $\mathscr{M}$;*
2. $\Delta^{it}\mathscr{H}^+_\omega = \mathscr{H}^+_\omega$ *for all* $t \in \mathbb{R}$;
3. *Given a positive-definite function f, then $f(\log\Delta)\mathscr{H}^+_\omega \subseteq \mathscr{H}^+_\omega$;*
4. *Given any $\psi \in \mathscr{H}^+_\omega$, then $J\psi = \psi$;*
5. $Aj(A)\mathscr{H}^+_\omega \subseteq \mathscr{H}^+_\omega$ *for any* $A \in \mathscr{M}$.

Next, we present two key results about the geometric properties of the cone and about its universality, which correspond to [BR97a, Propositions 2.5.28. and 2.5.30.].

Proposition 4.1.3. 1. *The natural positive cone $\mathscr{H}^+_\omega$ is self-dual, that is*

$$\mathscr{H}^+_\omega = \widehat{\mathscr{H}^+_\omega} \doteq \left\{\psi \in \mathscr{H}_\omega \,|\, \langle\psi|\varphi\rangle \geq 0 \;\forall\, \varphi \in \mathscr{H}^+_\omega\right\};$$

2. *$\mathscr{H}^+_\omega$ is pointed, that is $\mathscr{H}^+_\omega \cap -\mathscr{H}^+_\omega = \{0\}$;*
3. *If $\psi \in \mathscr{H}_\omega$ satisfies $J\psi = \psi$, than it has a unique orthogonal decomposition $\psi = \psi_1 - \psi_2$, where $\psi_1, \psi_2 \in \mathscr{H}^+_\omega$;*
4. *$\mathscr{H}_\omega$ is linearly spanned by $\mathscr{H}^+_\omega$.*

Proposition 4.1.4. *Let $\psi \in \mathscr{H}_\omega^+$ be fixed. Then:*

1. *ψ is cyclic for $\mathscr{M}$ if and only if ψ is separating for $\mathscr{M}$;*
2. *If ψ is cyclic, then the modular conjugation J_ψ and the natural positive cone $\mathscr{H}_\psi^+$ associated with the pair $(\mathscr{M},\psi)$[4] satisfy*

$$J_\psi = J, \qquad \mathscr{H}_\psi^+ = \mathscr{H}_\omega^+.$$

The importance of the natural cone is in the fact that every vector in it corresponds to a normal state, *i.e.* it is possible to establish a homeomorphism between $\mathscr{H}_\omega^+$ and $\mathscr{M}_*^+$ the positive elements of the predual of the algebra. This is expressed precisely by the following theorem

Theorem 4.1.2. *For every $\psi \in \mathscr{H}_\omega^+$ we define, as we may, a normal positive form $\omega_\psi \in \mathscr{M}_*^+$ by*

$$\omega_\psi(A) \doteq \langle \psi \,|\, A\psi \rangle \qquad \forall\, A \in \mathscr{M}.$$

Then the following hold:

- *For any $\eta \in \mathscr{M}_*^+$ there exists a unique $\psi \in \mathscr{H}_\omega^+$ such that $\eta \equiv \omega_\psi$;*
- *The map $\mathscr{H}_\omega^+ \ni \psi \mapsto \omega_\psi \in \mathscr{M}_*^+$ is a homeomorphism where both the spaces are endowed with the norm topology.*

One can find an inverse to the previous homeomorphism, defined as a map $\mathscr{M}_*^+ \ni \eta \mapsto \psi(\eta)$ and it is possible to prove that it is monotonously increasing and concave with respect to the ordering of the two cones. Moreover it is also possible to find an explicit form for the action of this map in certain cases, but we will not enter the details of that, but we demand to the literature, for instance [Ta02], or to the original papers of Araki, Connes and Haagerup [Ar74, Co73, Haa75], where the full theory is developed.

The last topic we would like to briefly discuss concerns the implementation of the dynamics and the analysis of the W^*-dynamical system obtained using the modular dynamics. First of all we introduce a bit of terminology:

Definition 4.1.5 (Standard Form)**.** A von Neumann algebra in a standard form is a quadruple $(\mathscr{M},\mathscr{H},J,\mathscr{H}^+)$, where $\mathscr{M} \subset \mathscr{B}(\mathscr{H})$ is a concrete von Neumann algebra acting on a Hilbert space $\mathscr{H}$, J is an antiunitary involution on $\mathscr{H}$ and $\mathscr{H}^+$ is a self-dual cone. In addition, the following properties are required:

- $J\mathscr{M}J = \mathscr{M}'$;
- $JAJ = A^*$, where A is in the centre of $\mathscr{M}$;
- $J\psi = \psi$ for all $\psi \in \mathscr{H}^+$;
- $AJA\mathscr{H}^+ \subset \mathscr{H}^+$ for all $A \in \mathscr{M}$.

[4] Here we are slightly abusing the notation identifying the vector ψ and the state to which it is associated.

If $\mathcal{N}$ is an abstract von Neumann algebra, we call $(\pi, \mathcal{H}, J, \mathcal{H}^+)$ its standard representation, where $\pi : \mathcal{N} \to \mathcal{B}(\mathcal{H})$ is an injective, unital representation and $(\pi(\mathcal{N}), \mathcal{H}, J, \mathcal{H}^+)$ is a standard form.

Actually, every von Neumann algebra admits a standard representation, which can be obtained applying the GNS construction using a faithful, normal state ω, as explained before, or weights in some particular case, see [Ta02]. An example of standard representation can be obtained by considering the left representation we used in the Introduction, the construction is explained in a very pedagogical way in [JOPP12, Chapter 2].

A big advantage of the standard representation is that it allows to unitarily implement every *-automorphism of the algebra, as per the following theorem

Theorem 4.1.3. *Given a von Neumann algebra in standard form $(\mathcal{M}, \mathcal{H}, J, \mathcal{H}^+)$, there exists a unique unitary representation* $\mathrm{Aut}(\mathcal{M}) \ni \rho \mapsto V(\rho)$ *on $\mathcal{H}$ such that*

1. $V(\rho)AV^*(\rho) = \rho(A)$ *for all* $A \in \mathcal{M}$*;*
2. $V(\rho)\mathcal{H}^+ \subset \mathcal{H}^+$*;*
3. *The implementation map is surjective and continuous if the two spaces are equipped with their norm topologies;*
4. $V(\rho)\Omega_\omega = \Omega_{(\rho^{-1})^*(\omega)}$ *for all* $\omega \in \mathcal{M}_*^+$*;*
5. $JV(\rho) = V(\rho)J$ *and* $V(\rho)\mathcal{M}'V^*(\rho) = \mathcal{M}'$.

The case of interest for us is when ρ is the dynamics τ_t of a W^*-dynamical system. The former theorem tells us that we can find a unitary $V(\tau_t) \equiv V_t$ which, by Stone Theorem, admits a unique self-adjoint generator L such that $V_t = e^{itL}$, which is called the *standard Liouvillian*. In particular, it is possible to prove that the standard Liouvillian is the unique self-adjoint operator such that

$$e^{itL}Ae^{-itL} = \tau_t(A), \qquad e^{itL}\mathcal{H}^+ \subset \mathcal{H}^+$$

for all $A \in \mathcal{M}$ and all $t \in \mathbb{R}$. In the case where we are considering the modular dynamics σ_t^ω, then the standard Liouvillian is given by $\log(\Delta)$ (often called the *relative Hamiltonian*), see for instance [Ar73, Don90].

This is not the first Liouvillian we have encountered in this thesis, in fact we have already encountered the Ω_ω-Liouvillian in the Introduction, hence we would like to finish this section by stating the relation between the two. This is given in [DJP03], see also the references therein quoted and it is summarised by the following proposition:

Proposition 4.1.5. *Let $(\mathcal{M}, \tau_t)$ be a W^*-dynamical system endowed with a stationary state ω and suppose that L is a self-adjoint operator such that $\tau_t(A) = e^{itL}Ae^{-itL}$. The following are equivalent:*

- $L\Omega_\omega = 0$
- $e^{itL}\mathcal{H}^+ \subset \mathcal{H}^+$ *for all* $t \in \mathbb{R}$.

This is telling us that, in presence of an invariant state, the standard Liouvillian and the Ω_ω-Liouvillian are the same.

4.1.2 The Relative Modular Operator and Araki's Relative Entropy

A generalisation of modular theory can be taken into consideration by taking into account two different states and studying how their modular dynamics are related. As we will see in this section, this leads to the introduction of the *relative conjugation*. This tool has turned out to have manifold applications, the most important for this thesis is Araki's definition of relative entropy, which is valid for general systems described using von Neumann algebras, see [Ar76, Ar77]. But this is not limited to that, for instance relative modular theory played a pivotal role in Connes' classification of type III factors [Co73]. A complete introduction and treatment of relative modular theory can be found in [AM82, Appendix C], where the whole framework is actually developed for weights and not only for states. Here we just limit ourselves to present some basic facts without proofs, so to fix the notations.

Let us consider a von Neumann algebra $\mathscr{M}$ in standard form and two normal states ψ and ϕ. Due to Proposition 4.1.4, they share the same natural positive cone $\mathscr{H}^+$ and, by normality and faithfulness, they are represented as two cyclic (and therefore separating) vectors Ψ and Φ respectively. Thence, likewise we did in the previous section, it is meaningful to consider the *relative conjugation operator*, which is defined as follows:

$$S_{\Psi,\Phi}A\Psi = A^*\Phi, \qquad \forall A \in \mathscr{M}.$$

This can be shown to be a closable operator, so we consider, as we may, its closure, which we denote again with $S_{\Psi,\Phi}$, slightly abusing the notation. It is now legit to consider the polar decomposition of $S_{\Psi,\Phi}$

$$S_{\Psi,\Phi} = J_{\Psi,\Phi}\Delta_{\Psi,\Phi}^{\frac{1}{2}},$$

where $J_{\Psi,\Phi}$ is an anti-unitary involution called *relative modular conjugation* and $\Delta_{\Psi,\Phi}$ is the *relative modular operator*.

The relative modular operator can be understood as the non-commutative version of the Radon-Nikodym derivative. In fact, in the classical picture the states are probability measures, which in particular are absolutely continuous due to the faithfulness and to the normality. What the relative modular operator actually does is exactly to interlace the two. Relative modular theory thus shows how the non-commutative picture is richer and different than the Abelian one.

Despite the very interesting features of relative moduar theory, we do not dwell on those any longer, demanding to [AM82, Appendix C] for further details, for instance about the structure of the cones in this case.

To close this quick overview we would like to spend just a few words about the relation between the modular dynamics of ψ and ϕ. This was first highlighted by Connes in [Co73] in its classification of factors, and it can be resumed in the following theorem:

Theorem 4.1.4 (Connes' Cocycle)**.** *Let ψ and ϕ be normal, faithful states on a von Neumann algebra $\mathscr{M}$ and let σ^ψ and σ^ϕ be the associated modular groups. Then there exists a strongly continuous one-parameter family of unitaries $t \mapsto U_t$ in $\mathscr{M}$ such that:*

$$\sigma_t^\phi(A) = U(t)\sigma_t^\psi(A)U^*(t), \qquad U(t+s) = U(t)\sigma_t^\psi(U(s)) \qquad \forall A \in \mathscr{M},\ \forall t,s \in \mathbb{R}.$$

A characterisation of this family of unitaries is given in the following theorem, also due to Connes:

Theorem 4.1.5 (Connes' Radon-Nikodym)**.** *For all ϕ, ψ normal, faithful states on a von Neumann algebra $\mathscr{M}$, there exists a continuous one-parameter family $t \mapsto [D\psi : D\phi]_t$ of unitaries in $\mathscr{M}$ such that:*

1. $\sigma_t^{\psi}(A) = [D\psi : D\phi]_t \, \sigma_t^{\phi}(A) \, [D\psi : D\phi]_t^*$;
2. $[D\psi : D\phi]_{t+s} = [D\psi : D\phi]_t \, \sigma_t^{\phi}([D\psi : D\phi]_s)$;
3. $[D\psi : D\phi]_t^* = [D\phi : D\psi]_t$;
4. $[D\psi : D\phi]_t [D\phi : D\eta]_t = [D\psi : D\eta]_t$;
5. *Given an unitary $V \in \mathscr{M}$, $\psi(A) = \phi(VAV^*)$ if and only if $[D\psi : D\phi]_t = V^* \sigma_t^{\phi}(V)$.*

Despite most of the tools of modular theory are not at disposal in pAQFT, (an analogue of) the Connes' co-cycle survives: This is precisely given by the co-cycle $U(t)$ defined in equation (2.3.29), which in fact interlaces the two dynamics under which the states ω^{β} and $\omega^{\beta,V}$ satisfy the KMS condition, so that they can be interpreted as modular evolutions. This will be clarified also in the following Working Example.

What is really important to us about modular theory is that, using the relative modular operator, Araki was able to define the *relative entropy* as

$$\mathrm{Ent}(\Psi, \Phi) \doteq - \left\langle \Psi \middle| \log\left(\Delta_{\Psi,\Phi}\right) \Psi \right\rangle . \tag{4.1.3}$$

This definition first appeared in [Ar76] and was designed for normal, faithful states, and then those hypothesis have been removed and the definition was extended to weights in [Ar77], but we will not take this last case into consideration for simplicity.

First of all we notice that the definition is well-posed, in particular one can make sense out of the logarithm by using the spectral theory for the relative modular operator. Moreover, we stress that the minus sign in the definition is purely conventional, very often it is omitted (for instance as in [BR97b]). The reason for that can be tracked back to the choice of $\beta = -1$ in the Tomita-Takesaki Theorem. We decided to follow Araki definition in order to have a positive relative entropy, according to the physical interpretation that "entropy always increases". Araki did not just limit himself to introduce it, but he also prove some structural properties of relative entropy, so explaining how his definition is meaningful. They are recollected in the following theorem, to whose proof is devoted the whole paper [Ar76].

Theorem 4.1.6. *The relative entropy* (4.1.3) *fulfills the following properties:*

Strict positivity: *If $\psi(\mathbb{1}) = \phi(\mathbb{1})$, then* $\mathrm{Ent}(\Psi, \Phi) \geq 0$*, where the equality holds if and only if $\phi \equiv \psi$;*

Lower semi-continuity: *Given two sequences $\{\psi_n\}_{n \in \mathbb{N}}$ and $\{\phi_n\}_{n \in \mathbb{N}}$ which are norm-convergent to ψ and ϕ respectively, then*

$$\lim_{n \to \infty} \mathrm{Ent}\left(\psi_n, \phi_n\right) \geq \mathrm{Ent}\left(\psi, \phi\right);$$

Convexity: $\mathrm{Ent}(\psi,\phi)$ *is jointly convex in* ψ *and* ϕ*, namely, given* $\lambda_j \geq 0$ *such that* $\sum_j \lambda_j = 1$*, we have*

$$\sum_j \lambda_j \mathrm{Ent}(\psi_j,\phi_j) \geq \mathrm{Ent}\left(\sum_j \lambda_j\psi_j, \sum_j \lambda_j\phi_j\right);$$

Monotonicity: *Let us consider the restriction map* $i_{\mathscr{N}} : \mathscr{M} \to \mathscr{N}$ *to a von Neumann subalgebra* $\mathscr{N}$*, which is assumed to be of one of the following:*

(a) $\mathscr{N} = \mathscr{A} \cap \mathscr{M}$*, where* $\mathscr{A} \subset \mathscr{M}$ *is a finite-dimensional, Abelian von Neumann subalgebra;*

(b) $\mathscr{M} = \mathscr{N} \otimes \mathscr{Z}$*,* $\mathscr{Z}$ *being the centre of* $\mathscr{M}$*;*

(c) $\mathscr{N}$ *is approximately finite, namely it is generated by an increasing net of finite-dimensional subalgebras.*

Then, denoting by $i^*_{\mathscr{N}}$ *the push-forward of* $i_{\mathscr{N}}$ *to states, it holds that*

$$\mathrm{Ent}\left(i^*_{\mathscr{N}}(\psi), i^*_{\mathscr{N}}(\phi)\right) \leq \mathrm{Ent}(\psi,\phi).$$

The relative entropy defined in equation (4.1.3) and its properties are what we would like to generalise. Unfortunately, as we saw in Chapter 2, in the context of pAQFT we deal with *-algebras only, hence the whole machinery of modular theory is not available. This implies that we can not hope to give a definition able to cover all possible states, but we have to do something limited to those we know, namely interacting KMS states of the form (2.3.42), possible composed with some time-evolution (the free one, or an interacting one generated with a different perturbation Lagrangian). In this case something can be done since the Araki's definition involves quantities which are at hand in pAQFT, such as the Connes' co-cycle $U(t)$ and its generator K. These expression are derived in the following example.

Working Example. As example of what we have discussed so far, we consider a finite dimensional W^*-dynamical system $(\mathscr{M},\tau_t)$. All the formulas we will obtain are valid in the infinite case, but finiteness allows us to avoid some technicalities in their derivation, which risks to hide the message of this example; for the details in infinite-dimension see [BR97b, Don90]. We suppose the dynamics to be generated by a self-adjoint Hamiltonian H, namely

$$\tau_t(A) = e^{\mathrm{i}tH} A e^{-\mathrm{i}tH} \qquad \forall\, A \in \mathscr{M},$$

and we endow our dynamical system with the extremal (τ_t,β)-KMS state ω^β, which is nothing but the usual Gibbs state

$$\omega^\beta(A) = \frac{\mathrm{Tr}\left(e^{-\beta H}A\right)}{Z_0}, \qquad Z_0 \doteq \mathrm{Tr}\left(e^{-\beta H}\right) \qquad \forall\, A \in \mathscr{M}.$$

Afterwards, we consider the GNS representation constructed out of ω^β, which is represented by the cyclic and separating vector Ω_0.

Then we consider a self-adjoint perturbation P and we have the Araki construction started, leading to the perturbed KMS state $\omega^{\beta,P}$, which in our case is simply given by

$$\omega^{\beta,P}(A) = \frac{\mathrm{Tr}\left(e^{-\beta(H+P)}A\right)}{Z_P}, \qquad Z_P \doteq \mathrm{Tr}\left(e^{-\beta(H+P)}\right) \qquad \forall\, A \in \mathscr{M},$$

and which is the extremal (τ_t^P, β)-KMS state, where the interacting dynamics is given by

$$\tau_t^P(A) = e^{\mathrm{i}t(H+P)} A e^{-\mathrm{i}t(H+P)} \qquad \forall A \in \mathscr{M}.$$

The free and the interacting evolution are intertwined by the co-cycle $U(t)$, that is

$$\tau_t^P(A) = U(t)\tau_t(A)U^*(t), \qquad U(t) = e^{\frac{1}{2}t(H+P)} e^{-\frac{1}{2}tH} \qquad \forall A \in \mathscr{M}.$$

Via this co-cycle we get back the known expression (2.3.42)

$$\omega^{\beta,P}(A) = \frac{\omega^\beta\left(AU(\mathrm{i}\beta)\right)}{\omega^\beta\left(U(\mathrm{i}\beta)\right)}.$$

In the GNS representation, the perturbed state is given by the vector

$$\Omega_P = \frac{1}{N} U\left(\mathrm{i}\frac{\beta}{2}\right)\Omega_0, \qquad N^2 = \left\langle \Omega_0 \middle| U^*\left(\mathrm{i}\frac{\beta}{2}\right) U\left(\mathrm{i}\frac{\beta}{2}\right)\Omega_0 \right\rangle,$$

where we denoted the implementation of the Connes' co-cycle with $U\left(\mathrm{i}\frac{\beta}{2}\right)$ again, with a slight abuse of the notation. We would like to compute the relative entropy between ω^β and $\omega^{\beta,P}$: First of all, by definition of the relative conjugation, we have

$$S_{\Omega_0,\Omega_P} A\Omega_0 = A^*\Omega_P = \frac{1}{N} A^* U\left(\mathrm{i}\frac{\beta}{2}\right)\Omega_0 = \frac{1}{N} S U^*\left(\mathrm{i}\frac{\beta}{2}\right) A\Omega_0,$$

where S is the conjugation operator obtained by the GNS representation with respect to ω^β. The former equation then implies (here the finite-dimension is crucial, some more work would have been needed otherwise)

$$S_{\Omega_0,\Omega_P} = \frac{1}{N} S U^*\left(\mathrm{i}\frac{\beta}{2}\right).$$

Hence, recalling that $\Delta_{\Omega_0,\Omega_P} = S^*_{\Omega_0,\Omega_P}$ and that $H = \log(\Delta) = \log(S^*S)$[5], we have

$$N^2 \Delta_{\Omega_0,\Omega_P} = U\left(\mathrm{i}\frac{\beta}{2}\right)\Delta U^*\left(\mathrm{i}\frac{\beta}{2}\right) = e^{-\frac{1}{2}\beta(H+P)} e^{\frac{1}{2}\beta H} e^{-\beta H} e^{-\frac{1}{2}\beta H} e^{\frac{1}{2}\beta(H+P)} = e^{\beta(H+P)},$$

by which

$$\mathrm{Ent}(\Omega_0, \Omega_P) = -\left\langle \Omega_0 \middle| \log(\Delta_{\Omega_0,\Omega_P}\Omega_0) \right\rangle = \\ -\left\langle \Omega_0 \middle| \beta P \Omega_0 \right\rangle + \log\left(N^2\right) = -\beta\omega^\beta(P) - \log\left(\omega^\beta\left(U\left(\mathrm{i}\beta\right)\right)\right). \quad (4.1.4)$$

Reasoning along the same lines, we also obtain

$$\mathrm{Ent}(\Omega_P, \Omega_0) = -\beta\,\omega^{\beta,V}(P) - \log\left(\omega^\beta\left(U\left(\mathrm{i}\beta\right)\right)\right). \quad (4.1.5)$$

As a next step, we would like to consider three self-adjoint perturbations $P_i \in \mathscr{M}$, $i \in \{1,2,3\}$ and the relative KMS states Ω_i obtained by means of the Araki's construction over Ω_0 as before. It holds that

$$\Omega_i = \frac{1}{N_i} U_i\left(\mathrm{i}\frac{\beta}{2}\right)\Omega_0, \qquad U_i = e^{-\frac{\beta}{2}(H+P_i)} e^{\frac{\beta}{2}H}, \qquad N_i^2 = \left\langle \Omega_0 \middle| U_i^*\left(\mathrm{i}\frac{\beta}{2}\right) U_i\left(\mathrm{i}\frac{\beta}{2}\right)\Omega_0 \right\rangle.$$

[5]Here we have denoted the Liouvillian and the Hamiltonian with the same symbol, abusing the notation. The abuse is justified by the choice of sticking to finite-dimensional case.

Let $W_i(t)$ be the weakly continuous one-parameter groups of unitary evolutions obtained by means of the Stone theorem from the generators $H+P_i$.

The relative modular operator between the states $\Psi \doteq W_2(t)\Omega_1$ and $\Phi \doteq \Omega_3$ is obtained starting from

$$S_{\Psi,\Phi} A W_2(t)\Omega_1 = A^*\Omega_3 = A^*\frac{1}{N_3}U_3\Omega_0 = \frac{N_1}{N_3}A^*U_3U_1^{-1}\Omega_1$$
$$= \frac{N_1}{N_3}W_2(t)W_2(t)^*A^*U_3U_1^{-1}\Omega_1 = \frac{N_1}{N_3}W_2(t)S_1U_1^{-1^*}U_3^*AW_2(t)\Omega_1,$$

where we have used S_1, the operator which realizes the conjugation $S_1A\Omega_1 = A^*\Omega_1$ and we have suppressed the argument of the U_i's, writing $U_i \equiv U_i\left(\mathrm{i}\frac{\beta}{2}\right)$. Hence

$$\Delta_{\Psi,\Phi} = \left(\frac{N_1}{N_3}\right)^2 U_3U_1{}^{-1}S_1^*S_1U_1^{-1^*}U_3^* = \left(\frac{N_1}{N_3}\right)^2 e^{-\beta(H+P_3)},$$

where we have used the fact that the modular operator of Ω_1 is $\Delta_1 = S_1^*S_1 = e^{-\beta(H+P_1)}$. Hence the relative entropy

$$\mathrm{Ent}(\Psi,\Phi) = -\beta\langle\Omega_1|(P_1-P_2)\Omega_1\rangle + \beta\langle W_2(t)\Omega_1|(P_3-P_2)W_2(t)\Omega_1\rangle - \log(N_1^2) + \log(N_3^2). \quad (4.1.6)$$

In particular, one finds

$$\mathrm{Ent}(\Omega_1,\Omega_3) = -\beta\langle\Omega_1|(P_1-P_3)\Omega_1\rangle - \log\left(N_1^2\right) + \log\left(N_3^2\right). \quad (4.1.7)$$

All the final expressions found involve only the Connes' co-cycles U_i and its generators P_i, though they may be generalised to the context of pAQFT. In particular, we will assume them as definitions of relative entropy in that case and we will prove that the definition is well-posed by showing that it fulfills all the desired properties.

4.2 Relative entropy in pAQFT

This section is devoted to the definition of the relative entropy for a perturbatively constructed massive scalar field theory on Minkowski space-time, with an interaction of the form (2.3.27). The relative entropy is defined regarding interacting KMS states as the one defined in Theorem 2.3.1 with formulas analogue to (4.1.4), (4.1.5) and (4.1.7).

In particular, we consider three interaction Lagrangians V_i, $i = 1,2,3$, of the form (2.3.27) and the perturbed KMS states ω^{β,V_i} generated out of them, possibly composed with the interacting dynamics $\alpha_t^{V_i}$. In this section we will not deal with the adiabatic limit, hence we will note make the dependance on the cutoff explicit in the notation. In addition, we suppose that the three potentials are smeared with the same function $h \in \mathscr{D}(\mathbb{R}^3)$.

We stress that, thanks to the identification between the free and the interacting algebras $\mathscr{A}_{V_i}$ given in Section 2.2.1, it is legit to compare the states ω^{β,V_i} among themselves and also with the free (α_t,β)-KMS ω^β and with the NESS ω^+. All along this chapter we will suppose to work with states on the free algebra $\mathscr{A}_{\omega^\beta}$.

In this setting, the definition of entropy is the following:

Definition 4.2.1. The relative entropy between $\omega^{\beta,V_1}\circ\alpha_t^{V_2}$ and ω^{β,V_3} is defined as

$$\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)\doteq -\omega^{\beta,V_1}(\beta K_1-\beta K_2)+\omega^{\beta,V_1}(\alpha_t^{V_2}(\beta K_3-\beta K_2))$$
$$-\log(\omega^{\beta}(U_1(\mathrm{i}\beta)))+\log(\omega^{\beta}(U_3(\mathrm{i}\beta))), \quad (4.2.8)$$

where K_i are the generators associated to V_i as in (2.3.33) and U_i the corresponding co-cycles, explicitly given in (2.3.36).

The definition above, in particular equation (4.2.8) has to be understood in terms of formal power series in the coupling constant λ. In particular, the expression for the logarithm $\log\left(\omega^{\beta,V_1}(U_1(\mathrm{i}\beta))\right)$ is given in equation (2.3.44). A first check of consistency of the previous definition is that, in the case where t and either V_1 or V_3 vanish, it gives

$$\mathrm{Ent}\left(\omega^{\beta},\omega^{\beta,V}\right)=\beta\omega^{\beta}(K)+\log\left(\omega^{\beta}(U(\mathrm{i}\beta))\right),\qquad \mathrm{Ent}\left(\omega^{\beta,V},\omega^{\beta}\right)=-\beta\omega^{\beta,V}(K)-\log\left(\omega^{\beta}(U(\mathrm{i}\beta))\right),$$

which are the direct extensions of equations (4.1.4) and (4.1.5) valid in statistical mechanics to the perturbative field theoretical framework.

Remark 4.2.1. The expression of entropy given in equation (4.2.8) is compatible with the definition of entropy as the difference of internal and free energies, divided by the temperature. In particular $\log\left(\omega^{\beta}(U(\mathrm{i}\beta))\right)/\beta$ is nothing but the difference of the free energies in the states ω^{β} and $\omega^{\beta,V}$, while the expectation value of K corresponds to the internal energy since K is the generator of the co-cycle $U(t)$. This agrees with the thermostatic formalism introduced in [Li13, Section 4.4.], where it is also performed a computation of the first non-trivial order for the free energy, showing that it agrees with the results present in the physical literature. This suggests that the present definition should have a direct counterpart in the standard perturbative QFT language, *i.e.* with the Keldysh contours formalism and perturbative expansions of the propagators through the Matsubara formalism. As said before, a direct connection between the two formalisms is still missing and future investigations in this direction are needed.

To make its definition meaningful, we shall prove that the generalised relative entropy for perturbed KMS states has similar properties as those shown by Araki in [Ar76], collected in Theorem 4.1.6, which in this case are going to be satisfied in the sense of formal power series. Actually, we have the following result.

Proposition 4.2.1. *The generalised relative entropy* $\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)$ *satisfies the following properties:*

(a) Quadratic quantity: *The lowest order contribution both in K_i (which are related to V_i as in* (2.3.33)*) and in the coupling constant λ in* $\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)$ *is the second.*

(b) Positivity: $\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)$ *is positive in the sense of formal power series for every t when $V_1\neq V_3$ or for $t\neq 0$ when $V_1=V_3\neq V_2$ and it vanishes in the remaining cases.*

(c) Convexity: $\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)$ *is convex in V_1, in V_2 and also in V_3 in the sense of formal power series.*

(d) Continuity: $\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)$ *is continuous in* V_i *in the sense of formal power series with respect to the topology of microcausal functionals.*

Proof. **(a)** Let us start observing that

$$\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)=\mathrm{Ent}\left(\omega^{\beta,V_1},\omega^{\beta,V_3}\right)+\omega^{\beta,V_1}\left((\alpha_t^{V_2}-\alpha_t^{V_1})(\beta K_3-\beta K_2)\right). \tag{4.2.9}$$

Expanding ω^{β,V_i} and $\omega^{\beta}(\log(U_i(\mathrm{i}\beta)))$ in equation (4.2.8) with (2.3.43) and (2.3.44) we obtain the following expansion in powers of K:

$$\begin{aligned}\mathrm{Ent}\left(\omega^{\beta,V_1},\omega^{\beta,V_3}\right)&=\int_0^\beta\omega^{c,\beta}(\beta K_1\otimes\alpha_{iu}K_1)du-\int_0^\beta\omega^{c,\beta}(\beta K_3\otimes\alpha_{iu}K_1)du\\&\quad-\int_{\beta S_2}\omega^{c,\beta}(\alpha_{iu_1}K_1\otimes\alpha_{iu_2}K_1)dU_2+\int_{\beta S_2}\omega^{c,\beta}(\alpha_{iu_1}K_3\otimes\alpha_{iu_2}K_3)dU_2+O(K^{\otimes 3}).\end{aligned} \tag{4.2.10}$$

Furthermore, in view of (2.3.40),

$$\begin{aligned}&\omega^{\beta,V_1}\left(\left(\alpha_t^{V_2}-\alpha_t^{V_1}\right)(\beta K_3-\beta K_2)\right)=\\&\quad=-\mathrm{i}\beta\int_0^t\left[\omega^{\beta,c}\left(\alpha_s(K_1-K_2)\otimes\alpha_t(K_3-K_2)-\alpha_t(K_3-K_2)\otimes\alpha_s(K_1-K_2)\right)\right]ds+O(K^{\otimes 3}).\end{aligned} \tag{4.2.11}$$

Since K is at least of order 1 in λ, equations (4.2.9), (4.2.10) and (4.2.11) prove *a*).

(b) In order to prove that $\mathrm{Ent}(\omega^{\beta,\lambda V_1}\circ\alpha_t^{\lambda V_2},\omega^{\beta,\lambda V_3})$ is positive in the sense of formal power series we have to be sure that the lowest order contribution in the coupling constant is positive and that the higher contributions are real. Notice that every term in the expansion in powers of K in $\mathrm{Ent}\left(\omega^{\beta,\lambda V_1}\circ\alpha_t^{\lambda V_2},\omega^{\beta,\lambda V_3}\right)$ is real because K_i is formally self-adjoint for every i. If we prove that the second order in K in (4.2.9), which is obtained from (4.2.10) and from (4.2.11), is strictly positive, we get the assert because the lowest contribution in the λ expansion of the second order expansion in K remains positive. Notice that the second order contributions in K are given in (4.2.10) and in (4.2.11) in terms of connected functions with two entries. We thus proceed analysing the following connected functions for any copies of formally selfadjoint microcausal functionals A,B

$$\omega^{\beta,c}(A\otimes B)=\sum_l\frac{1}{l!}\Gamma^l_{12}(A\otimes B)\Big|_{(0,0)}=\sum_l\frac{1}{l!}\left\langle A^{(l)},\left(\omega_2^\beta\right)^{\otimes l}B^{(l)}\right\rangle_l\Big|_{(\phi,\phi)=(0,0)},$$

where ω_2^β is the operator obtained by the Schwartz kernel theorem from the 2-point function of the free KMS state at temperature β given in (1.3.70), hence

$$\omega^{\beta,c}(\alpha_{\mathrm{i}u_1}A\otimes\alpha_{\mathrm{i}u_2}B)=\sum_{l=1}^\infty\frac{1}{l!}\int\left(\prod_{j=1}^l\frac{e^{-E(j)(u_2-u_1)}\lambda_+(p_j)+e^{E(j)(u_2-u_1-\beta)}\lambda_-(p_j)}{2E(j)(1-e^{-\beta E(j)})}\right)\widehat{\Psi_l}(-P_l,P_l)dP_l,$$

where $P_l=(p_1,\dots,p_l)$ with $p_j=(p_{j0},\mathbf{p}_j)\in\mathbb{R}^4$ and $E(j)=\sqrt{\mathbf{p}_j^2+m^2}$. Furthermore, $\lambda_\pm(p_j)=\delta(p_{j0}\mp E(j))$, where δ is the Dirac delta function and thus $\lambda_\pm(p_j)$ impose the restriction on the positive or negative mass shell of the domain of the p_j-integration. Finally, $\widehat{\Psi_l}$ is the Fourier transform of the distribution

$$\Psi_l(X,Y)=A^{(l)}(X)\otimes B^{(l)}(Y)\Big|_{(\phi,\phi)=(0,0)},\qquad\forall X,Y\in\mathbb{M}^l.$$

Notice that, since A,B are formally self-adjoint, $\widehat{A^{(l)}}(-P) = \overline{\widehat{A^{(l)}}(P)}$. The integrals over every p_{i0} can now be performed thanks to the delta functions supported on the mass shells which are present in $\lambda_{\pm}$. We obtain

$$\omega^{\beta,c}(\alpha_{iu_1}A \otimes \alpha_{iu_2}B) = \sum_{l=1}^{\infty} \frac{1}{l!} \int \prod_{j=1}^{l} \left(\frac{e^{-\frac{\beta}{2}E(j)}}{2E(j)(1-e^{-\beta E(j)})} \right) \sum_{\{\mathbf{E}_+,\mathbf{E}_-\}} e^{-\sum_k p_{k0}\left(u_2-u_1-\frac{\beta}{2}\right)} \widehat{\Psi}_l(-P_l,P_l)\Big|_{\substack{p_{a0}=\pm E(a) \\ \forall a\in E_\pm}} d\mathbf{P}_l \quad (4.2.12)$$

where the sum is taken over all possible partitions of $\{1,\dots,l\}$ in two subsets $\{\mathbf{E}_+,\mathbf{E}_-\} \subset \mathscr{P}_2\{1,\dots,l\}$ which can also be empty.

Let us start using equation (4.2.12) to expand the second order contributions in (4.2.10). Notice that the integrals over u_1, u_2 and u can be taken before the integration over P because $\widehat{\Psi}(-P,P)$ is not of rapid decrease for large momenta only for the directions P for which $f = \sum_k p_{k0} = 0$ and $\mathbf{p}_i = 0\ \forall i$. Furthermore, if $f = 0$ and $\mathbf{p}_i = 0$, $\forall i$, $\widehat{\Psi}(-P,P)$ is polynomially bounded in P and its growth is tamed by the factor $e^{-\frac{\beta}{2}\sum_j E(j)}$. See Theorem 4 and its proof in [FL14] for further details. In particular, using the fact that

$$\int_0^\beta e^{-ua+\frac{\beta}{2}a} du = 2\frac{\sinh\left(\frac{\beta}{2}a\right)}{a}, \qquad \int_0^\beta du_2 \int_0^{u_2} du_1 e^{-u_2 a + u_1 a + \frac{\beta}{2}a} = \beta \frac{\sinh\left(\frac{\beta}{2}a\right)}{a} + R(a),$$

where R is antisymmetric for changes of a to $-a$, symmetrising the summand over the partitions $\{\mathbf{E}_+,\mathbf{E}_-\}$ and noticing that under that symmetrization $2\overline{\widehat{K_i^{(l)}}}\widehat{K_j^{(l)}}(P_0,\mathbf{P})$ is mapped to $\overline{\widehat{K_i^{(l)}}}\widehat{K_j^{(l)}}(P_0,\mathbf{P}) + \widehat{K_i^{(l)}}\overline{\widehat{K_j^{(l)}}}(P_0,-\mathbf{P})$ we obtain

$$\begin{aligned} \mathrm{Ent}(\omega^{\beta,V_1},\omega^{\beta,V_3}) = \sum_{l\geq 1} \frac{1}{l!} \int \prod_{j=1}^{l} \left(\frac{e^{-\frac{\beta}{2}E(j)}}{2E(j)(1-e^{-\beta E(j)})} \right) \\ \times \sum_{\{\mathbf{E}_+,\mathbf{E}_-\}} \frac{\beta \sinh\left(\frac{\beta}{2}f\right)}{f} \left(\overline{\widehat{K_1^{(l)}}} - \overline{\widehat{K_3^{(l)}}} \right) \left(\widehat{K_1^{(l)}} - \widehat{K_3^{(l)}} \right) \Big|_{p_{a0}=\pm w_a,\, a\in E_\pm} d\mathbf{P}_l + O(K_i^{\otimes 3}), \end{aligned} \quad (4.2.13)$$

where

$$f \doteq \sum_k p_{k0}, \quad (4.2.14)$$

and where the minus sign appearing in front of $-\mathbf{P}$ is removed by a change of integration variables. Notice that since the right hand side of (4.2.13) is a sum of positive quantities, hence the sought positivity is proven for the case $t = 0$ and $V_1 \neq V_3$.

In order to analyse the remaining cases, in view of (4.2.9), we need to discuss

$$\omega^{\beta,V_1}\left((\alpha_t^{V_2} - \alpha_t^{V_1})(\beta K_3 - \beta K_2) \right). \quad (4.2.15)$$

Let us start observing that

$$\omega^{\beta,V_1}\left((\alpha_t^{V_2} - \alpha_t^{V_1})(\beta K_3 - \beta K_2) \right) = -\mathrm{i}\beta \int_0^t \omega^\beta([\alpha_s(K_1-K_2), \alpha_t(K_3-K_2)])\, ds + O(K^{\otimes 3}). \quad (4.2.16)$$

Furthermore, from (4.2.12) we have that for any A,B formally self-adjoint microcausal functionals

$$-\mathrm{i}\beta\int_0^t \omega^\beta([\alpha_s(A),\alpha_t(B)])ds = \beta\sum_{l=1}^{\infty}\frac{1}{l!}\int\prod_{j=1}^{l}\left(\frac{e^{-\frac{\beta}{2}E(j)}}{2E(j)(1-e^{-\beta E(j)})}\right)\sum_{\{\mathbf{E}_+,\mathbf{E}_-\}}\sinh\left(\frac{f\beta}{2}\right)$$
$$\times\left(\frac{1}{f}(1-\cos(ft))\left(\overline{\widehat{A^{(l)}}}\widehat{B^{(l)}}+\overline{\widehat{B^{(l)}}}\widehat{A^{(l)}}\right)-i\frac{\sin(ft)}{f}\left(\overline{\widehat{A^{(l)}}}\widehat{B^{(l)}}-\overline{\widehat{B^{(l)}}}\widehat{A^{(l)}}\right)\right)\Big|_{\substack{p_{a0}=\pm w_a\\ \forall a\in E_\pm}}d\mathbf{P}_l, \quad (4.2.17)$$

where f is given in (4.2.14) and we have symmetrysed the summands over $\{\mathbf{E}_+,\mathbf{E}_-\}$. Notice that if both $A=B=K_1-K_2$, the terms proportional to $\overline{\widehat{A}}\widehat{B}-\overline{\widehat{B}}\widehat{A}$ in (4.2.17) vanish, while the remaining terms are all formally positive.

We now proceed with the discussion of the generic case. If

$$A=K_1-K_2,\qquad B=K_3-K_2$$

we have that

$$\left(\overline{\widehat{A^{(l)}}}\widehat{B^{(l)}}+\overline{\widehat{B^{(l)}}}\widehat{A^{(l)}}\right)=2\left|\frac{\widehat{K_1^{(l)}}+\widehat{K_3^{(l)}}}{2}-\widehat{K_2^{(l)}}\right|^2-\frac{1}{2}\left|\widehat{K_1^{(l)}}-\widehat{K_3^{(l)}}\right|^2. \quad (4.2.18)$$

Furthermore, since $0\leq 1-\cos(ft)\leq 2$, recalling (4.2.13), we argue that the negative contributions proportional to $\left|\widehat{K_1^{(l)}}-\widehat{K_3^{(l)}}\right|^2$ are controlled by $\mathrm{Ent}(\omega^{\beta,V_1},\omega^{\beta,V_3})$ and that the terms proportional to $\left|\widehat{K_1^{(l)}}+\widehat{K_3^{(l)}}-2\widehat{K_2^{(l)}}\right|^2$ are formally positive. Moreover,

$$\left(\overline{\widehat{A^{(l)}}}\widehat{B^{(l)}}-\overline{\widehat{B^{(l)}}}\widehat{A^{(l)}}\right)=\overline{\widehat{K_1^{(l)}}}\widehat{K_3^{(l)}}-\overline{\widehat{K_3^{(l)}}}\widehat{K_1^{(l)}}-\overline{\widehat{K_2^{(l)}}}\widehat{K_3^{(l)}}+\overline{\widehat{K_3^{(l)}}}\widehat{K_2^{(l)}}+\overline{\widehat{K_2^{(l)}}}\widehat{K_1^{(l)}}-\overline{\widehat{K_1^{(l)}}}\widehat{K_2^{(l)}}. \quad (4.2.19)$$

Finally, summing (4.2.13) and (4.2.17) composed with (4.2.18) and with (4.2.19) we get

$$\mathrm{Ent}(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3})=$$
$$\beta\sum_{l=1}^{\infty}\frac{1}{l!}\int\prod_{j=1}^{l}\left(\frac{e^{-\frac{\beta}{2}E(j)}}{2E(j)(1-e^{-\beta E(j)})}\right)\sum_{\{\mathbf{E}_+,\mathbf{E}_-\}}\frac{\sinh\left(\frac{f\beta}{2}\right)}{f}\widehat{F}\overline{\widehat{F}}\Big|_{\substack{p_{a0}=\pm w_a\\ \forall a\in E_\pm}}d\mathbf{P}_l+O(K^{\otimes 3}), \quad (4.2.20)$$

where

$$F=\sin\left(\frac{ft}{2}\right)(K_1+K_3-2K_2)+i\cos\left(\frac{ft}{2}\right)(K_1-K_3), \quad (4.2.21)$$

and where f is given in (4.2.14). Expression (4.2.20) implies that the second order contribution of the relative entropy $\mathrm{Ent}(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3})$ is non-negative.

To conclude the proof of the positivity of the relative entropy we need to prove that the second order contributions are non-vanishing, unless very special conditions are met.

Since the generic contribution to (4.2.20) corresponding to an arbitrary but fixed partition $\{\mathbf{E}_+,\mathbf{E}_-\}$ is non-negative, it is sufficient to analyse in details only one of them, so let us consider only the contributions to (4.2.20) in which $E_-=\emptyset$. So we get

$$C_{E_-=\emptyset}=\beta\sum_{l=1}^{\infty}\frac{1}{l!}\int\prod_{j=1}^{l}\left(\frac{e^{-\frac{\beta}{2}E(j)}}{2E(j)(1-e^{-\beta E(j)})}\right)\frac{\sinh\left(\frac{f\beta}{2}\right)}{f}\widehat{F}\overline{\widehat{F}}\Big|_{p_{a0}=E(a)\,\forall a}d\mathbf{P}_l,$$

where $f = \sum_k w_k$ in this case. If $K_1 \neq K_3$, $\cos(\frac{ft}{2})^2 (K_1 - K_3)^2$ at fixed t is positive for almost every f. Furthermore, if $K_1 = K_3 \neq K_2$, $\sin\left(\frac{ft}{2}\right)^2 (K_1 + K_3 - 2K_2)^2$ at fixed $t \neq 0$ is positive for almost every f. In the remaining case, that is when $V_1 = V_3 = V_2$, the relative entropy is trivial because $\omega^{\beta,V_1} \circ \alpha_t^{V_1} = \omega^{\beta,V_1}$ and the same holds whenever $t = 0$ and $V_1 = V_3$, because $\mathrm{Ent}(\omega^{\beta,V}, \omega^{\beta,V}) = 0$ for every $\omega^{\beta,V}$. This concludes the proof of point b).

(c) The convexity in V_i for every i can be proved in the sense of perturbation theory analysing the lowest non-vanishing order in λ of (4.2.20). This gives a sum of quadratic elements, namely, all possible $F\overline{F}$ in (4.2.20) for various l, $\mathbf{p}_l$ and $E_\pm$. Since all these elements are convex, the thesis is proven.

(d) The perturbative expansion of the relative entropy (4.2.20) guarantees continuity for V_i in $\mathscr{A}_{\omega^\beta}$ with respect to the topology of microcausal functionals in the sense of perturbation theory. □

Remark 4.2.2. The positivity of both $\mathrm{Ent}(\omega^{\beta,V_1} \circ \alpha_t^{V_2}, \omega^{\beta,V_3})$ and $\mathrm{Ent}(\omega^{\beta,V_1}, \omega^{\beta,V_3})$ shown in point (**b**) does not guarantee the positivity of their difference

$$\mathrm{Ent}\left(\omega^{\beta,V_1} \circ \alpha_t^{V_2}, \omega^{\beta,V_3}\right) - \mathrm{Ent}\left(\omega^{\beta,V_1}, \omega^{\beta,V_3}\right) = \beta \omega^{\beta,V_1}\left((\alpha_t^{V_2} - \alpha_t^{V_1})(K_3 - K_2)\right),$$

as can be seen composing (4.2.9) with (4.2.16) and then with (4.2.17). This will be important in Section 4.4, when we will deal with the entropy production.

Remark 4.2.3. An alternative (shorter) proof of the positivity of $\mathrm{Ent}(\omega^{\beta,V_1} \circ \alpha_t^{V_2}, \omega^{\beta,V_3})$ given in (4.2.9) can be obtained introducing the Kubo-Mari sesquilinear product:

$$\langle A \mid B \rangle_\beta \doteq \frac{1}{\beta} \int_0^\beta \omega^{c,\beta}(A^* \otimes \alpha_{iu}(B)) du,$$

see [BR97b, Section 5.3] for more details and for its properties.

Consider the second order contributions in K in (4.2.10), which is the first term in $\mathrm{Ent}(\omega^{\beta,V_1} \circ \alpha_t^{V_2}, \omega^{\beta,V_3})$ as displayed in (4.2.9). The KMS condition permits to rewrite the integrals over the simplex S_2 as integrals over a single variable, namely

$$\int_{\beta S_2} \omega^{\beta,c}\left(\alpha_{iu_1} K_1 \otimes \alpha_{iu_2} K_1\right) dU_2 = \frac{\beta}{2} \int_0^\infty \omega^{\beta,c}\left(K_1 \otimes \alpha_{iu} K_1\right) du.$$

Using the Kubo-Mari product we obtain

$$\mathrm{Ent}\left(\omega^{\beta,V_1}, \omega^{\beta,V_3}\right) = \frac{\beta^2}{2} \langle K_1 - K_3 \mid K_1 - K_3 \rangle_\beta + O(K^{\otimes 3}) \tag{4.2.22}$$

and since, $\langle \cdot \mid \cdot \rangle_\beta$ is a positive semidefinite sesquilinear form and $K_1 - K_3$ is formally self-adjoint, the positivity of $\mathrm{Ent}(\omega^{\beta,V_1}, \omega^{\beta,V_3})$ follows.

The other second order contributions in (4.2.11) or in (4.2.16) can be treated using the analyticity property of the state ω^β and its time-translation so to switch the time integration into an imaginary time one, and then recognizing again the Kubo-Mari product:

$$\omega^{\beta,V_1}\left((\alpha_t^{V_2} - \alpha_t^{V_1})(\beta K_3 - \beta K_2)\right) = \\ \beta^2 \langle K_1 - K_2 \mid K_3 - K_2 \rangle_\beta - \beta^2 \langle K_1 - K_2 \mid \alpha_t(K_3 - K_2) \rangle_\beta + O(K^{\otimes 3}) \tag{4.2.23}$$

Combining the two contributions (4.2.22) and (4.2.23), appealing to the sesquilinearity of $\langle\cdot\,|\,\cdot\rangle_\beta$ and its time-translation invariance, we obtain

$$\mathrm{Ent}\Big(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\Big)=\frac{\beta^2}{2}\,\langle F\,|\,F\rangle_\beta+O(K^{\otimes 3})$$

where, in analogy with (4.2.21), F is the formal selfadjoint element

$$F=\frac{1}{2}(-\alpha_{t/2}(K_1+K_3-2K_2)+\alpha_{-t/2}(K_1+K_3-2K_2)+\alpha_{t/2}(K_1-K_3)+\alpha_{-t/2}(K_1-K_3)).$$

Hence, the sesquilinearity of the Kubo-Mari product and the form of K_i implies that $\mathrm{Ent}(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3})$ is positive semidefinite in the sense of formal power series. The strict positivity follows from the expansion given in (4.2.20).

4.3 Adiabatic limits

In the adiabatic limit $h\to 1$ the relative entropy given in (4.2.8) diverges due to the integration over an infinite space. As we saw in Section 2.3, $\omega^{\beta,V}(A)$ is well-defined in the adiabatic limit if A is of compact support. Moreover, in [Li13, Chapter 4.4.] Lindner had been able to proof the finiteness of the van Hove limit $\text{vH-lim}_{h\to 1}\log(\omega^\beta(U^h(\mathrm{i}\beta)))/I(h)$ where we introduced

$$I(h)\doteq\int_{\mathbb{R}^3}h(\mathbf{x})d\mathbf{x}. \tag{4.3.24}$$

Furthermore, we recall another kind of infrared divergences, that appear if the adiabatic limit is performed in $\omega^\beta(\alpha_t^V(A))$, see *e.g.* [Al90, LW87, LeB00, Ste95] and Proposition 3.3.2, whose proof provides an explicit computation showing this fact.

The discussion above makes us confident about the well-posedness of the adiabatic limit of expressions of the form

$$\mathrm{e}=\underset{h\to 1}{\text{vH-lim}}\,\frac{1}{I(h)}\,\mathrm{Ent}(\omega^{\beta,V_1}\circ\alpha_t,\omega^{\beta,V_3}),$$

which has the dimension of an entropy density. In other words, the infinite-volume integration leading to the divergent behaviour of the relative entropy is expected to be cured by taking densities. Actually, we get to the following definition.

Definition 4.3.1. Let V_i^h for $i\in\{1,3\}$ be two interaction Lagrangians of the form (2.3.27) with the same spatial cutoff $h\in\mathscr{D}(\mathbb{R}^3)$. We define the relative entropy per unit volume as

$$\mathrm{ent}(\omega^{\beta,V_1}\circ\alpha_t,\omega^{\beta,V_3})\doteq\underset{h\to 1}{\text{vH-lim}}\,\frac{1}{I(h)}\,\mathrm{Ent}(\omega^{\beta,V_1^h}\circ\alpha_t,\omega^{\beta,V_3^h}), \tag{4.3.25}$$

where $I(h)$ is the integral of the cutoff function over the volume $\mathbb{R}^3$ given in (4.3.24) and the limit $h\to 1$ is taken in the sense of van Hove, as per Definition 2.3.1.

In order for this definition to be meaningful, we shall prove that the relative entropy per unit volume is finite. To do so, we first prove a technical lemma, which states that the expectation values of the interacting Hamiltonian densities H_i (2.3.35) in the interacting state obtained out of the potential V_j for any $i,j=1,2,3$ is constant in the spatial variables and uniformly bounded in time.

Lemma 4.3.1. *Consider the function*

$$l(t,\mathbf{x}) \doteq \omega^{\beta,V_1}\left(\alpha_t\left(\beta H_3(\mathbf{x})\right)\right)$$

constructed with V_1 and V_3 of the from (2.3.27)*, with H_3 given as in* (2.3.35) *and where the limit $h \to 1$ has already been taken both in V_1 and V_3. The function $l(r,\mathbf{x})$ is constant in $\mathbf{x}$ and uniformly bounded in t.*

Proof. The proof proceeds along the same line of the one of Theorem 3.4.1. Many of the formulas will actually be the same, with very little modifications, but in order to reach a self-consistent proof, we prefer to report them here.

Let us thus start by expanding $\omega^{\beta,V}$ in terms of connected functions using equation (2.3.43). This leads to an analogue of equation (3.4.18), which reads:

$$\omega^{\beta,V}(\alpha_t(A)) = \omega^{\beta}(\alpha_t(A)) + \sum_{n=1}^{\infty}\int_{\beta S_n} dU_n \int_{\mathbb{R}^3} d^3\mathbf{x}_1 \ldots \int_{\mathbb{R}^3} d^3\mathbf{x}_n\, \omega^{\beta,c}\left(\alpha_t(A)\otimes\alpha_{iu_1,\mathbf{x}_1}(R)\otimes\cdots\otimes\alpha_{iu_n,\mathbf{x}_n}(R)\right),$$

where $R \doteq -R_V(H(\dot{\chi}^- \delta_0))$ and $\alpha_{t,\mathbf{x}}$ indicates the automorphisms implementing Minkowski space-time translations of $(t,\mathbf{x})$. Furthermore, as in the proof of [FL14, Theorem 4.], the connected $n-$point functions can be written by means of the following graphical expansion

$$\begin{aligned}\omega^{\beta,c}(\alpha_{\mathrm{i}u_0,\mathbf{x}_0}(A)\otimes\alpha_{\mathrm{i}u_1,\mathbf{x}_1}(R)\otimes\cdots\otimes\alpha_{\mathrm{i}u_n,\mathbf{x}_n}(R)) = \\ \sum_{G\in\mathscr{G}^c_{n+1}}\prod_{k<j}\left(\frac{\Gamma_{kj}^{l_{kj}}}{l_{kj}!}\right)\left(\alpha_{\mathrm{i}u_0,\mathbf{x}_0}(A)\otimes\alpha_{\mathrm{i}u_1,\mathbf{x}_1}(R)\otimes\cdots\otimes\alpha_{\mathrm{i}u_n,\mathbf{x}_n}(R)\right)\Big|_{(\phi_0,\ldots,\phi_n)=0} \\ \doteq \sum_{G\in\mathscr{G}^c_{n+1}}\frac{1}{\mathrm{Symm}(G)}F_{n,G}(u_0,\mathbf{x}_0;u_1,\mathbf{x}_1;\ldots;u_n,\mathbf{x}_n),\end{aligned}$$

where the sum is taken over the oriented connected graphs joining $n+1$ vertices and $\mathrm{Symm}(G)$ is a normalisation factor. Following the proof of Theorem 4 in [FL14], $F_{n,G}$ can be computed as

$$F_{n,G}(u_0,\mathbf{x}_0;u_1,\mathbf{x}_1;\ldots;u_n,\mathbf{x}_n) = \int_{\mathbb{R}^n}\prod_{l\in\mathbf{E}(G)}\frac{e^{\mathbf{i}\mathbf{p}_l(\mathbf{x}_{s(l)}-\mathbf{x}_{r(l)})}(\lambda_+(p_l)+\lambda_-(p_l))}{2E(l)\left(1-e^{-\beta E(l)}\right)}\widehat{\Psi}(-P,P)\,dP, \tag{4.3.26}$$

where $\mathbf{E}(G)$ is the set of lines of the graph G, $s(l)$ and $r(l)$ are respectively the indexes of the source and the range of the points joined by the line l. Furthermore, $\widehat{\Psi}(-P,P)$ is the Fourier transform of the function $\Psi(X,Y)$, that is defined as

$$\Psi(X,Y) = \prod_{l\in\mathbf{E}(G)}\frac{\delta^2}{\delta\phi_{s(l)}(x_l)\delta\phi_{r(l)}(y_l)}(A\otimes\underbrace{R\otimes\cdots\otimes R}_{n\text{ times}})\Big|_{(\phi_0,\ldots,\phi_n)=0},$$

X and Y standing for $(x_1,\ldots,x_k)$ and $(y_1,\ldots,y_k)$ respectively and k indicates the number of lines in $\mathbf{E}(G)$. Similarly, in the Fourier transform $\widehat{\Psi}(-P,P)$, we have used the shorthand $P=(p_1,\ldots,p_k)$. $\lambda_+(p_l)$ and $\lambda_+(p_l)$ are the positive and negative frequency contributions to Γ_{ij} respectively and they are defined according to equation (3.4.23).

Then we expand the products of the sums of positive and negative frequencies parts in (4.3.26) and we perform the spatial integrals over $\mathbf{x}_1,\dots,\mathbf{x}_n$ in $F_{n,G}$. Arguing as in the proof of Theorem 3.4.1, we obtain that each graph G in $\mathscr{G}_n^c$ contributes to $\omega^{\beta,V}(\alpha_t(A))$ with a term proportional to

$$\int_{\beta S_n} dU_n \int_{\mathbb{R}^3} d^3\mathbf{x}_1 \dots \int_{\mathbb{R}^3} d^3\mathbf{x}_n \, F_{n,G}(u_0 - \mathrm{i}t, \mathbf{x}_0; u_1, \mathbf{x}_1; \dots; u_n, \mathbf{x}_n) =$$

$$\sum_{\{\mathbf{E}_+,\mathbf{E}_-\}\in\mathscr{P}_2(\mathbf{E}(G))} \int_{\beta S_n} dU_n \int d^3\mathbf{p} \prod_{l_+\in E_+} \frac{e^{-E(l_+)(u_{r(l_+)}-u_{s(l_+)})}}{2E(l_+)\left(1-e^{-\beta E(l_+)}\right)} \prod_{l_-\in E_-} \frac{e^{E(l_-)(u_{r(l_-)}-u_{s(l_-)}-\beta)}}{2E(l_-)\left(1-e^{-\beta E(l_-)}\right)} \hat{\Psi}(-P,P)\Big|_{\substack{p_{k0}=\pm E(k),\\ \forall k\in\mathbf{E}_\pm}}$$

$$e^{\mathrm{i}\mathbf{x}_0\left(\sum_{\substack{l\in\mathbf{E}(G)\\ s(l)=0}}\mathbf{p}_l\right)} \prod_{j\in\{1,\dots,n\}} \delta\left(\sum_{\substack{l\in\mathbf{E}(G)\\ s(l)=j}}\mathbf{p}_l - \sum_{\substack{l\in\mathbf{E}(G)\\ r(l)=j}}\mathbf{p}_l\right) \prod_{\substack{e_+\in\mathbf{E}_+\\ s(e_+)=0}} e^{-\mathrm{i}tE(e_+)} \prod_{\substack{e_-\in\mathbf{E}_-\\ s(e_-)=0}} e^{\mathrm{i}tE(e_-)},$$

where the product of delta functions expresses the momentum conservation. The exponentials $e^{-\mathrm{i}tE(e_+)}$ and $e^{\mathrm{i}tE(e_-)}$ are uniformly bounded in time, and the same holds for the results of the remaining integrations over P and U. Finally, we observe that, because of the delta functions implementing momentum conservation, $\sum_{\substack{l\in\mathbf{E}(G)\\ s(l)=0}}\mathbf{p}_l = 0$. This implies that $F_{n,G}$ becomes constant in $\mathbf{x}_0$ after integration over the other spatial variables for every graph, thus concluding the proof. □

Remark 4.3.1. The adiabatic limit can be decomposed in two limits, namely the limit $h\to 1$ can be taken in different steps without altering the final result. More precisely, following [FL14, Theorem 3.] and [DrHaPi16, Lemma C.1.], it can be shown that the following limits are equal:

$$\operatorname*{vH-lim}_{h\to 1}\frac{1}{I(h)}\omega_h^{\beta,V}(R_{V_h}(\dot{V}_h)) = \operatorname*{vH-lim}_{h_1\to 1}\operatorname*{vH-lim}_{h_2\to 1}\frac{1}{I(h_1)}\omega^{\beta,V^{h_2}}(R_{V^{h_2}}(\dot{V}^{h_1})), \tag{4.3.27}$$

where $K_h = R_{V_h}(\dot{V}_h)$.

Proposition 4.3.1. *The relative entropy per unit volume $s(\omega^{\beta,V_1}\circ\alpha_t,\omega^{\beta,V_3})$ given in* (4.3.25) *is finite.*

Proof. In [Li13, Prop. 4.4.2] it has been shown that the van Hove limit

$$L \doteq \operatorname*{vH-lim}_{h\to 1}\frac{\log\left(\omega^\beta\left(U(\mathrm{i}\beta)\right)\right)}{I(h)} \tag{4.3.28}$$

exists and is finite. Recalling the definition of relative entropy (4.2.8), to ensure the finiteness of the relative entropy density (4.3.1) in the adiabatic limit we just need to prove the finiteness of the following two limits

$$L_1 \doteq \operatorname*{vH-lim}_{h\to 1}\frac{1}{I(h)}\omega^{\beta,V_1^h}(\beta K_1^h), \qquad L_2 \doteq \operatorname*{vH-lim}_{h\to 1}\frac{1}{I(h)}\omega^{\beta,V_1^h}(\alpha_t(\beta K_3^h)). \tag{4.3.29}$$

We shall now consider only L_2 because the same conclusions for L_1 can be follows fixing $t=0$ and $V_3 = V_1$. Let us decompose K_3 as in (2.3.35) by introducing the hamiltonian density $H_3(\mathbf{x}) \equiv R_{V_3}(\dot{V}_3^{\delta_{\mathbf{x}}})$. Equation (4.3.27) discussed in the remarks above implies that

$$L_2 \doteq \operatorname*{vH-lim}_{h_1\to 1}\operatorname*{vH-lim}_{h_2\to 1}\frac{1}{I(h_1)}\int h_1(\mathbf{x})\omega^{\beta,V_1^{h_2}}(\alpha_t(\beta H_3^{h_2}(\mathbf{x})))d^3\mathbf{x}.$$

We taken now the limit $h_2 \to 1$ and thanks to Lemma 4.3.1 we have that

$$l_2(\mathbf{x}) \doteq \underset{h_2 \to 1}{\text{vH-lim}}\, \omega^{\beta, V_1^{h_2}}(\alpha_t(\beta H_3^{h_2}(\mathbf{x})))$$

exists, is constant in $\mathbf{x}$ and bounded in t. We can now take the limit $h_1 \to 1$ and from (4.3.24) we have that $L_2 = l_2$ thus concluding the proof. □

Proposition 4.3.2. *The relative entropy per unit volume* $\mathrm{ent}(\omega^{\beta,V_1} \circ \alpha_t, \omega^{\beta,V_2})$ *is positive.*

Proof. First of all notice that if $V_1 = V_2$ and $t = 0$ the relative entropy per unit volume vanishes because $\mathrm{Ent}(\omega^{\beta,V_1}, \omega^{\beta,V_1})$ is zero for every h. In the other cases consider a van Hove sequence h_n converging to 1. Notice that $I(h_n)$ is positive for every n because h_n are positive functions. The relative entropy Ent is also positive for every n as shown in proposition 4.2.1. The limit for $n \to \infty$ of positive quantities is positive, thus we have the thesis. □

4.4 Entropy production

The definition of entropy production for C^*- or W^*-dynamical systems has been given in [JP01, JP02, JP02b], see also the previous works [OHI88, Oj89, Oj91] and [Ru01, Ru02] for the case of spin systems. Consider state ω fulfilling the KMS condition with respect to a continuous one-parameter group of automorphisms α_t and let α_t^V be the dynamics perturbed by a self-adjoint observable V. The entropy production[6] of α_t^V with respect to α_t in the state η is usually defined as

$$\mathrm{Ep}_V(\eta) \doteq \eta(\sigma_V), \qquad \text{where} \qquad \sigma_V \doteq -\frac{\mathrm{d}}{\mathrm{d}t}\alpha_t(\beta V)\Big|_{t=0} = -\frac{\mathrm{d}}{\mathrm{d}t}\alpha_t^V(\beta V)\Big|_{t=0},$$

where the last equality can be obtained from the cocycle condition of U and the definition of its generator, see equations (2.3.31), (2.3.33). Even if the form of the Hamiltonian generating α_t is not available in the case of field theories, and hence σ_V can not be computed, a generalization of the definition of entropy production can be obtained for any stationary η. In particular, if η is a $\alpha_t^{V_1}$-invariant state, it holds that

$$\mathrm{Ep}_{V_2}(\eta) = \frac{\mathrm{d}}{\mathrm{d}t}\eta\left(\alpha_{-t}^{V_1}\alpha_t(-\beta V_2)\right)\Big|_{t=0}, \qquad \mathrm{Ep}_{V_2}(\eta \circ \alpha_s) = \frac{\mathrm{d}}{\mathrm{d}t}\eta\left(\alpha_{-t}^{V_1}\alpha_t(-\beta V_2)\right)\Big|_{t=s},$$
$$\mathrm{Ep}_{V_2}\left(\eta \circ \alpha_s^{V_2}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\eta\left(\alpha_{-t}^{V_1}\alpha_t^{V_2}(-\beta V_2)\right)\Big|_{t=s}.$$

These expressions can be directly extended to the case of perturbative quantum field theories via the following definition.

Definition 4.4.1. Let V_i, for $i \in \{1,2,3\}$, be three perturbation Lagrangians of the form (2.3.27) constructed with the same cutoff function $h \in \mathscr{D}(\mathbb{R}^3)$ which are past compact and of compact spatial support. Consider η, a state which is invariant under the one parameter group of automorphisms $\alpha_t^{V_1}$. The entropy production in the state η of $\alpha_t^{V_2}$ relative to $\alpha_t^{V_3}$ (or to ω^{β,V_3}) is defined as

$$\mathrm{Ep}_{V_3}^{V_2}(\eta) \doteq \frac{\mathrm{d}}{\mathrm{d}t}\eta\left(\alpha_{-t}^{V_1}\alpha_t^{V_2}(\beta(K_3 - K_2))\right)\Big|_{t=0}. \tag{4.4.30}$$

[6] The sign of Ep_V, which descends from the sign of σ_V, is the same as in the definition of [JP01] because there the authors assume $\beta = -1$, as customary in the context of Tomita-Takesaki theory.

Analogously, the entropy production in the state $\eta\circ\alpha_t^{V_2}$ of $\alpha_t^{V_2}$ relative to $\alpha_t^{V_3}$ is defined as

$$\mathrm{Ep}_{V_3}^{V_2}(\eta\circ\alpha_s^{V_2}) \doteq \frac{\mathrm{d}}{\mathrm{d}t}\eta\left(\alpha_{-t}^{V_1}\alpha_t^{V_2}(\beta(K_3-K_2))\right)\Big|_{t=s}. \tag{4.4.31}$$

The following proposition, extending [JP01, Theorem 1.1.] valid in the C^*- or W^*-dynamical systems case, motivates the name entropy production.

Proposition 4.4.1. *Consider V_i for $i\in\{1,2,3\}$ three perturbation potentials which are past compact and with spatially compact supports and the KMS state ω^{β,V_3} then*

$$\mathrm{Ent}\left(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}\right)=\mathrm{Ent}\left(\omega^{\beta,V_1},\omega^{\beta,V_3}\right)+\int_0^t\mathrm{Ep}_{V_3}^{V_2}\left(\omega^{\beta,V_1}\circ\alpha_s^{V_2}\right)ds, \tag{4.4.32}$$

where $\mathrm{Ep}_{V_3}^{V_2}(\omega^{\beta,V_1}\circ\alpha_s^{V_2})$ is the entropy production relative to the KMS state ω^{β,V_3}.

Proof. Equation (4.2.9), the invariance of ω^{β,V_1} with respect to $\alpha_t^{V_1}$ and the fact that $\alpha_0^{V_2}\equiv\mathbb{1}$ imply that

$$\mathrm{Ent}(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3})-\mathrm{Ent}(\omega^{\beta,V_1},\omega^{\beta,V_3})=\beta\omega^{\beta,V_1}((\alpha_t^{V_2}-\beta\alpha_t^{V_1})(K_3-K_2))=$$
$$\beta\omega^{\beta,V_1}(\alpha_{-t}^{V_1}\alpha_t^{V_2}(K_3-K_2))-\beta\omega^{\beta,V_1}(\alpha_0^{V_1}\alpha_0^{V_2}(K_3-K_2))=\beta\int_0^t\frac{d}{ds}\omega^{\beta,V_1}(\alpha_{-s}^{V_1}\alpha_s^{V_2}(K_3-K_2))\,ds.$$

The proof can thus be concluded recalling the definition 4.4.1. □

Remark 4.4.1. As observed also in Remark 4.2.2, the entropy production can not be always positive because the difference $\mathrm{Ent}(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3})-\mathrm{Ent}(\omega^{\beta,V_1},\omega^{\beta,V_3})$ is not necessarily positive. However, in the following we will prove that if ergodic means (infinite time average) are considered, the positivity of entropy production is recovered.

By Definition 4.4.1, $\mathrm{Ep}_{V_3}^{V_1}(\omega^{\beta,V_1}\circ\alpha_t^{V_2})$ vanishes if $V_2=V_3$. Furthermore, by Proposition 4.4.1, the entropy production vanishes also if $V_1=V_2$.

We shall now rewrite the entropy production in a way which shall be useful in the analysis of time averages, which we must be able to treat so to include the NESS ω^+ given in (3.4.17) in our analysis.

Proposition 4.4.2. *In the case of $V_2=0$ it holds that*

$$\mathrm{Ep}_{V_3}(\omega^{\beta,V_1}\circ\alpha_t)=\beta\,\omega^{\beta,V_1}(\alpha_t(\Phi_t)),\qquad \textit{with}\qquad \Phi_t=-\mathrm{i}[\alpha_{-t}K_1,K_3],$$

the commutator being computed with respect to the $\star$ product.

Proof. Notice that

$$\alpha_t^V(A)=U_h(t)\star\alpha_t(A)\star U_h(t)^*,$$

furthermore, the cocycle condition and the form of the generator K imply

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U_h(t)=U_h(t)\star\alpha_t(K_h).$$

Denoting U_1 the co-cycle obtained with the perturbation V_1^h, by definition of entropy production (4.4.31) we have

$$\begin{aligned}
\mathrm{Ep}_{V_3}(\omega^{\beta,V_1}\circ\alpha_t) &= \beta\,\omega^{\beta,V_1}\left(\frac{\mathrm{d}}{\mathrm{dt}}\alpha_{-t}^{V_1}\alpha_t(K_3)\right)\\
&= \beta\,\omega^{\beta,V_1}\left(\frac{\mathrm{d}}{\mathrm{dt}}\left(U_1(-t)\star K_3\star U_1(-t)^*\right)\right)\\
&= -\mathrm{i}\beta\,\omega^{\beta,V_1}\left(U_1(-t)\star\alpha_{-t}([K_1,\alpha_t(K_3)])\star U_1(-t)^*\right)\\
&= -\mathrm{i}\beta\,\omega^{\beta,V_1}\left(\alpha_{-t}^{V_1}\alpha_t([\alpha_{-t}K_1,K_3])\right)\\
&= -\mathrm{i}\beta\,\omega^{\beta,V_1}\circ\alpha_t([\alpha_{-t}K_1,K_3])\,.
\end{aligned}$$

Hence, the thesis holds. □

Similar results have been obtained by Haag and Trych-Pohlmeyer in [HTP77], although in a different context.

The strategy then is to estimate how far ω^+ is from the free equilibrium state ω^β. The most direct way would be to evaluate their relative entropy, but, unfortunately, (4.2.8) can not be directly applied to ω^+. This led us in [DFP18b] to analyse the entropy production in ω^+. So to be able to compute it in the case $\eta\equiv\omega^+$, we must first discuss the adiabatic limits of the entropy production, together with its relations with the relative entropy per unit volume introduced in Definition 4.3.1. In fact, recall that this state is defined as a by-product of the study of return to equilibrium, which actually fails if we perturb the system with a spatially non-compact perturbation potential, *i.e.* if the adiabatic limit is takes, even though an ergodic mean is considered. Hence, to avoid infrared problems, the entropy production per unit volume of a NESS ω^+ is described via an extension of Definition 4.4.1 to the infinite volume case following what we did for the relative entropy in Definition 4.3.1. Hence, in close analogy to [JP01, Equation (1.2)], the entropy production per unit volume of α_t in the state $\omega^+_{V_1}$ is defined as

$$\mathrm{ep}_{V_3}(\omega^+_{V_1}) \doteq \lim_{t\to\infty}\,\mathrm{vH}\text{-}\lim_{h\to 1}\frac{1}{t}\frac{1}{I(h)}\int_0^t \omega_h^{\beta,V_1}\circ\alpha_s\left(\beta\Phi_s\right)ds, \qquad \Phi_s=-\mathrm{i}\left[\alpha_{-s}K_1^h,K_3^h\right], \tag{4.4.33}$$

where $I(h)$ is given in (4.3.24) and where we used the reformulation of $\mathrm{Ep}(\omega^{\beta,V_1}\circ\alpha_t)$ given in Proposition 4.4.2.

From Proposition 4.2.1, if $V_1=V_3=V$, we obtain that the entropy production per unit volume $e_V(\omega_V^+)$ is positive:

$$\begin{aligned}
\mathrm{ep}_V(\omega_V^+) &= \lim_{t\to\infty}\,\mathrm{vH}\text{-}\lim_{h\to 1}\frac{1}{t}\frac{1}{I(h)}\int_0^t \omega_h^{\beta,V}\circ\alpha_s\left(\beta\Phi_s\right)ds = \lim_{t\to\infty}\,\mathrm{vH}\text{-}\lim_{h\to 1}\frac{1}{t}\frac{1}{I(h)}\int_0^t \mathrm{Ep}\left(\omega_h^{\beta,V}\circ\alpha_s\right)ds\\
&= \lim_{t\to\infty}\,\mathrm{vH}\text{-}\lim_{h\to 1}\frac{1}{t}\frac{1}{I(h)}\left(\mathrm{Ent}\left(\omega_h^{\beta,V}\circ\alpha_t,\omega^{\beta,V^h}\right)-\mathrm{Ent}\left(\omega_h^{\beta,V},\omega_h^{\beta,V}\right)\right)\\
&= \lim_{t\to\infty}\,\mathrm{vH}\text{-}\lim_{h\to 1}\frac{1}{t}\frac{1}{I(h)}\mathrm{Ent}\left(\omega_h^{\beta,V}\circ\alpha_t,\omega_h^{\beta,V}\right),
\end{aligned}$$

where in the last but one equality we used the fact that $\mathrm{Ent}(\omega^{\beta,V},\omega^{\beta,V})=0$. Moreover, $\mathrm{Ent}(\omega^{\beta,V}\circ\alpha_t,\omega^{\beta,V})$ and $I(h)$ are positive for every h fulfilling the hypothesis in equation (2.3.28) respectively by item (**b**) in Proposition 4.2.1 and by hypothesis, hence the right hand side of the previous

equation is also positive. However, the next proposition shows that the entropy production per unit volume is zero also in the generic case because Ent/I is bounded uniformly in h and t by Lemma 4.3.1.

Theorem 4.4.1. *Let V_1, V_3 be two interaction Lagrangians of the form* (2.3.27) *constructed with the same cutoff function h, the NESS ω^+_V obtained with the time average as described in* (3.4.17) *is thermodynamically simple, namely*

$$\mathrm{ep}_{V_3}(\omega^+_{V_1}) = 0\,.$$

In other words, the entropy production per unit volume referred to any interacting KMS state vanishes.

Proof. Starting from (4.4.33), then Proposition 4.4.1 implies that

$$\mathrm{ep}_{V_3}(\omega^+_{V_1}) = \lim_{t\to\infty} \underset{h\to 1}{\mathrm{vH\text{-}lim}} \frac{1}{t}\frac{1}{I(h)}\left(\mathrm{Ent}(\omega_h^{\beta,V_1}\circ\alpha_t, \omega_h^{\beta,V_3}) - \mathrm{Ent}(\omega_h^{\beta,V_1}, \omega_h^{\beta,V_3})\right),$$

hence, usin (4.2.9), we obtain

$$\mathrm{ep}_{V_3}(\omega^+_{V_1}) = \lim_{t\to\infty} \underset{h\to 1}{\mathrm{vH\text{-}lim}} \frac{1}{t}\frac{1}{I(h)}\left(\omega_h^{\beta,V_1}(\alpha_t(\beta K_3^h)) - \omega^{\beta,V_1^h}(\beta K_3^h)\right).$$

In order to study the limits $h\to 1$ and $t\to\infty$ we notice that

$$\omega^{\beta,V_1}\left(\alpha_t\left(\beta K_3\right)\right) = \int_{\mathbb{R}^3} h(\mathbf{x}_0)\,\omega^{\beta,V_1}\left(\alpha_t\left(\beta H_3(\mathbf{x}_0)\right)\right) d^3\mathbf{x}_0$$

Furthermore, as discussed in the Remark 4.3.1 and in Lemma 4.3.1, the result of

$$L = \underset{h\to 1}{\mathrm{vH\text{-}lim}} \frac{1}{I(h)}\omega^{\beta,V_1}(\alpha_t(\beta K_3)),$$

is equal to

$$l(t,\mathbf{x}_0) = \underset{h\to 1}{\mathrm{vH\text{-}lim}}\,\omega^{\beta,V_1}(\alpha_t(\beta H_3(\mathbf{x}_0)))\,.$$

Furthermore, $l(t,\mathbf{x}_0)$ is bounded by some constant C uniformly in t and it is constant in $\mathbf{x}_0$, so it holds that

$$|L| = |l| \le C.$$

This implies that

$$\left|e_{V_3}(\omega^+_{V_1})\right| \le \frac{C}{t},$$

for every $t>0$ hence, $\mathrm{ep}_{V_3}(\omega^+_{V_1})$ vanishes. □

Theorem 4.4.1 and Proposition 4.4.1 characterise the non-equilibrium steady state ω^+ as a thermodynamically trivial state, namely as a state which possesses vanishing entropy production per unit volume. Physically, this means that ω^+ is thermodynamically close to ω^β, that is ω^+ is not far from being an equilibrium state. In the language of Statistical Mechanics, this would mean that the NESS is in the normal folium of the free KMS ω^β.

CONCLUSIONS AND OUTLOOK

The main subject of the present thesis is perturbative Quantum Field Theory at finite temperature, which is studied following the way tracked by Fredenhagen and Lindner in [FL14, Li13], where they have defined an interacting KMS state for a massive scalar field theory on Minkowski space-time in the algebraic framework. The construction of this state and an introduction of the framework are the subject of Chapters 1 and 2.

The personal contributions are recollected in the remaining two chapters, in particular Chapter 3, which is based on [DFP18a], deals with the study of the stability and return of equilibrium of the interacting KMS state. There, we proved that if the interaction potential is of spatially-compact support, *i.e.* if the adiabatic limit is not considered, then both stability and return to equilibrium hold. On the other hand, if the adiabatic limit is taken in advance, they fail, even if an ergodic mean is considered. In the case of the stability, we obtained severe infrared divergencies which break the validity of perturbation theory, while return to equilibrium surprisingly gives a finite result. Actually, we proved that the outcome in this case is a stationary state for the free theory which does not fulfill the KMS condition, though we interpreted it as a non-equilibrium steady state according to [Ru00].

In order to better characterise this new state, in Chapter 4, following [DFP18b], we addressed the problem of the definition of relative entropy and of entropy production in the framework of pAQFT. Generalising the works of Araki [Ar76, Ar77] and of Jakšić and Pillet [JP01, JP02, JP02b] we manage to give satisfactory definitions. Unfortunately, these definitions are limited to the states at our disposal only, and they do not provide a way for computing entropies for general states. On the other hand, concerning the positive aspects, we proved that they still hold if the adiabatic limit is taken if densitised quantities are considered, as usual in QFT. Furthermore, they allowed us to compute the entropy production of the NESS, showing that it is zero: This state is then a thermodynamically trivial one, in the sense that it is actually very close to the equilibrium one.

The results achieved in this thesis constitutes some significant steps towards a better understanding of the non-equilibrium features of interacting QFT. Of course they are far from being fully satisfactory and a lot of additional work is required. First of all we point out the very in-

teresting work by Hack and Verch [HV18], where another NESS is constructed and where its stability and entropic properties are studied, taking our work as a starting point.

Something which in our humble opinion will require a deeper study is the NESS defined in [DFP18a]: As we proved, actually this state has vanishing entropy production, but at the same time it does not satisfy the KMS condition with respect to the free dynamics, under whose action it is stationary. This situation is a bit puzzling after all. In the von Neumann algebras framework, the vanishing of entropy production would signify that the NESS is in the normal folium of the free KMS, but in our case such is not available.

Possible interpretation would be that this state is in fact a KMS, but with respect to a different time-evolution, which however is unknown. It must be said that it may also be pretty complicated to find it, due to the lack of an explicit expression for the state ω^+.

Another possibility would be that this state is actually a convex combination of equilibrium states, in the spirit of what is done by Buchholz, Ojima and Roos [BOR02]. This is suggested by the fact that the NESS seems to satisfy the passivity condition, but not the ancillary requirement which has to be fulfilled for the passivity to imply the state to be a KMS or a ground, see [FV03, PW78, SV00]. Actually, we stress that those are just speculation under current investigation, supported by some preliminary computations.

A different possible way to characterise this state may come by taking into consideration the results coming from the literature which deals with equilibration, thermalisation and generalised Gibbs ensambles, see for instance [Doy17, GE16] and references therein. The idea is that the state ω^+ would not be a proper NESS because it is constructed perturbatively, *i.e.* the large-time limit is taken order by order in the perturbative expansion. Actually this procedure, though being the only correct one in the realm of formal power series, might prevent us to have access to the true non-equilibrium state of the theory. Thus, what we are dealing with may be just an "approximation" of it. Those objects are known in the literature with the name of *pre-relaxed states* and have already been studied in some statistical mechanical system [GE16].

By the way, the study of the NESS is not the only interesting thing that may be done within this algebraic approach to thermal field theory. First of all it would be very interesting to establish a direct connection between the framework deleted in this thesis and the one present in the usual physical literature, see for instance [LW87, LeB00]. The methods used in the physical literature are based on Schwinger-Keldysh contour integration and on expansions in Matsubara frequencies. Unfortunately, those methods are somehow not fully satisfactory since they lead to infrared divergencies. On the other hand, the Fredenhagen and Lindner techniques are absolutely free of them, hence a direct comparison between the two methods would lead also to an improvement of the physical picture and it will constitutes another evidence of the validity and of the advantages of the algebraic approach.

Another novelty present in this thesis is the definition of relative entropy (density) and of (density of) entropy production in the framework of perturbative QFT which, despite restricted

to a limited case, to our knowledge has never appeared in the literature before. The understanding of entropy in QFT (mainly concerning the free case) has emerged as a hot topic in the last years research and it has been studied under many points of view, from entanglement entropy to entropy in CFT's passing through black hole entropy. Just to quote some, we recall [HS17, KL05, LX18, Wi18]. It would be nice trying to understand possible relations between our work and the present literature, in particular with [HS17], where the entanglement entropy for a free scalar field is defined, hence it would be nice to understand if how this ideas transfer in the interacting case and how they are related to the one introduced in [DFP18b].

Finally, we would like to mention one last development. It is known from physicists by long time that the $\lambda\phi^4$ scalar field theory on (4-dimensional) Minkowski presents a critical behaviour, see [PS95, Zi02], whose study is based on renormalisation group techniques and that relies on the computation of expectation values in the vacuum state. In our humble opinion, it would be interesting to try to explore those features also for expectation values computed in our new thermal equilibrium state. Actually, this is for sure a very ambitious task, but as a starting point one can try to look at how the renormalisation group influence the interacting KMS state. In particular, the state exhibits an explicit dependance on the coupling constant due to the presence of the cocycle U in its definition, so we expect the expectation values to be influenced by renormalisation in a non-trivial way.

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