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Thermal equilibrium states in perturbative Algebraic Quantum Field Theory in relation to Thermal Field Theory

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Abstract

In the first part, we analyse the properties of an interacting, massive scalar field in an equilibrium state over Minkowski spacetime. We compare the known real- and imaginary-time formalisms of Thermal Field Theory with the recent construction by Fredenhagen and Lindner of a KMS state for perturbative interacting theories in the context of perturbative Algebraic Quantum Field Theory, in the adiabatic limit. In particular, we show that the construction of Fredenhagen and Lindner reduces to the real-time formalism only if the cocycle which intertwines between the free and interacting dynamics can be neglected. Furthermore, the Fredenhagen and Lindner construction reduces to the ordinary imaginary-time formalism if one considers the expectation value of translation invariant observables. We thus conclude that a complete description of thermal equilibrium for interacting scalar fields is generally obtained only by means of the state constructed by Fredenhagen and Lindner, which combines both formalisms of Thermal Field Theory. We also discuss the properties of the expansion of the Fredenhagen and Lindner construction in terms of Feynman diagrams in the adiabatic limit. We finally provide examples showing that the real- and the imaginary-time formalisms fail to describe thermal equilibrium already at first or second order in perturbation theory. The results presented in this part are summarized in [BDP19].

In the second part, we discuss the so-called secular effects, characterized by the appearance of polynomial divergences in the large time limit of truncated perturbative expansions of expectation values in Quantum Field Theory. We show that, although such effect is an artifact of perturbation theory, and thus may not be obtained via exactly solving the dynamical equation (whenever this is possible), they do not represent the breakdown of perturbation theory itself. Instead, we show that the polynomial divergences follow from a bad choice of state, and we present examples of states which produce expectation values whose perturbative expansion does not present secular effects. In particular, we point that it is possible to obtain non time-divergent perturbative expressions from thermal equilibrium states for the interacting theory. This last part is based on a research project which, by the time this thesis was delivered, had not been concluded yet.

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Introduction

Quantum field theory (QFT) corresponds to a general, abstract terminology for the physical description of force fields, in accordance with the laws of relativity and quantum physics. Based on the results of different experiments, it is possible to say that many theories, all considered within the broad terminology of *Quantum Field Theories*, provide very accurate descriptions of certain physical systems. For instance, the experimental value of the electron magnetic momentum has a relative uncertainty of the order of 3×10^{-10},[1] and agrees with theoretical predictions up to order 10^{-9}, (cf. [Fre]) which illustrates the accuracy obtained in the context of quantum electrodynamics. Moreover, results obtained from the many experiments in the Large Hadron Collider (LHC) have been abble to confimr theoretical previsions such as the existence of quark-gluon plasma, besides the validity of the standard model of particles physics. Classical references for QFT in the physics literature are [IZ80; BS80; PS95].

From the theoretical perspective, QFT involves different and complex theories, supported in different areas of mathematics. From its early days after the pubblication of Dirac's paper *"The Quantum Theory of the Emission and Absorption of Radiation"* in 1927[2]) to the present, it continues to motivate the analysis of PDEs, different aspects of geometry, commutative and non-commutative algebra, harmonic analysis, logic, category theory and number theory, for instance.

Following the ideas presented in [BC97; Em0], the general description of a physical system may be structured upon *states* and *observables*, which may be described by different mathematical objects depending on the context. For instance, an observable may be given by a self-adjoint operator over some Hilbert space in the realm of Quantum Mechanics, or it may be a functional over the space of smooth sections of a vector bundle, as we shall see later in this thesis. In general, however, one should heuristically think of observables as the the elements of the physical system which are measured, and the states as the configurations of the experimental apparatus at the moment prior to the measurement. A clear and elegant description of this basic description of physical systems in the context of QFT may be found also in [Ara99]. An abstract and general characterization of quantum field theories, directly based upon observables and states, was formulated along these lines by R. Haag and D. Kastler in [HK64] in the early 1960s.

[1] According to the 2018 Committee on Data for Science and Technology (CODATA) publication. See the USA National Institute of Standards and Technology Reference on Constants, Units and Uncertainty, https://physics.nist.gov/cgi-bin/cuu/Value?muem.

[2] P.A.M. Dirac, Proc. Royal Soc. Lond. A 114, pp. 243–265, (1927).

Given the fact that the set of observables of a quantum field theory may be endowed with an algebra structure, their work explores a net of such $*$-algebras, labeled by relatively compact regions of spacetime. The authors recollected the basic physical assumptions for a QFT in a list of axioms for the net of algebras of obserables, which result in an algebraic description of quantum field theories. Though in [HK64] the authors address theories on the flat Minkowski spacetime, in [Dim80] Dimock showed how this formalism may be extended to quantum field theories over more generic spacetimes. We may consider the Haag-Kastler formalism via the following set of axioms for the observables of a physical QFT.

Although the concepts below will be further discussed in chapter I, for now one may think of a spacetime as a particular four dimensional smooth manifold, endowed with a Lorentzian metric, a non positive-definite metric with signature $(+,-,-,-)$. A Cauchy surface would then be thought in terms of a hypersurface $\{t\} \times \mathbb{R}^3$ for some fixed $t \in \mathbb{R}$, and a spacetime which may be differentially foliated by Cauchy surfaces is what we shall call a globally hyperbolic spacetime. All the precise definitions may be found in the first section of chapter I. In this context, the Haag-Kastler axioms may be summarized as follows.

I. Let M be a globally hyperbolic spacetime[3]. To each relatively compact region $O \subset M$, it is associated a unital $*$-algebra $\mathscr{A}(O)$, interpreted as the local algebra of observables of O.

II. **(Isotony)** If $O_1 \subset O_2 \subset M$, then $\mathscr{A}(O_1) \subset \mathscr{A}(O_2)$.

III. Given a net of local algebras $\big(\mathscr{A}(O_n)\big)_{n\in I}$ with $\mathscr{A}(O_n) \subset \mathscr{A}(O_{n+1})$ and I an ordered indexing set such that $\bigcup_{n\in I} O_n = M$, then we define the universal algebra of observables via the indutive limit

$$\mathscr{A}(M) := \lim_{n\to\infty} \mathscr{A}(O_n).$$

IV. **(Causality)** Let $O_1, O_2 \subset M$ be two causally separated, relatively compact regions of M.[4] Then the respective algebras commute, i.e.

$$\big[\mathscr{A}(O_1), \mathscr{A}(O_2)\big] = \{0\}.$$

V. **(Time-slice condition)** If $O_1 \subset O_2$ have a common Cauchy surface[5], then $\mathscr{A}(O_1)$ and $\mathscr{A}(O_2)$ are isomorphic.

It is evident, however, that the above axioms address only observables and not states, which are given by suitable (linear, positive and normalized) functionals over the $*$-algebra $\mathscr{A}(M)$. In this manner, the combination of observables and states produce

[3] Cf. definitions 2 and 3

[4] Cf. subsection I.1.1.

[5] See subsection I.1.1.

numbers, interpreted as expectation values of observables, or mean values of repeated measurements of the the same observable in a given state. We shall discuss states in chapter I, section I.3. The fact that the above list of axioms considers only observables turns out to be a great advantage of AQFT. Since states are to be considered separately from the basic axioms for quantum theories, the algebra itself is independent of states. This is not the case, for instance, in the Wightman description of QFT described in [SW00].

The abstract formulation of a quantum field theory based on the above axioms has been called **Algebraic QFT (AQFT)**. In this thesis, the $*$-algebra of observables will be considered in the sense of formal power series in the quantum parameter $\hbar$, as will be described in the first chapter. We anticipate that the time-slice condition, which may be seen as a week form of determinism by initial conditions, plays an important role in the work by Fredenhagen and Lindner, [FL14; Lin13], on which we shall base our analysis.

The usual description of quantum field theories is developed considering systems at very low temperatures, with the either implicit or explicit assumption of vanishing temperature $T = 0\,K$. Though this may provide a good approximation for some physical systems, that may not be the case in different contexts, and one is then forced to search for a description of quantum systems at finite temperature. Systems out of thermal equilibrium are considerably more complex and beyond the scope of this thesis. Hence, the main problem consists of the characterization of thermal equilibrium in quantum field theory. This analysis may be physically motivated also by the high temperature thermal equilibrium achieved in the early universe during some time, for instance, in addition to other examples of physical systems provided below. Such characterization is usually implemented by means of a proper construction of thermal equilibrium states which depends on the temperature of the system. In other words, the analysis of thermal systems in equilibrium concerns the construction of suitable states, which, according to the work of Haag, Hugenholtz and Winnink [HHW67], are determined by the inverse temperature $\beta > 0$ of the system and which are characterized by the so-called KMS condition (after Kubo, Martin and Schwinger). This is motivated as follows. In the context of quantum statistical mechanics, an ideal gas contained in a finite volume, once it achieves thermal equilibrium with the walls of its container acting as a thermal reservoir, is described in terms of a density matrix, given as the exponential of the Hamiltonian operator times the inverse temperature $0 < \beta < +\infty$. This permits to construct states, the so-called Gibbs states, which are completely characterized by the analytic continuation of expectation values into a strip of the complex plane. In general, states fulfilling analogous analytic conditions are called β-KMS states. This will be properly explained in definitions 34 and 35, chapter II. Hence, when considering thermal equilibrium states in other, more general situations, according to [HHW67] we shall adopt the KMS condition as a characterization of thermal equilibrium states.

For the case of free scalar theories, the construction of a KMS state is then straightforward, as we shall see in section II.1. If one is interested in interacting theories, however, the situation is considerably more complex. Considering the quantum scalar field ϕ as an algebraic-valued distribution over Minkowski spacetime $\mathbb{M}$ for what concerns this introduction, we examine a system described by the Lagrangian functional

$$\mathcal{L}(\phi) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \mathcal{L}_I(\phi), \tag{1}$$

where $m > 0$ is interpreted as a mass constant, and $\mathcal{L}_I(\phi)$ is some polynomial in the field ϕ, which is interpreted as a field self-interaction term. This contribution to the total Lagrangian will be discussed in section I.4, where interacting fileds will be constructed with perturbation methods over the free theory. Since the KMS condition concerns the group of automorhisms which implement dynamics over the algebra of observables, as the introduction of an interaction term $\mathcal{L}_I(\phi)$ perturbs this dynamics, the KMS state for the free state is not expected to correspond to a KMS state of the interacting theory. In the physical literature, the problem of describing thermal equilibrium states for interacting theories originated what is often called *Thermal Field Theory* (TFT). We briefly recall some of its basic aspects, and refer to the classical references [LW87; Bel00] for further details.

Thermal Field Theory is also seen as a combination of quantum field theory and aspects proper to statistical mechanics, and it has been founded more than fifty years ago with the pioneering works of Matsubara [Mat55a], Keldysh [Kel65] and Schwinger [Sch61] (see also [NS84], [Hov86]). At that time, one of the main physical motivations was the analysis of phase transitions of hadronic matter predicted to occur at high temperature in quantum cromodynamics, (cf. [McL84]), the quantum theory describing the strong interaction between quarks and gluons. The formalism of thermal field theory has also been applied, for instance, to the analysis of baryogenesis in the early-universe (see e.g. [Kaj85; CH88; PSW04a; PSW04b]) and to derive transport equations for a system of quantum fields, such as in the study of the dynamics of a quark-gluon plasma (for a more recent application, see [CM05]).

Although in particular situations the differential equation describing the dynamical behaviour of expectation values, which descends from the Lagrangian functional (1), may be solved exactly, this in general is not the case in theoretical and mathematical physics. In this thesis, an exactly solvable interacting system will be discussed in light of the *Principle of Perturbative Agreement*, to be discussed at the end of I.4. In the absence of an exact solution to the dynamical equation, interactions are treated by means of perturbation theory. In this way, considering the polynomial interaction term $\mathcal{L}_I(\phi) = \lambda\phi^n$, $\lambda \in \mathbb{C}$ is treated as a perturbation parameter. In this approach to interacting quantum field theories, the interacting observables are then represented within the algebras of the free theory, introduced in the Haag-Kastler axioms, as a subalgebra of formal power series in λ. This representation concerns only the algebraic level, and thus it does not consider the effect the interaction term $\mathcal{L}_I$ may have upon states. For perturbative computations, it is particularly convenient to have expectation values of the interacting theory written in terms of some state of the free theory. This is possible at zero temperature, and for the vacuum state one obtains the so-called Gell'Mann-Low formula for the interacting state Green function, which contains the dynamical information for expectation values. In more generic situation, a similar expression is not possible, and one has to consider the modifications upon the state produced by the interaction. In TFT, however, we may find a representation of thermal Green function in terms of free states, where the effect of $\mathcal{L}_I$ upon states is transferred to the product of fields, which are now to be ordered along a certain contour in the complex plane. The generic description is the following.

Consider a free quantum field theory, described by the Lagrangian functional

$$\mathcal{L}_0(\phi) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2. \tag{2}$$

Suppose this system had been initially prepared in a free thermal equilibrium state at some inverse temperature $0 < \beta < +\infty$, and as of a certain time t_i, the perturbative interaction was switched on, so that the system is then described by Lagrangian (1). With both the state and the dynamics perturbed, the system has then been left to evolve. One is now interested in expectation values of observables supported in the future of t_i, and, in particular, the n-point Green functions for points located in this region are formally given by

$$G(x_1,\ldots,x_n) = \frac{1}{Z(0)}\frac{\delta^n}{\delta j(x_1)\ldots\delta j(x_n)}\left\langle T_{\mathscr{C}} \exp i\int_{\mathscr{C}} dx_0 \int_{\mathbb{R}^3} d\mathbf{x}\,\mathcal{L}_I(x) + j(x)\phi(x)\right\rangle\bigg|_{j=0}. \tag{3}$$

Here the brackets correspond to averaging with respect to the initial free equilibrium state, and j is a complex-valued source. The time ordering $T_{\mathscr{C}}$ and the integral of the interaction Lagrangian $\mathcal{L}_I$ over the time coordinate x_0 is performed along a contour $\mathscr{C}$ in the complex plane. The standard contour in TFT is known as Keldish-Schwinger contour (see fig. II.1, page 86), which usually has three pieces. It starts at t_i, goes on to some later $t_f > t_i$, chosen in such a way that it is also later than the time coordinates of every point x_i. The second branch then goes back from t_f to t_i, and the final one goes from t_i to $t_i - i\beta$. The first two lines take into account the perturbation of the fields in the interaction picture, while the last one, on the other hand, is necessary in order to modify the free into an interacting equilibrium state. As we shall consider only the Keldysh-Schwinger contour, we shall write $\mathscr{C} = C \cup C_v$, where C represents the two real lines, and C_v the vertical, imaginary one. In resume, according to the discussion presented throughout chapter II and III, the contour C formally corresponds to the effect of the interaction over fields, while C_v accounts for the modification upon the state.

In some situation, when one is interested in computing expectation values of observables which do not depend on time, it is possible to discard the real contour C and consider an integration from t_i directly to $t_i - i\beta$. This analysis is named **imaginary-time**, or **Matsubara formalism**. The very same analysis holds if one is interested in computing correlation functions at imaginary times. We notice the n-point functions with all the time arguments along this vertical complex contour are correlation functions of an Euclidean field theory. Arguably, one of the greatest advantages of this formalism lies on the fact that the set of Feynman rules, which provide a prescription for the calculation of expectation values, obtained with such analysis is quite similar to those of a field theory in a vacuum state. However, in order to obtain time dependent

Green functions in Minkowski spacetime, it is necessary to perform an extension of the propagators obtained in the Matsubara formalism for real times, a task which is usually non trivial. We refer to [OS75a; OS75b] for details about the analytic continuation of correlation functions. An alternative method is possible if the imaginary contribution to (3) factorizes from the correlation functions instead. If this is the case, the computational scheme obtained is known as **real-time formalism**. As a result, in this case equation (3) involves the free state only, and one ends up with a thermal equivalent to Gell'Mann-Low formula. That is, if the C_v-contribution to equation (3) does factorize, it is possible to obtain expectation values of the interacting theory without considering any modification on the initial state.

For a generic contour other than the immaginary Matsubara contour C_v, however, it is not easy to obtain a set of Feynman rules for the perturbative representation of (3). Furthermore, if the interaction is switched on instantaneously, divergences in certain correlation functions are expected. This problem could be overcome using an adiabatic or smooth switching on function. Unfortunately, in this way the interaction Hamiltonian is not local in time, hence the integration over the imaginary part of the path turns out to be problematic. Moreover, in the limit where $t_i \to -\infty$ the contribution of relative partition function, (i.e. the integration of the last path from t_i to $t_i - i\beta$) factorizes only in very special cases, see [DFP18] for further details.

Recently, Fredenhagen and Lindner presented in [FL14; Lin13] an alternative construction of a thermal equilibrium state in perturbative AQFT, which will serve as starting point ans basis for our discussion. Their analysis follows the work of Araki in the context of quantum statistichal mechanics [Ara73]. The state is constructed after the perturbative formulation of a cocycle $U(t)$, which relates the one-parameter group of automorphisms implementing dynamics in the free theory, with the analogous dynamics of the interacting theory. The result is a thermal equilibrium state that may be written in terms of a thermal equilibrium state of the free theory at the same inverse temperature β, but which also considers the effect of interaction. In fact, in their work the authors show that it is necessary to modify the initial state, in order to obtain a thermal equilibrium state for the perturbative theory.

In the first chapter we shall present the basic aspects of quantum field theory upon which this thesis is based. We shall start by setting the basic concepts and notation for the background geometry. Since AQFT provides a suitable description of quantum systems over a curved, globally hyperbolic background, we shall first introduce its basic aspects in a more general form and later on restrict to Minkowski spacetime. We shall then properly address the algebraic approach to free field theories, in order to consider perturbative models later on. The construction of the algebras of observables will be performed in steps. That is, we shall first consider the algebra of observables of a classical theory, and address its quantization via the construction of a non commutative product which implements the so-called *canonical commutation relations (CCR)* of quantum physics. As will be discussed then, the result of this construction, at this stage, will not be enough to contain some physically interesting observables, and in fact already the squared field is not present within this first algebra of quantum observables. In order to include objects which are more singular than the linear observables obtained in the previous step, we have to deform the quantum product, and then to extend the algebra, in a state-independent way, in order to obtain the final algebra of the free theory $\mathscr{A}^0$. Then, considering perturbative interacting theories, an important topic depicted in the first chapter will be the representation of interacting observables into the free algebra, as mentioned previously, by means of the Bogolubov map $\mathcal{R}_V$, which is constructed as the (functional) derivative of a formal scattering matrix. This requires the construction of a time-ordered product of observables, which will be briefly discussed in light of Epstein and Glaser analysis [EG73]. This formalism permits to obtain the algebra of observables of the interacting theory as a subalgebra $\mathscr{A}^I \subset \mathscr{A}^0$. All this construction, of a broad algebra of observables for the interacting quantum theory, will be performed for observables supported in some relatively compact region of Minkowski spacetime, and considering a compactly suported interaction term. In order to obtain a universal algebra $\mathscr{A}(\mathbb{M})$, as discussed in point III of the above Haag-Kastler axioms, we shall first extend the support of functionals, considering the interaction term supported within a neighbourhood of a Cauchy surface. This will be made possible thanks to two observations. First, we shall notice that such an extension of the interaction term is possible as an inductive limit in its support. Second, due to the validity of time-slice property for perturbative theories, cf. proposition 16, chapter I, as proved in [CF09], we shall observe that restricting the interaction term to a neighbourhood of the Cauchy surface is enough to describe the whole algebra, up to terms which vanish on-shell. We shall conclude the first chapter with a brief discussion about graphic representations for the product of observables.

At this point, since a state has been defined as a suitable functional $\omega : \mathscr{A}^0 \to \mathbb{C}$ over the algebra of the free theory, due to the representation of interacting observables into $\mathscr{A}^0$ in the sense of formal power series, it will be possible to consider an interacting state from the restriction of ω to the subalgebra $\mathscr{A}^I \subset \mathscr{A}^0$. The definition of an interacting state as $\omega^I := \omega \circ \mathcal{R}_V$ in terms of a free state ω, where $\mathcal{R}_V$ is the Bogolubov map mentioned in the previous paragraph, may not be suitable for the same physical interpretations as ω. The most important example of this fact in this thesis will be precisely a thermal equilibrium state, to be properly defined in chapter II. That is, if ω is a thermal equilibrium state for a free theory, extending the same interpretation to $\omega \circ \mathcal{R}_V$ as a thermal equilibrium state for the interacting theory results in an incomplete analysis, as will be shown in chapter III, even though the object $\omega \circ \mathcal{R}_V$ may be a well defined state over $\mathscr{A}^I$. This incompleteness manifest the necessity of considering the effect of interaction upon states.

In [FL14; Lin13], the state obtained by the authors is written in terms of a KMS state of the free theory at the same inverse temperature, ω^β, but it also involves the change in the dynamics produced by the interaction upon states. More precisely, with $U(t)$ a cocycle intertwining the interacting dynamics $\alpha_t^{\mathcal{L}_I}$ and the one-parameter group of $*$-automorphisms $(\alpha_t)_{t\in\mathbb{R}}$ as

$$\alpha_t^V \mathcal{R}_V A = U(t)\alpha_t \mathcal{R}_V(A) U(t)^{-1} \tag{4}$$

for a suitable observables A, Fredenhagen and Lindner showed that the function

$$\mathbb{R} \ni t \mapsto \frac{\omega^\beta\big(\mathcal{R}_V A U(t)\big)}{\omega^\beta\big(U(t)\big)},$$

where ω^β is a KMS state of the free theory, has an analytic extension onto the strip $\{z \in \mathbb{C} : \Im z \in (0,\beta)\}$ and is continuous along its borders. In addition, they showed that, cf. equation (II.23),

$$\omega^{\beta,V}(A) := \frac{\omega^\beta\big(\mathcal{R}_V A U(i\beta)\big)}{\omega^\beta\big(U(i\beta)\big)} \tag{5}$$

satisfies the KMS condition with respect to the interacting dynamics, and hence it corresponds to a thermal equilibrium state of the interacting theory. We then see that the thermal equilibrium state is not of the form $\omega \circ \mathcal{R}_V$, since the cocycle U presents an important contribution. Throughout this thesis we shall present arguments attesting that ignoring the cocycle contribution produces a different state, which may not be regarded as describing an interacting system in thermal equilibrium.

Starting from the Fredenhagen and Lindnder's analysis, in this thesis we shall establish a formal relation between the FL-state and the Keldish-Schwinger formalism, respectively summarized in equations (5) and (3). In fact, a relation between TFT and the analysis by Fredenhagen and Lindner may be established from noticing that the real-time formalism is formally equivalent to neglecting the term $U(i\beta)$ in $\omega^{\beta,V}$. By justifying this claim, we shall be able to affirm the inequivalence between the formalisms, and to discuss in which situations the real-time formalism produces a precise description of thermal equilibrium. In this thesis we are interested in the modifications produced by interaction terms upon thermal equilibrium states. We shall discuss the relation between a thermal equilibrium state for the perturbative theory, constructed by Fredenhagen and Lindner [FL14; Lin13], and the usual description of thermal equilibrium systems in the physics literature in chapter II.

In the third chapter we establish the relation between the two approaches to thermal theories. In particular, we shall show that the Fredenhagen and Lindner state reduces to either the Matsubara or to the real-time formalism in particular cases, but that a complete and general description of thermal systems is obtained only via the state $\omega^{\beta,V}$, when the two are altogether considered. To the best of our knowledge, this was the first time the two formalisms where combined to provide a complete characterization of thermal equilibrium. We shall also present a graphic representation scheme for the perturbation series of expectation values $\omega^{\beta,V} \circ \mathcal{R}_V(A)$. We shall conclude the chapter presenting two concrete computations showing the importance of considering the cocycle U, the first considering $\mathcal{L}_I \simeq \lambda\phi^2$, a situation which will permit to discuss also the case with $\mathcal{L}_I \simeq \lambda\phi^4$, and the second with $\mathcal{L}_I \simeq \lambda\phi^3$ interaction. Therefore, in the last section of the third chapter we shall present an explicit calculation for the difference between the estimations for the self-energy in the real-time and in the Fredenhagen-Lindner formalism. We shall see differences in the first order terms of the perturbation series for the quadratic interaction, but we shall have to consider second order terms in the cubic theory in order to see the effect of $U(i\beta)$. Considering the $\lambda\phi^3$-theory, we shall conclude that this difference in the self-energy estimated with the state $\omega^{\beta,V}$ and with the real-time, it depends on the time cutoff function of the interaction term, introduced in (I.37), via the Fourier transform of its derivative. This result allows us to conclude that, in this case, the real-time formalism presents a sensibility with respect to how the interaction is turned on, which is absent from the Fredenhagen-Lindner formalism. Therefore, the more abruptly the interaction is turned on, the larger will be the contribution this difference between formalisms.

In addition, we shall see in (III.30) that this difference between $\omega^{\beta,V}$ and real-time estimations involves a term which depends on the renormalization constant c, but not on the time cutoff of the interaction term. Since the renormalization constant has to be state independent, due to the principle of general covariance described in [HW01; BFV03], it may not depend on the inverse temperature β. It is possible to consider $c = 0$ in particular, but, in the limit of zero temperature $\beta \to \infty$, the whole difference between formalisms vanishes either way. We highlight the fact that this regards only the case of a $\lambda\phi^3$-interaction, and that the situation is considerably different in the case of a $\lambda\phi^2$ interaction, which produces inequivalent results if we consider the FL state or the real time formalism. As we shall see then, this result permits to obtain the same conclusion for the $\lambda\phi^4$ theory.

The results presented in chapter III are also described in the reference [BDP19], on which the first part of this thesis is based.

Chapter IV addresses a different problem, in the same lines. In the physics literature such as [AAP14; AP15; AGP16], secular effects are described as the presence of unbounded terms with respect to time in the perturbative expansion of expectation values of QFT. Though the perturbation series for interacting quantum field theories hardly ever converges, it is possible to obtain accurate results from its truncation at a certain order in the perturbation parameter, as may be seen e.g. in [PS95]. The presence of terms with a polynomial dependence on time in the perturbative theory, whose degree grows with the perturbation order, however, changes the situation considerably. In the truncated series, for whatever $\lambda \ll 1$ fixed, if after a long enough time the nth term, in presenting a factor t^n, becomes comparable or lager than each term of lower order, then the basic assumption justifying the truncation of the perturbative series in a first place is itself violated. Such secular effects have been said in the mentioned references to be a consequence of the break down of perturbation theory. However, considering the analysis by Fredenhagen and Lindner, we do know that perturbation theory may produce time-translation invarian results. As we shall see in chapter IV, this divergences are expected if we consider a perturbation theory upon certain states out of thermal equilibrium, but are not present in certain exact theories. Furthermore, we shall also explicitly describe how perturbation theory for a thermal equilibrium state must not present such effect, considering also the fact that thermal equilibrium states are translation invariant. In order to do so, we shall consider an interaction term similar to the one the considered in [AAP14] (see also comments in [AP15]). We shall finally conclude that secular effects follow from an imprecise choice of state, instead of being an intrinsic result to perturbative representations of expectation values.

This last chapter is based on a research project which, by the time this thesis was written, had not been concluded yet. We shall then present the first results obtained, but only indicate a dynamical stability result for certain states.

Notation and conventions

Though many of the following objects will be properly defined throughout this thesis, we have decided to add this section for the reader's convenience.

- Mathematical definitions will be denoted with the symbols ":=" or "=:". The symmetric symbol "≡" will be used both to denote uniform equality (i.e., $f|_{x>0} \equiv 1$ meaning the same as $f(x) = 1\ \forall x > 0$) and to present an alternative notation to an already defined object.

- We shall employ the notations

$$\mathbb{N} = \{1, 2, 3, \dots\}, \quad \mathbb{N}_0 = \mathbb{N} \cup \{0\}.$$

  In addition, if A is a set, its cardinality will be denoted as $\#A$.

- For any $n \in \mathbb{N}$, a multindex is a n-tuple $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$. Its absolute value is defined as the sum of its components, $|\alpha| := \alpha_1 + \cdots + \alpha_n$. If α, β are two multindices, then we denote $\alpha \leq \beta$ if and only if $\alpha_i \leq \beta_i$ for all $i = 1, \dots, n$. For $x \in \mathbb{R}^n$, $x^\alpha := x_1^{\alpha_1} \times \cdots \times \alpha_n^{\alpha_n}$. In addition, higher order partial derivatives are denoted with multindices as $\partial^\alpha := \partial_1^{\alpha_1} \dots \partial_n^{\alpha_n}$, where $\partial_i^{\alpha_i} \equiv \partial^{\alpha_i}/\partial x_i^{\alpha_i}$.

- Minkowski spacetime will be denoted as $\mathbb{M}$, and we shall adopt the convention $(+, -, -, -)$ for its metric's signature.

- The space of smooth, complex-valued functions over $\mathbb{M}$ will be denoted $\mathcal{E}(\mathbb{M})$, where by smooth we shall always mean of class C^∞. The subspace of real-valued smooth functions on $\mathbb{M}$ will be denoted as $\mathcal{C}^\infty(\mathbb{M}) \subset \mathcal{E}(\mathbb{M})$. In addition, the subspace of compactly supported functions in $\mathcal{E}(\mathbb{M})$ will be denoted $\mathscr{D}(\mathbb{M}) \subset \mathcal{E}(\mathbb{M})$, whereas compactly supported functions in $\mathcal{C}^\infty(\mathbb{M})$ will be denoted as $\mathcal{C}_0^\infty(\mathbb{M}) \subset \mathcal{C}^\infty(\mathbb{M})$. We shall also eventually substitute the symbol $\mathbb{M}$ by $\mathbb{R}^4$, when considering only the topological space structure over the set $\mathbb{R}^4$.

- We shall adopt for the Fourier transform of a function on $\mathbb{R}^n$ the convention

$$\big(\mathcal{F}f\big)(p) \equiv \hat{f}(p) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} dx\, f(x) e^{-ipx}, \quad \big(\mathcal{F}^{-1}f\big)(p) = \int_{\mathbb{R}^n} dx\, \hat{f}(p) e^{ipx}.$$

- The following propagators will be properly defined in chapter I, but we anticipate that the two point function of some state ω over an algebra of observables will be denoted as Δ^+. If $\omega = \omega_0$ is the vacuum state, then its two-point function (Wightman function) will be denoted as Δ_0^+. On the other hand, the two point function of a β-KMS state ω^β will be denoted as Δ_β^+. (**Remark:** one should **not** interpreted from this notation the vacuum state as the limit of a β-KMS state for $\beta \to 0$. In fact, β corresponds to an inverse temperature, and the index 0 is not related to β). However, in some points in chapter IV, there will be far too many symbols to characterize the propagators, and we shall eventually interchange the position of symbols 0 or β and $+$, for instance, in order to obtain a cleaner notation. We hope and believe the object of our interest will then be kept clear in the given context.

- We shall in general adopt a system o physical units such that

$$k_B = \hbar = c = 1.$$

In some situations, however, we shall keep the parameter $\hbar$ explicitly written, in order to keep explicitly the fact that observables in the perturbative theory are given as formal power series in $\hbar$.

I. Basic Aspects of Perturbative Algebraic Quantum Field Theory

In this chapter we shall present the basic aspects of quantum field theory upon which this thesis is based. We shall address the algebraic approach to field theories, and of our particular interest will be perturbative interacting models. As the general description of a physical theory is based on expectation values as the composition of observables and states of a system, in this chapter we intend to lay down the basic concepts which allow for a precise and physically meaningful definition of these objects and their mutual relations. We emphasize that we shall consider only real scalar field theories in this thesis, and the formalism presented in this chapter restricts to this purpose.

We shall begin by discussing aspects of the background geometry. Although in the chapters to come we shall restrict our analysis to quantum field theories on the flat Minkowski spacetime, we shall discuss such first aspects in a rather more general form than it shall be required later. This choice is justified by the fact that a great advantage of the algebraic approach lies precisely on its description of quantum systems over curved, globally hyperbolic spaces. We shall work on the so called functional formalism of quantum field theory, to be explained in section (I.3), and hence we shall present a brief discussion of functional calculus and distributions theory.

After that, we shall consider the algebra of observables for the quantum field theory, which will be constructed in steps. We first consider the algebra of observables of the free theory, which will contain only regular functionals. Next, the process of quantization of this algebra, which produces the observables of the free quantum theory, will be considered via the introduction of a non-commutative product which implements the canonical commutation relations. The construction of an algebra of observables of the quantum theory in this form will be called deformation quantization. However, we anticipate that, at that point, physically meaningful objects such as ϕ^4 will remain excluded from the algebra of observables. The last step, concerning free systems, will therefore consist of the extension of the quantum algebra of regular observables to more singular objects, via the algebraic implementation of Wick powers. This will require a discussion on states over the algebra. This last step itself is actually composed of two parts, a further deformation of the product followed by an extension of the algebra, in order to include more singular, local observables.

Finally, we shall address the perturbative approach to interacting quantum field theories, considering a local interaction term. The construction of the algebra of observables for the interacting theory will follow the formalism established in [BS80]. This is based on the implementation of the time-ordered product of local functionals within the algebra of the free theory, and, subsequently, the description of interacting observables in terms of the formal S-matrix, constructed as the time-ordered exponential of the interacting term. We shall briefly discuss the essential properties of the time-ordered product and renormalization procedure in the sense of [EG73]. In addition, given the scope of this thesis we may content ourselves with stating that such a product may be extended to globally hyperbolic spacetimes, as it has been shown in a series of publications about algebraic quantum field theory in curved spacetimes [HW01; HW02; HW05].

We conclude this chapter with a brief discussion about graphic representations for the product of observables and expectation values, which will prove to be an important and elegant way of formulating the analysis in the chapters to come.

I.1 Background geometry and dynamical equation

We start this thesis by addressing aspects of the background spacetime geometry. We have no intention to extend this part any further than the proper establishment of the notation and conventions employed in this thesis. Subsequently, we shall discuss the structure of a field over a given spacetime and the form of its equation of motion. The latter will then be considered within the algebraic structure of observables, or upon physical states.

I.1.1 Lorentzian Geometry: conventions and basic notions.

Let M be a smooth, connected, Hausdorff manifold with dimension $n < \infty$. A **Riemannian metric** on M is a positive-definite, symmetric and continuous bilinear form over the tangent bundle TM. We define a **pseudo-Riemannian metric** by excluding the requirement of positive-definiteness. A pseudo-Riemannian metric g is then said to have signature (p, q) if its associated quadractic form at each point of M has signature (p, q). In particular, if $p = +1$ then g is called a **Lorentzian metric**. A manifold M as above, endowed with a Lorentzian metric, is called a **Lorentzian manifold**. We shall denote the pair $(M, g) \equiv M$ whenever the choice of g is unambiguous. In addition, we shall always consider M **orientable**, i.e. we suppose it is endowed with a nowhere vanishing volume form. The Lorentzian manifold of our particular interest in this thesis will be the Minkowski space $\mathbb{M}$, i.e. $\mathbb{R}^4$ endowed with a metric with signature $(+, -, -, -)$.

The Lorentzian structure over M allows for a classification of separation between its points which mimics that of Minkowski space. Consider some $x \in M$ and let $v \in T_xM$ be a tangent vector. We say v is spacelike, if $g(v, v) < 0$; timelike, if $g(v, v) > 0$; lightlike, if $g(v, v) = 0$. In addition, v is called **causal** if it is either timelike or lightlike – i.e., if $g(v, v) \geq 0$.

We say a Lorentzian manifold is time-oriented if it admits a smooth, non-vanishing time-like vector field. Let $\mathbf{e}_0$ denote the time-orientation over M. We say v is **past-directed** (resp. future-directed), and denote $v \lhd 0$ if $g(\mathbf{e}_0, v) < 0$ (resp. $v \rhd 0$, $g(\mathbf{e}_0, v) > 0$). Let now $\gamma : I \subset [0,1] \to M$ a regular curve on M whose tangent vector has its character (past/future-pointing form) preserved throughout the image of γ, $\gamma(I) \equiv Im\,\gamma$. We say that γ is timelike, spacelike, lightlike or causal if so is its tangent vector, respectively. We may say, then, that two-points $x, y \in M$ are causally separated if there exist a causal curve γ connecting x to y. We may also define timelike, spacelike and lightlike separation in the analogous manner. Besides that, a regular curve $\gamma_1 : I_1 \subset [0,1] \to M$ is called extendable if there exists $\gamma_0 : I_0 \subset [0,1] \to M$ such that $Im\,\gamma_1 \subset Im\,\gamma_0$; a curve which is not extendable will be called **unextendable**.

Let now $x \in M$, and let $J(x)$ the set of points of M which are causally separated from x,

$$J(x) := \{y \in M | \exists\, \gamma : I \subset [0,1] \to M \text{ causal and s.t. } x, y \in Im\gamma\}.$$

This set has two connected components, formed by points of M connected to x by causal, past/future oriented curves. I.e., $J(x) = J_-(x) \cup J_+(x)$ with

$$\begin{aligned} J_+(x) &:= \{y \in J(x) | \exists\, \gamma :\subset [0,1] \to M \text{ causal, future oriented s.t. } x = \gamma(0),\ y = \gamma(1)\}; \\ J_-(x) &:= \{y \in J(x) | \exists\, \gamma :\subset [0,1] \to M \text{ causal, past oriented s.t. } x = \gamma(0),\ y = \gamma(1)\}; \end{aligned}$$

These are called the **causal past** and the **causal future** of x, respectively, whereas $J(x)$ is called **causal lightcone** of x. The subset $I_\pm(x) \subset J_\pm(x)$ obtained by requiring the causal curve γ in the latter definitions to be also timelike is called **chronological future/past** of x. The **chronological light-cone** of x is defined in a similar way.

For a non empty subset $O \subset M$, we define its causal future/past as the union of the causal futures/pasts of its points, i.e. $J_\pm(O) := \cup_{x \in O} J_\pm(x)$. The notions of chronological future and past for the region O are then defined in an analogous way, and so are the causal/chronological light-cones $J(O)$, $I(O)$. In addition, a hypersurface $S \subset M$ is called **acausal** if every unextendable causal curve in M crosses S at most once. Finally, let $\mathcal{D}(O)$ denote the **Cauchy development** of O: it is the set of points $x \in M$ such that every unextendable causal curve passing through x intersects O. Heuristically, the Cauchy development of a region $O \subset M$ represents the subset of M of points which are completely causally related to events in O. A related concept of particular interest of ours is the following.

Definition 1. *A connected hypersurface $\Sigma \subset M$ is called a **Cauchy surface** if every unextendable causal curve on M intersects Σ at most once and if its Cauchy development $D(\Sigma)$ coincides with M.*

That is, Σ is a Cauchy surface if every unextendable causal curve in M intersects Σ at one point and at one point only.

Let M be a Lorentzian manifold, let $x \in M$, and, for every open neighbourhood N_x of x, suppose there exists $U_x \subset N_x$ an open neighbourhood of x such that every causal curve γ on M starting and ending within U_x is entirely contained within N_x. If this condition is satisfied for all $x \in M$, M is then said to satisfy the **strong causality condition**.

Finally, we define the basic structure for the construction of physical models to come.

Definition 2. *A four-dimensional, oriented and time-oriented Lorentzian manifold M which satisfies the strong causality condition is called a* ***spacetime****.*

We shall be particularly interested in a special class of spacetimes, characterized after the following proposition.

Proposition 1. *Let M denote a oriented, time-oriented Lorentzian manifold. Then, the following three statements are equivalent:*

(i). For all $x, y \in M$, $J_+(x) \cap J_-(y)$ is compact;

(ii). there exists a Cauchy surface $\Sigma \subset M$;

(iii). M admits a differentiable foliation by Cauchy surfaces. I.e., M is isometric to $\mathbb{R} \times \Sigma_0$ with metric $\beta dt \otimes dt - h_t$, where β is a positive, smooth function and h is a Riemannian metric on Σ_0 depending smoothly on $t \in \mathbb{R}$, in such a way that $\Sigma_t := \{t\} \times \Sigma_0$ is a smooth spacelike Cauchy surface of M for every $t \in \mathbb{R}$.

The proof of this proposition may be found in [BS05]. This allows us to define the following structure.

Definition 3. *A spacetime M such that one, and hence all the above conditions (i)-(iii) in proposition 1 hold is called a* ***globally hyperbolic spacetime****.*

Our particular interest in globally hyperbolic spacetimes is justified, first, by the well-posedness of the Cauchy problem, and the existence of unique solutions. We shall address this topic shortly after the introduction of other important objects.

Definition 4. *Let M, E be smooth manifolds, $\dim M = n$, $\dim E = n + k$ for $n, k \in \mathbb{N}$. Let $\pi : E \to M$ be a smooth, surjective map and let V be a k-dimensional $\mathbb{K}$-vector space, $\mathbb{K} = \mathbb{R}, \mathbb{C}$. Suppose that*

(i). for each $x \in M$, $\pi^{-1}(x) \equiv E_x$ is a $\mathbb{K}$-vector space isomorphic to V;

(ii). for each $x \in M$, there exist an open neighbourhood $N_x \subset M$ of x and a diffeomorphism

$$\phi : \pi^{-1}(N_x) \to N_x \times V$$

such that each restriction to some $E_y \to \{y\} \times V$, $y \in N_x$, is a vector space isomorphism, for each $y \in N_x$.

Then, the quadruple (E, M, π, V) is called a ***vector bundle*** *of rank k. The space E is called* ***total space****, whereas M is called* ***base space*** *and V is the* ***typical fiber****. In addition, the set N_x in point (ii) is called a trivializing open neighbourhood, and the pair (N_x, ϕ) is called a* ***local trivialization*** *for E. Finally, each vector space E_x is called a* ***fiber****.*

We denote a vector bundle (E, M, π, V) as $E \to \mathbb{M}$, keeping the surjective map π and the typical fiber implicit. A continuous map $s : M \to E$ such that $\pi \circ s = id_M$ is called a **section** of the vector bundle $E \to M$. It may be seen as an inverse of π at each fiber. The support of a section makes sense when considering the null vector of a certain fiber. That is, $\operatorname{supp} s$ is the closure of the set $\{x \in M : s(x) \neq 0 \in E_x\}$, with the closure with respect to the topology of M. The space of smooth sections of E will be denoted by $\Gamma(E) \equiv C^\infty(M, E)$, and we shall denote as $\Gamma_0(E)$ the subspace of smooth, compactly supported sections.

In this way, we shall later regard a field configuration as a smooth section of an abstract vector bundle over M. The structure of quantum field theories, built upon the smooth section of a vector bundle over M, will be the subject of the next sections of this chapter. First, the dynamical law of propagation of the field lies at the geometrical level as follows.

I.1.2 Differential operator and the Cauchy problem.

Definition 5. *Let $E \to M$ and $F \to M$ be two $\mathbb{K}$-vector bundles over the same base space M, with M a globally hyperbolic Lorentzian manifold with dimension $dim\, M = n$, and $\mathbb{K} = \mathbb{R}, \mathbb{C}$. A $\mathbb{K}$-linear map $P : \Gamma(E) \to \Gamma(F)$ is a* ***differential operator*** *if for each $x \in M$ there exists an open neighbourhood $N_x \ni x$ and local trivializations (N_x, ψ_E), (N_x, ψ_F), and if there exists a family of maps $A_\alpha : N_x \to Hom(V_E, V_F)$, with respect to which P may be written as*

$$P = \sum_{|\alpha| \leq k} A_\alpha \frac{\partial^{|\alpha|}}{\partial x^\alpha} \tag{I.1}$$

on N_x, for some $k \in \mathbb{N}$. The summation in taken over all multiindices $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ such that $|\alpha| := \alpha_1 + \cdots + \alpha_n \leq k$. In this case P is said to be of order at most k. If P is of order at most k but not of order at most $(k-1)$, then it is called a differential operator of order k.

The dynamical equations of our interest in this thesis are obtained from a particular class of differential operators. Let P be a differential operator of order k from $\Gamma(E) \to \Gamma(F)$. Let the map

$$\sigma_P : T^*M \to Hom(V_E, V_F)$$

be locally defined as follows. For some $x \in M$, let P be written such as in equation (I.1) for some coordinate system in a neighbourhood of x. For every $k \in T^*_x M$, we consider $k = \sum_{j=1}^n k_j dx^j$ and define

$$\sigma_P(\xi) := \sum_{|\alpha|=k} k^\alpha A_\alpha(x), \quad k^\alpha := k_1^{\alpha_1} \ldots k_n^{\alpha_n}.$$

We call σ_P the principal symbol of P. Heuristically it corresponds to the highest degree term in P. Restricting to the case of a unique bundle $E \to M$ and considering a differential operator $P : \Gamma(E) \to \Gamma(E)$ of order at most two acting on its smooth sections, we may consider the case of the homomorphisms A_α given in terms of components of the metric g on M, in such a way that P is given by

$$P = \sum_{\mu,\nu=0}^{3} \mathbf{1}_E g^{\mu\nu}(x) \frac{\partial^2}{\partial x^\mu \partial x^\nu} + \sum_{\mu=0}^{3} a_\mu(x) \frac{\partial}{\partial x^\mu} + b(x), \tag{I.2}$$

where $a_\mu(x), b(x), \in Hom(V_E)$, $\mu = 0, \ldots, 3$, and $\mathbf{1}_E \in Hom(V_E)$ is the identity. This defines a particular class of differential operators.

Definition 6. *A differential operator of order at most two which may be locally written as in equation* (I.2) *for some $a_\mu(x), b(x) \in Hom(V_E)$, $\mu = 0, \ldots, 3$, is called* ***normally hyperbolic****.*

From now on we shall omit the symbol $\mathbf{1}_E \in Hom(V_E)$ when considering a normally hyperbolic operator. In addition, these have the following important characteristic. Let ∇ be any connection on the bundle $E \to M$. This is a map $\nabla : \Gamma(E) \to \Gamma(E) \otimes T^*M$ such that

$$\nabla(sf) = (\nabla s)f + s \otimes df,\ \forall s \in \Gamma(E),\ \forall f \in C^\infty(M, \mathbb{R}). \tag{I.3}$$

Together with the Levi-Civita connection on T^*M, we then obtain a connection on $\Gamma(E) \otimes T^*M^{\otimes k}$ via multiple composition $\nabla \circ \cdots \circ \nabla$ (k times) for arbitrary $k \in \mathbb{N}$. We recall that a Levi-Civita connection is an affine connection which preserves the metric and which is torsion-free; we refer to [BGP07] for details. This permits us to define of the normally hyperbolic operator $\Box^\nabla$ over $\Gamma(E)$.

Definition 7. *Let $E \to M$ be a vector bundle over the globally hyperbolic spacetime M. Let $E \to M$ be endowed with a connection ∇. Together with the Levi-Civita connection on T^*M, we obtain a connection on $\Gamma(E) \otimes T^*M^{\otimes k}$ for all $k \in \mathbb{N}$, as above, again denoted as ∇. This induces a map $\Box^\nabla := -\nabla^2 \circ (Tr \otimes \mathbf{1}_E)$ as the composition*

$$\Gamma(E) \xrightarrow{\nabla} \Gamma(E) \otimes T^*M \xrightarrow{\nabla} \Gamma(E) \otimes T^*M^{\otimes 2} \xrightarrow{Tr \otimes \mathbf{1}_E} \Gamma(E), \tag{I.4}$$

where $Tr : T^*M^{\otimes 2} \to \mathbb{R}$ is given in terms of the metric as $k \otimes \xi \mapsto g(k, \xi)$. The operator $\Box^\nabla$ is usually called d'Alembertian operator induced by ∇.

The fact that $\Box^\nabla$ is a normally hyperbolic operator may be seen from the explicit computation of its principal symbol: according to the above definitions, we have that

$$\sigma_\Box(\xi) = -Tr \otimes \mathbf{1}_E \circ \sigma_\nabla(\xi) \circ \sigma_\nabla(\xi) = -g(\xi, \xi) \otimes \mathbf{1}_E, \tag{I.5}$$

which justifies our previous statement. The important characteristic of normally hyperbolic operator we mentioned is then presented in the proposition below.

Proposition 2. *Let M be a Lorentzian manifold and let $P : \Gamma(E) \to \Gamma(E)$ be a normally hyperbolic operator. Then, there exist a unique connection ∇ on $\Gamma(E)$, and a unique $B \in C^\infty(M, Hom(E))$ such that $P = \Box^\nabla + B$, where $\Box^\nabla$ is induced by the connection ∇ cf. equation* (I.4).

For the proof of this proposition, see [BGP07, prop. 1.5.5]. In view of this statement, a differential operator P is therefore said to be **compatible** with a connection ∇ on E if there exist $B \in C^\infty(M, Hom(E))$ and ∇ such that $P = \Box^\nabla + B$, with $\Box^\nabla$ induced by ∇. In addition, from now on we shall omit the subscript ∇ when denoting the d'Alembert operator, and the connection shall be held implicit.

Let the map $\langle \cdot, \cdot \rangle_E : \Gamma(E) \times \Gamma(E) \to C^\infty(M, \mathbb{R})$ such that, for each pair $\phi, \psi \in \Gamma(E)$, $\langle \phi, \psi \rangle_E$ is an inner product at each fiber. I.e., $M \ni x \mapsto \langle \phi, \psi \rangle(x) \equiv \langle \phi(x), \psi(x) \rangle$, $\phi(x), \psi(x) \in E_x$, is a bilinear, positive-definite map which is null if and only if $\phi(x)$ or $\psi(x)$ is the null vector in E_x, for all $x \in M$. Let then $P : \Gamma(E) \to \Gamma(F)$ a differential operator between the fibers of bundles E and F, and let the differential operator $P^* : \Gamma(F) \to \Gamma(E)$ such that

$$\langle \psi,\, P\phi \rangle_F =: \langle P^*\psi,\, \phi \rangle_E \quad \forall \psi \in \Gamma(F), \forall \phi \in \Gamma(E).$$

Then P^* is called the **formal adjoint** of P, and the operator P is called **formally self-adjoint** if $P, P^* : \Gamma(E) \to \Gamma(E)$ and $P = P^*$.

Let then $P : \Gamma(E) \to \Gamma(E)$ a normally hyperbolic operator acting on the smooth sections of the bundle $E \to M$ over the spacetime M. A differential equation

$$P\phi = f, \quad \phi,\, f \in \Gamma(E). \tag{I.6}$$

is called a **dynamical equation** for $\phi \in \Gamma(E)$. Concerning the Cauchy problem regarding equation (I.6), we set the following. Let $\Sigma \subset M$ a Cauchy surface of M and let $\mathbf{n}$ be a future-directed normal vector-field over Σ. As ∇ denotes a connection on $\Gamma(E)$ as per (I.3), we denote $\nabla_{\mathbf{n}} : \Gamma(E) \to \Gamma(E)$ the induced linear differential operator, obtained by the restriction to $\mathbf{n} \in T^*M$. Solving the **Cauchy problem** with initial data ϕ_0, ϕ_1 means obtaining $\phi \in \Gamma(E)$ fulfilling (I.6), for fixed $f \in \Gamma(E)$, and such that $\phi|_\Sigma = \phi_0$, $\nabla_{\mathbf{n}}\phi|_\Sigma = \phi_1$, with P compatible with ∇. One may find in [BGP07] the proof of the following proposition.

Proposition 3. (Existence and uniqueness of solutions of the Cauchy problem). *Let $E \to M$ a vector bundle over the globally hyperbolic spacetime M. Given a normally hyperbolic operator $P : \Gamma(E) \to \Gamma(E)$, for each $f \in \Gamma(E)$ and for each pair of initial conditions $\phi_0, \phi_1 \in \Gamma(\Sigma)$, there is a unique $\phi \in \Gamma(E)$ such that $P\phi = f$, $\phi|_\Sigma = \phi_0$, $\nabla_{\mathbf{n}}\phi|_\Sigma = \phi_1$, with P compatible with ∇. Furthermore, $\mathrm{supp}\,\phi \subset J(K)$, where $K := \mathrm{supp}\,\phi_0 \cup \mathrm{supp}\,\phi_1 \cup \mathrm{supp}\, f \subset M$.*

At this point we should then address the characterization of solutions to the Cauchy problem in proposition 3 above. Such characterization, however, will not be made in terms of sections only. The dynamical equation for the field theory will be regarded in the sense of distributions or functionals over the space $\Gamma(E)$, and at that level we shall obtain a complete description of such solutions. Considering the scope of this thesis, limited to the analysis of real scalar field theories over Minkowski spacetime, we shall focus on aspects of the theory of distributions over $\mathbb{R}^4$, and then in the next section we shall extend the results below to functionals over the space of field configurations. We refer to [Hör90; FJ99; BGP07] for details.

Definition 8. *Considering the space of smooth sections of the complex bundle $\mathbb{R}^4 \times \mathbb{C} \to \mathbb{M}$ with typical fiber $\mathbb{R}$,*

*(i). we denote by $\mathcal{E}(\mathbb{M})$ the space of smooth, complex-valued functions over $\mathbb{M}$, endowed with a locally convex topology as follows: a sequence $(\phi_n)_{n\in\mathbb{N}}$ is said to converge to $\phi \in \mathcal{E}(\mathbb{M})$ if for any $K \subset \mathbb{M}$ compact, $\partial^k \phi_n \to \partial^k \phi$ uniformly on K, for all $k \in \mathbb{N}_0$. The topological dual of $\mathcal{E}(\mathbb{M})$ is the **space of compactly supported distributions**, denoted $\mathcal{E}'(\mathbb{M})$;*

*(ii). we denote by $\mathscr{D}(\mathbb{M}) \subset \mathcal{E}(\mathbb{M})$ the space of compactly supported functions in $\mathcal{E}(\mathbb{M})$, also called **test functions**. This space is endowed with the following locally convex topology: we say $f_n \to f$ for $f_n, f \in \mathcal{C}_0^\infty(\mathbb{M})$ for all $n \in \mathbb{N}$ if there exists $K \subset \mathbb{M}$ compact such that supp f_n, supp $f \subset K$ and $\partial^k f_n \to \partial^k f$ for all $k \in \mathbb{N}_0$. The topological dual of $\mathcal{C}_0^\infty(\mathbb{M})$ is the **space of distributions**, i.e. the space of continuous linear functionals $\mathcal{C}_0^\infty(\mathbb{M}) \to \mathbb{C}$, which we denote by $\mathscr{D}'(\mathbb{M})$.*

The above spaces fulfill the inclusion relations $\mathscr{D}(\mathbb{M}) \subset \mathcal{E}(\mathbb{M})$, $\mathcal{E}'(\mathbb{M}) \subset \mathscr{D}'(\mathbb{M})$.

In the future, as we shall restrict our analysis to real scalar fields, we shall be particularly interested in the subspaces of real-valued functions om $\mathbb{M}$. We shall hence denote

$$\mathcal{C}^\infty(\mathbb{M}, \mathbb{R}) \equiv \mathcal{C}^\infty(\mathbb{M}) := \{f \in \mathcal{E}(\mathbb{M}) : f : \mathbb{M} \to \mathbb{R}\},$$

and analogously

$$\mathcal{C}_0^\infty(\mathbb{M}, \mathbb{R}) \equiv \mathcal{C}_0^\infty(\mathbb{M}) := \{f \in \mathscr{D}(\mathbb{M}) : f : \mathbb{M} \to \mathbb{R}\}.$$

Due to the duality relations between the spaces of functions and distributions or compactly supported distributions, we may denote the action of $u \in \mathscr{D}'(\mathbb{M})$ in the two manners $f \mapsto u(f) \equiv \langle f, u\rangle$ for all $f \in \mathscr{D}(\mathbb{M})$, with the analogous for compactly supported distributions. We recall that if $u \in \mathscr{D}'(\mathbb{M})$ is a distribution and if $\psi \in \mathscr{D}(\mathbb{M})$, then the product between u and ψ is defined as $\psi u(\phi) := u(\psi\phi)$ for all $\phi \in \mathscr{D}(\mathbb{M})$. Let $u \in \mathscr{D}'(M)$ and $x \in \mathbb{M}$. A **localization** of u in a neighbourhood $N_x \subset \mathbb{M}$ of x is a distribution $fu \in \mathscr{D}'(\mathbb{M})$ with $f \in \mathcal{C}_0^\infty(\mathbb{M})$, such that for some larger neighbourhood $U \supset N_x$ of x, $\operatorname{supp} f \subset U$ and $f|_{N_x} \equiv 1$. For $x \in \mathbb{M}$, we denote $\mathfrak{N}_x$ the collection of neighbourhoods $N \subset \mathbb{M}$ of x. We then recall that the **support of a distribution** $u \in \mathscr{D}'(\mathbb{M})$, denoted $\operatorname{supp} u$, is defined as the closure of the complement of

$$\{x \in \mathbb{M} : \forall N \in \mathfrak{N}_x, \forall f \in \mathscr{D}(\mathbb{M}) \text{ s.t. } \operatorname{supp} f \subset N, fu = 0\}.$$

It consists of the points of $\mathbb{M}$ which have no neighbourhood over which the restriction of u is identically zero.

We define the derivative of $u \in \mathscr{D}'(\mathbb{M})$ as the distribution u' given by

$$u'(\phi) := -u(\phi') \quad \forall \phi \in \mathscr{D}(\mathbb{M}).$$

This definition may be extended to $\phi \in \mathcal{E}(\mathbb{M})$, if $\operatorname{supp} u \cap \operatorname{supp} \phi$ is compact.

In view of the above definition, we may lift the action of a normally hyperbolic operator to distributions in the following manner.

Definition 9. *Let $P : \mathcal{E}(\mathbb{M}) \to \mathcal{E}(\mathbb{M})$ a differential operator. We define the differential operator $P : \mathscr{D}'(\mathbb{M}) \to \mathscr{D}'(\mathbb{M})$ on distributions, denoted with the same symbol, in the sense of the pairing*

$$\big(Pu\big)(\phi) = \langle \phi, Pu \rangle := \langle P^* \phi, u \rangle = u(P^* \phi),$$

where P^* is the formal adjoint of $P : \mathcal{E}(\mathbb{M}) \to \mathcal{E}(\mathbb{M})$.

In this thesis, the latter notation $f \mapsto \langle f, u \rangle$ via the dual pairing will be frequently written as a formal integral

$$u(f) \equiv \int_{\mathbb{M}} dx\, f(x) u(x) \tag{I.7}$$

where dx denotes the volume form over $\mathbb{M}$. In fact, we shall denote the action of a distribution or of a functional over a space of functions as in above, even if the formal kernel $u(x)$ is to be understood only in the sense of generalized functions.

In view of the definition 9, we address the dynamical equation (I.6) in the sense of distributions,

$$Pu = f, \quad u, f \in \mathscr{D}'(\mathbb{M}). \tag{I.8}$$

Let first $\delta_x \in \mathscr{D}'(\mathbb{M})$ denote the Dirac delta function at $x \in \mathbb{M}$, $\mathscr{D}(\mathbb{M}) \ni f \mapsto f(x) \in \mathbb{C}$.

Definition 10. *A distribution $F \in \mathscr{D}'(\mathbb{M})$ is called a **fundamental solution**, or **Green operator** of* (I.8) *at $x \in \mathbb{M}$ if $PF = FP^* = \delta_x$, in the sense of distributions.*

We then obtain two fundamental solutions to the Cauchy problem, completely characterized by their supports, by lifting the previous result in proposition 3 to distributions [cf. in BGP07]. For the rest of this section we shall restrict to the case $f \equiv 0$ in equation (I.8).

Proposition 4. *Consider the Cauchy problem for a given normally hyperbolic operator $P : \mathcal{E}(\mathbb{M}) \to \mathcal{E}(\mathbb{M})$. There exist maps $\Delta_{R/A} : \mathscr{D}(\mathbb{M}) \to \mathcal{E}(\mathbb{M})$, unique fundamental solutions for P such that supp $\Delta_{R/A}(f) \subset J_{+/-}($supp $f)$ for all $f \in \mathscr{D}(\mathbb{M})$. In addition, $\Delta_R^* = \Delta_A$.*

The maps $\Delta_{R/A}$ are called **retarded** and **advanced propagator**, respectively. Each of these maps defines a bidistribution $\Delta_{R/A} : \mathscr{D}(\mathbb{M}) \times \mathscr{D}(\mathbb{M}) \to \mathbb{C}$, $(f, g) \mapsto \langle f, \Delta_{R/A} g \rangle$ which we denote by the same symbol. The difference $\Delta := \Delta_R - \Delta_A$, named **causal propagator**, completely characterizes any solution of the Cauchy problem regarding a normally hyperbolic operator, in the following sense.

Proposition 5. *If $\phi \in \mathcal{E}(\mathbb{M})$ is a solution of the Cauchy problem $P\phi = 0$ for a normally hyperbolic P with initial conditions $\phi_0, \phi_1 \in \mathscr{D}(\Sigma)$ for some Cauchy surface $\Sigma \subset \mathbb{M}$, then $\phi = \Delta(f)$ for some $f \in \mathscr{D}(\mathbb{M})$. Furthermore, if $f \in \mathscr{D}(\mathbb{M})$ is such that $\Delta(f) = 0$, then $f = Pg$ for some $g \in \mathcal{E}(\mathbb{M})$.*

The causal propagator, seen as a map $\mathscr{D}(\mathbb{M}) \to \mathcal{E}(\mathbb{M})$, induces a bidistribution Δ on $\mathscr{D}(\mathbb{M}) \times \mathscr{D}(\mathbb{M})$ as $(f, g) \mapsto \Delta(f, g) := \langle f, \Delta g \rangle$, due to the inclusion $\mathcal{E}(\mathbb{M}) \subset \mathscr{D}'(\mathbb{M})$. Let $f, g \in \mathscr{D}(\mathbb{M})$. in view of the above proposition, we define $f \sim_P g$ if $f - g = Ph$ for some $h \in \mathcal{C}_0^\infty(\mathbb{M})$. In other words, we shall consider smooth, compactly supported sections equivalent if their difference has the form Ph, for some $h \in \mathcal{C}_0^\infty(\mathbb{M})$, where P is the normally hyperbolic operator from equation (I.8). Considering the quotient of $\mathcal{C}_0^\infty(\mathbb{M})$ with respect to this equivalence relation, we obtain a characterization of the space of solutions of (I.8) with compact spacial support.

Definition 11. *Let I_P be the closed ideal generated by elements $Pf \in \mathcal{E}(\mathbb{M})$, $f \in \mathscr{D}(\mathbb{M})$. The space $Sol(P) := \{\phi \in \mathscr{D}(\mathbb{M}) | P\phi = 0, \phi|_{\Sigma \subset \mathbb{M}}, \nabla_{\mathbf{n}}\phi|_{\Sigma \subset \mathbb{M}} \in \mathscr{D}(\Sigma)\}$ of solutions of the Cauchy problem with smooth compactly supported initial data over some Cauchy surface $\Sigma \subset \mathbb{M}$, cf. in proposition 3, forms the symplectic space of solutions of equation $P\phi = 0$, endowed with the symplectic form*

$$\zeta : Sol(P) \times Sol(P) \to \mathbb{C}, \quad (f, g) \mapsto \Delta(f, g).$$

In addition, the quotient $\mathcal{E}(\mathbb{M})/\sim_P = \mathcal{E}(\mathbb{M})/Ker\,\Delta$ with the symplectic form $\tilde{\zeta}\big([f], [g]\big) := \Delta(f, g)$ is isomorphic to $(Sol(P), \zeta)$.

The proof of the above proposition may be found in [BGP07]. Moreover, the symplectic structure obtained as the space of solutions provides a Poisson bracket dynamical structure to the field theory via the causal propagators. That, in resume, highlights the cornerstone role played by Δ in the construction of both the classical and the quantum algebra of free observables, as will be presented later.

In the context of scalar fields propagating over Minkowski space, as the normally hyperbolic operator is the Klein-Gordon operator, and equation (I.6) assumes the particular form

$$\big(\Box + m^2\big)\phi \equiv \Big(\partial_0^2 - \partial_x^2 + m^2\Big)\phi = j, \quad \phi \in \mathcal{E}(\mathbb{M}) \tag{I.9}$$

for $m \geq 0$ a mass term and $j \in \mathscr{D}(\mathbb{M})$ a source term. As per proposition 4, in the sense of distributions, equation (I.9) with $j \equiv 0$ has two fundamental solutions given in terms of the integral kernels

$$\Delta_{R/A}(x, y) = \lim_{\varepsilon \to 0^+} \frac{1}{(2\pi)^4} \int_{\mathbb{R}^4} dp \frac{e^{ip(x-y)}}{(p^0 \pm i\varepsilon)^2 - w_p^2}, \tag{I.10}$$

with $w_{\mathbf{p}} := \sqrt{\mathbf{p}^2 + m^2}$. The choice of sign $p^0 + i\varepsilon$ defines the retarded propagator for the Klein-Gordon operator $\Box + m^2$, whereas the difference $p^0 - i\varepsilon$ defines the advanced one. The integral kernel of the causal propagator may be written as

$$\Delta(x, y) = \theta(x^0 - y^0)\Delta_R(x, y) - \theta(x^0 - y^0)\Delta_A(x, y), \tag{I.11}$$

or also in terms of the sign function $\varepsilon(p_0) := \theta(p_0) - \theta(-p_0)$ as

$$\begin{aligned} i\Delta(x,y) =& \frac{1}{(2\pi)^3} \int_{\mathbb{R}^4} dp\, \varepsilon(p_0)\delta(p_0^2 - w_{\mathbf{p}}^2) e^{ip(x-y)} \\ =& - \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p}\, \frac{\sin\big(w_{\mathbf{p}}(x^0 - y^0)\big) e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{w_p} \end{aligned} \tag{I.12}$$

if $(x^0 - y^0)^2 \geq 0$, it being 0 otherwise. This latter property of Δ, which is equivalent to $\Delta(f, g) = 0$ for $\operatorname{supp} f, \operatorname{supp} g$ spacelike-separated, also justifies the use of the causal propagator in the implementation of the canonical commutation relations, as will be described in the next section.

I.1.3 The wave front set of a distribution and the propagation of singularities

The Fourier transform of a distribution $u \in \mathcal{E}'(\mathbb{R}^n)$ is given by the analytic function

$$\mathbb{C}^n \ni k \mapsto \hat{u}(k) := \langle u, x \mapsto e^{-ikx} \rangle. \tag{I.13}$$

It is also polynomially bounded, in the sense that for some $N \in \mathbb{N}$ there exists $C_N \in \mathbb{R}$ such that

$$|\hat{u}(k)| \leq C_N (1 + |k|)^N, \quad \forall k \in \mathbb{R}^n \tag{I.14}$$

In addition, if $u \in \mathcal{E}'(\mathbb{R}^n)$, then $u \notin \mathscr{D}(\mathbb{R}^n)$ if and only if there exist a direction in frequency space along which the Fourier transform of u is not **fast decreasing**, in the following sense.

Definition 12. *Let $u \in \mathcal{E}'(\mathbb{R}^n)$. A vector $k_0 \in \mathbb{R}^n$ is called a direction of fast (or rapid) decrease for u if there exists a conic*[1] *neighbourhood $\mathcal{V} \subset \mathbb{R}^n$ of k_0 such that, for all $N \in \mathbb{N}$, there exists $C_N \in \mathbb{R}$ satisfying*

$$|\hat{u}(k)| \leq C_N (1 + |k|)^{-N} \quad \forall k \in \mathcal{V}. \tag{I.15}$$

We refer to [Hör90] for details. This motivates an analysis on the regular behaviour of a distribution, based on the properties of its Fourier transform, a topic to which we dedicate the next few paragraphs.

The set of points of $\mathbb{R}^n$ where u is not given by a smooth function is called its **singular support**. It is the set of points of $\mathbb{R}^n$, denoted $\operatorname{singsupp} u$, which have no neighbourhood where u reduces to a smooth function, and so it is defined as the complement of

$$\{x \in \mathbb{M} : \exists N \in \mathfrak{N}_x, \exists f \in \mathscr{D}(\mathbb{M}) \text{ s.t. } \operatorname{supp} f \subset N,\ fu \in \mathscr{D}(\mathbb{M})\}.$$

[1] Let V be a $\mathbb{K}$-vector space. A **cone** is a subset $C \subset V$ such that for any $v \in C$ and for any $\lambda \in \mathbb{K}\backslash\{0\}$, $\lambda v \in C$. If $O \subset \mathbb{R}^n$ is open, $\Gamma \subset T^*O\backslash\{0\}$ is called a cone if $(x,k) \in \Gamma$ implies $(x, \lambda k) \in \Gamma$ for all $\lambda > 0$

In addition to the set singsupp u of points where the distribution $u \in \mathscr{D}'(\mathbb{M})$ is not given in terms of a regular function, we might consider the set of directions along which it is singular, i.e. the directions along which the Fourier transform of u does not rapidly decreases , as per definition 12. This brings us to the concept of wave front set of distribution.

Definition 13. *Let $u \in \mathscr{D}'(\mathbb{R}^n)$ be a distribution in $\mathbb{R}^n$. A point $p = (x_0, k_0) \in \mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$ is called a* ***regular directed point*** *of u if there exists a localization of u around x_0 such that* (I.15) *holds for all k in some conic neighbourhood of k_0.*

The wave front set of a distribution $u \in \mathscr{D}'(\mathbb{R}^n)$, $WF(u)$, is the complement in $\mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$ of the set of regular directed points of u. Due to the covector action of $k \in \mathbb{R}$ in (I.13), we properly define the wave front set in the following manner.

Definition 14. *The* ***wave front set*** *of $u \in \mathscr{D}'(\mathbb{M})$, denoted as $WF(u)$, is defined as the closure of the complement in $T^*\mathbb{M}\backslash\{0\}$ of the set of regular directed points of u. The subset $\{0\} \subset T^*\mathbb{M}$ is called* ***zero section*** *of $T^*\mathbb{M}$.*

The following properties of the wave front set of a distribution are true, see [Hör90].

Proposition 6. *Let $u \in \mathscr{D}'(\mathbb{M})$, its wave front set is such that*

(i). if $(x, k) \in WF(u)$, then $x \in$ singsupp u;

(ii). if $u \in C^\infty(\mathbb{R}^n)$, then $WF(u) = \emptyset$;

(iii). for any localization f of u, $WF(fu) \subset WF(u)$;

(iv). let $P : \mathscr{D}(\mathbb{M}) \to \mathscr{D}(\mathbb{M})$ be any liner partial differential operator, then $WF(Pu) \subset WF(u)$.

For details concerning distributions and their wave front sets over smooth manifolds, see also [BFK96]. In the context of this thesis, however, much of this discussion will not be required as we, as stated before, shall work only on fields propagating over Minkowski space.

In chapter IV we shall make explicit use of the so called propagation of singularities theorem. Though a more general formulation may be found in [Hör94], and in particular in [Rad96b] and references there mentioned, we shall restrict our discussion to a particular version of this theorem, which suffices for the scope of our future discussion. We star by introducing some basic concepts.

As before, let $E \to \mathbb{M}$ a $\mathbb{K}$-vector bundle over $\mathbb{M}$. If P is a normally hyperbolic differential operator as in equation (I.2), consider the set

$$N := \{(x, k) \in T^*\mathbb{M}\backslash\{0\} : g^{\mu\nu}(x) k_\mu k_\nu = 0\},$$

called **bicharacteristic strip** of P. In addition, let

$$C := \big\{\big((x_1, k_1), (x_2, k_2)\big) \in N \times N : (x_1, k_1) \sim (x_2, k_2)\big\},$$

where $(x_1, k_1) \sim (x_2, k_2)$ means there exists a null geodesics γ in M connecting x_1 to x_2, with k_i coparallel to γ at x_i, $i = 1, 2$, and such that k_1 is parallel-transported to k_2 along the γ. Denoting the diagonal of $N \times N$ as $diag(N \times N) := \{\big((x_1, k_1), (x_2, k_2)\big) \in N \times N : x_1 = x_2,\, k_1 = k_2, \}$, we notice that the set $C \backslash diag(N \times N)$ decomposes into the two connected components $C^{\pm}$, the first given as

$$C^+ := \big\{\big((x_1, k_1), (x_2, k_2)\big) \in N \times N : x_1 \in J^+(x_2), k_1 \rhd 0 \text{ or } x_1 \in J^-(x_2), k_1 \lhd 0\big\}.$$

Again, with respect to the time orientation on M, $k \rhd 0$ (resp. $k \lhd 0$) denotes k future (resp. past) directed. The component C^- is defined analogously, interchanging the orientation of k in each condition above. Let be the splitting $C \backslash diag(N \times N)$ as $C \backslash diag(N \times N) = C^1 \cup C^2$ with C^1, C^2 open subsets of $C \backslash diag(N \times N)$ such that $\big((x_1, k_1), (x_2, k_2)\big) \in C^1$ if and only if $\big((x_2, k_2), (x_1, k_1)\big) \in C^2$. We call C^1, C^2 orientations on C, and so $C^{\pm}$ are two orientations on C. In [Rad96b; Rad92] the author shows that an orientation for $C \backslash diag(N \times N)$ always exists, also in more general contexts, and that both C^1 and C^2 cannot be neither empty nor the whole of $C \backslash diag(N \times N)$.

The set N for a four-dimensional spacetime has the two connected components

$$N^+ := \{(x, k) \in N : k^0 \rhd 0\}, \quad N^- := \{(x, k) \in N : k^0 \lhd 0\}.$$

Let $\tilde{N}$ denote the set of all connected components of N, and let $\nu \subset \tilde{N}$ denote a partition of N. Specifically, in the present case we have four options, $\nu = \{N_+, N_-\}, N_+, N_-$, and $\nu = \emptyset$. Set now

$$N^+_\nu := \bigcup_{N' \in \nu} N', \quad N^-_\nu := \bigcup_{N' \in \tilde{N} \backslash \nu} N'.$$

We then obtain $N^+_\nu = N, N^{\pm}, \emptyset$, and N^-_ν the corresponding complement. Finally, let $C^{\pm}_\nu$ be the orientation of C corresponding to $N^{\pm}_\nu$, respectively. See the mentioned references for the details. We may now state the following.

Proposition 7. *Let P a real normally hyperbolic operator. For every orientation ν of $C \backslash diag(N \times N) = C^+_\nu \cup C^-_\nu$, there exist fundamental solutions of P such that*

$$WF'(u^{\pm}_\nu) = D^* \cup C^{\pm}_\nu,$$

where D^* denotes the diagonal of $T^*\mathbb{M} \times T^*\mathbb{M}$, and

$$WF'(u) := \big\{\big((x_1, k_1), (x_2, k_2)\big) \in T^*\mathbb{M} : \big((x_1, k_1), (x_2, -k_2)\big) \in WF(u)\big\}.$$

In addition, any fundamental solution u of P equals $u^{\pm}_\nu$ up to smooth terms.

The important point in the above proposition, whose proof may be found in [DH72] (see [Rad92] for a detailed discussion), is that the wavefront set of fundamental solutions for real normally hyperbolic operators over globally hyperbolic spacetimes, such as the Klein-Gordon operator, depends only on the principle symbol of P. In conclusion, we observe that a transformation of P, altering its terms of order at most one only, preserves its wave front set, although it might change its fundamental solutions. This will be of particular importance in chapter IV. In addition, we affirm that the above result generalizes to all globally hyperbolic spacetimes.

The concept of wave front set provides a sufficient condition for the existence of the product between two distributions. Given two distributions $u, v \in \mathscr{D}'(\mathbb{M})$, we define the Whitney sum of their wave front sets as

$$WF(u) \oplus WF(v) := \{(x, k + k') \in T^*\mathbb{M} : (x, k) \in WF(u),\ (x, k')WF(v)\} \tag{I.16}$$

We then have the following theorem, see [Hör90], theorem 8.2.10.

Proposition 8. (Hörmander criterium for the product of distributions.)*If $u, v \in \mathscr{D}'(\mathbb{M})$, then the product uv is well defined if the Whitney sum of their wave front sets does not intersect the zero section. I.e., if for any $(x, k) \in WF(u)$, $(x, -k) \notin WF(v)$.*

I.2 Functionals over field configurations

In the functional formalism of algebraic quantum field theory, observables are described as functionals over the space of field configurations. In general, one considers the space of field configurations as the space of smooth sections of some abstract vector bundle $E \to M$. However, as in the present case we shall focus on a real, scalar field propagating over Minkowski space, this abstract structure reduces to the space $\mathcal{C}^\infty(\mathbb{M})$ of smooth, real valued functions over $\mathbb{M}$. We shall then consider observables among functionals over $\mathcal{C}^\infty(\mathbb{M})$, in particular those which satisfy certain properties, as will be described in this section. This perspective towards the description of observables of a physical system may be introduced with the following example[2].

Consider a field describing the Universe's temperature: in a certain configuration, this should be given by a smooth function $\phi : \mathbb{M} \to \mathbb{R}$, which assigns to each point $x \in \mathbb{M}$ a certain value, corresponding to the temperature of that point. If we are interested in the weighted average of the field in a finite region of spacetime, this corresponds to the smearing $\phi \mapsto \langle f, \phi \rangle \in \mathbb{R}$, performed in the region of $\mathbb{M}$ determined by $\operatorname{supp} f$, for some weight $f \in \mathcal{C}_0^\infty(\mathbb{M})$. Therefore, the compactly supported function describing the region of spacetime considered in the measuring process, it will always be regarded as an intrinsic part of the observable. Subsequently, the dynamical equation for observables is obtained from the lifting of the differential operator over field configurations to distributions, as presented in definition 9.

This example presents the field as a linear functional over $\mathcal{E}(\mathbb{M})$, which we represent as

$$\mathcal{E}(\mathbb{M}) \ni \phi \mapsto \Phi_f(\phi) := \int_{\mathbb{M}} dx\, f(x)\phi(x), \quad f \in \mathscr{D}(\mathbb{M}). \tag{I.17}$$

In practical situations, we are also interested in more complex observables, which correlate different regions of spacetime or which simply are not contemplated within this

[2] Adapted from Thomas-Paul Hack's PhD thesis, see [Hac10, pg. 56]

example, such as already the observable $\mathcal{C}^\infty(\mathbb{M}) \ni \phi \mapsto \langle f, \phi^2 \rangle$ is not. Pondering upon these rather simplistic cases, we think of observable as functionals over the space $\mathcal{C}^\infty(\mathbb{M})$ of smooth field configurations.

The functionals described in the last few paragraphs correspond to particular observables. As mentioned above, one is usually interested in more complex and singular objects, than simply linear or local functionals. The general aspects of the observables we shall be interested in will be described further below in the present section.

We now intend to provide a brief introduction to functional calculus and describe the particular classes of functionals which will be employed later. For a a deeper and more detailed survey on functional calculus, we refer to [Rej16; FR15b] which contains a briefer, quantum field-oriented introduction to the argument, and to [Nee05; Bro+18] for a detailed discussion on the topic. Further, more specific references will be pointed throughout the text. We start with a proper characterization of what we shall call the space of field configurations, after some recollection of other fundamental aspects of distributions. For details on the following topics, we refer to [Hör90; FJ99].

I.2.1 Functionals over $\mathcal{C}^\infty(\mathbb{M})$

In the present subsection we examine general aspects of functionals over the space $\mathcal{C}^\infty(\mathbb{M})$ of field configurations, and present a basic discussion on functional calculus. As in the previous section, we shall maintain the formal notation of pairing as an integration. I.e., for some functionals we may write

$$\langle f, F(\phi) \rangle \simeq \int dx\, f(x)\mathcal{F}(\phi)(x), \quad f \in \mathscr{D}(\mathbb{M}),$$

even if the above integral kernel $\mathcal{F}(\phi)(x)$ is to be understood as a generalized function.

We now address functionals over the space of field configurations.

Definition 15. *Let the continuous functional $F : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$, and let $\phi \in \mathcal{C}^\infty(\mathbb{M})$ arbitrary but fixed. Then, F is said to be C^1-differentiable at ϕ if the map*

$$\psi \in \mathcal{C}^\infty(\mathbb{M}) \mapsto F'(\phi)(\psi) := \frac{d}{d\lambda} F(\phi + \lambda\psi)\Big|_{\lambda=0} \in \mathbb{C} \tag{I.18}$$

with $\lambda \in \mathbb{R}$ exists and is continuous for all $\psi \in \mathcal{C}^\infty(\mathbb{M})$. If F is C^1-differentiable at every $\phi \in \mathcal{C}^\infty(\mathbb{M})$, then we say F is C^1- differentiable, and the map $F' : \mathcal{C}^\infty(\mathbb{M}) \times \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$ defined as in (I.18) *is called its (first)* ***functional derivative****.*

Higher order derivatives may then be defined recursively, and thus the n-th functional derivative of F, whenever it exists, is the map

$$\begin{aligned} \frac{\delta^n F}{\delta \phi^n} \equiv F^{(n)} &: \mathcal{C}^\infty(\mathbb{M}) \times \mathcal{C}^\infty(\mathbb{M})^{\otimes n} \to \mathbb{C}, \\ (\phi, \psi_1 \otimes_s \cdots \otimes_s \psi_n) &\mapsto \frac{\partial^n}{\partial\lambda_1 \cdots \partial\lambda_n} F\Big(\phi + \sum_{j=1}^n \lambda_j \psi_j\Big)\Big|_{\boldsymbol{\lambda}=0}, \end{aligned} \tag{I.19}$$

where we have denoted $\boldsymbol{\lambda} := (\lambda_1, \dots, \lambda_n) \in \mathbb{R}^n$ and $\otimes_s$ is the symmetrized tensor product. Whenever the n-th functional derivative of $F : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$ exists, we shall use both notations presented in the last equation to denote it.

As an example, consider again the linear functional $\Phi \equiv \Phi_f : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$ given by equation (I.17). Its functional derivative at ϕ in the direction ψ is

$$\Phi'(\phi)(\psi) = \frac{d}{d\lambda} \int dx\, f(x)\big(\phi + \lambda\psi\big)(x)\Big|_{\lambda=0} = \int dx\, f(x)\psi(x) \in \mathbb{C}, \quad \forall \psi \in \mathcal{C}^\infty(\mathbb{M})$$

It is then evident that $\Phi^{(2)} = 0$. In the same manner, the functional

$$\phi \mapsto \int dx\, f(x)\phi^2(x), \quad f \in \mathcal{C}_0^\infty(\mathbb{M})$$

is such that

$$\frac{\delta}{\delta\phi}\left[\int dx\, f(x)\phi^2(x)\right](\psi) = \frac{d}{d\lambda}\int dx\, f(x)\big(\phi + \lambda\psi\big)^2(x)\Big|_{\lambda=0} = 2\int dx\, f(x)\phi(x)\psi(x).$$

As the nth functional derivative of a differentiable functional defines a map over $\mathcal{C}^\infty(\mathbb{M})^{\otimes n}$ for each $\phi \in \mathcal{C}^\infty(\mathbb{M})$, we conclude that, for the generic non linear functional

$$\phi \mapsto \int dx\, f(x)\phi^p(x),$$

it equals

$$\begin{aligned}\frac{\delta^n}{\delta\phi^n}&\left[\int dx\, f(x)\phi^p(x)\right](\psi_1 \otimes \cdots \otimes \psi_n) = \\ &= \frac{p!}{(p-n)!}\int dx_1 \dots dx_n f(x_1)\phi^{p-n}(x_1)\delta(x_1, \dots, x_n)\prod_{j=1}^{n}\psi_j(x_j),\end{aligned}$$

for $n \leq p$, and it is null otherwise.

If the C^1-functional derivative of F' exists and is continuous, then F is said to be of class C^2. If the same is true for all the subsequent derivatives of F, we obtain a particular class of functionals.

Definition 16. *A functional $F : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$ is called* ***differentiable*** *or* ***smooth*** *if its nth functional derivative, defined as per equation* (I.19)*, exists and is a continuous map from $\mathcal{C}^\infty(\mathbb{M})^n \to \mathbb{C}$ for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$ and for all $n \in \mathbb{N}_0$.*

We now define the support of a functional.

Definition 17. *Let $F : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$. Then, the* ***support*** *of F, denoted supp F, is defined as the closure of the set*

$$\{x \in \mathbb{M} : \forall N \in \mathfrak{N}_x,\, \exists\, \phi, \psi \in \mathcal{C}^\infty(\mathbb{M}),\, \mathit{supp}\, \psi \subset N,\, \text{s.t. } F(\phi + \psi) \neq F(\phi)\}.$$

If supp F is compact, then F is called a ***compactly supported*** *functional.*

The support of a functional may be completely characterized by the support of its first functional derivative.

Proposition 9. *Let $F : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$ a C^1-differentiable functional over $\mathcal{C}^\infty(\mathbb{M})$. Then*

$$\mathit{supp}\, F = \overline{\bigcup_{\phi \in \mathcal{C}^\infty(\mathbb{M})} \mathit{supp}\, F'(\phi)}.$$

Proof. See [BFR19] or [Bro+18]. □

Before moving to the next section, where we intend to present how the above functionals enter the context of quantum field theory, we provide a few examples of particularly interesting functionals.

Definition 18. *Let $\mathscr{F}(\mathbb{M})$ the space of smooth functionals $\mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$. A functional $F \in \mathscr{F}(\mathbb{M})$ is called*

(i). ***regular****, if it is everywhere given by a smooth, compactly supported function. I.e., if $WF(F^{(n)}(\phi)) = \emptyset$ for all $n \in \mathbb{N}_0$ and for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$. The subset of regular elements of $\mathscr{F}(\mathbb{M})$ will be denoted $\mathscr{F}_{reg}(\mathbb{M})$;*

(ii). ***additive****, if for all $\phi, \psi, \xi \in \mathcal{C}^\infty(\mathbb{M})$ such that $\mathit{supp}\, \phi \cap \mathit{supp}\, \psi = \emptyset$ and regardless of further assumptions upon the form of the support of ξ, $F(\phi+\psi+\xi) = F(\phi+\xi)+F(\psi+\xi) - F(\xi)$.*

In addition,

(iii). let $V_\pm(x)$ denote the future/past lightcone at $x \in \mathbb{M}$ in the cotangent space $T^*\mathbb{M}$, and let $V_\pm := \cup_{x\in\mathbb{M}} V_\pm(x) \subset T^*\mathbb{M}$; F is called ***microcausal****, if $WF(F^{(n)}(\phi)) \cap \left(\overline{V}^n_+ \cup \overline{V}^n_-\right) = \emptyset$ for all $n \in \mathbb{N}$, for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$. The set of microcausal functionals in $\mathscr{F}(\mathbb{M})$ will be denoted $\mathscr{F}_{\mu C}(\mathbb{M})$;*

(iv). a microcausal functional $F \in \mathscr{F}_{\mu C}(\mathbb{M})$ is called ***local*** *if it is additive and, moreover, if its wave front set is normal to the tangent space of the thin diagonal on $\mathbb{M}$. I.e., if $WF(F^{(n)}(\phi)) \perp T^*diag(\mathbb{M}^n)$, where $diag(\mathbb{M}^n) := \{(x_1, \ldots, x_n) \in \mathbb{M}^n : x_1 = \cdots = x_n\}$, $\forall n \in \mathbb{N}$. The subset of local elements of $\mathscr{F}(\mathbb{M})$ is denoted $\mathscr{F}_{loc}(\mathbb{M})$;*

Notice that the definition of the support of a functional is motivated by the form of locality condition. The first example of a local functional is the Dirac δ-distribution, in the following sense. Let

$$F(\phi) := \int dxdy\, \phi(x)\phi(y)\delta(x-y)f(y), \quad f \in \mathscr{D}(\mathbb{M}).$$

Then, the wave front set of its second functional derivative is given by

$$WF\big(F^{(2)}\big) = WF(f\delta) = \{(x, x, k, -k) \in T^*\mathbb{M}^2 : x \in \operatorname{supp} f,\ k \neq 0\}.$$

See [BDH14], for instance. In [Bro+18], on the other hand, the authors provide what they call a "local definition of locality". For $\phi \in \mathcal{C}^\infty(\mathbb{M})$, the k-jet of ϕ at $x \in \mathbb{M}$ is the polynomial $y \mapsto j^k_x\phi(y) := \sum_{n\geq 0} \phi^{(n)}(x)y^n/n!$. Let then $J^k\mathbb{M}$ denote the k-jet bundle over $\mathbb{M}$, let $U \subset \mathbb{M}$ be an open subset, and let $F : U \to \mathbb{C}$ a smooth functional. We may alternatively call it a local functional if for every $\phi \in \mathcal{C}^\infty(\mathbb{M})$ there exists $N \subset \mathcal{C}^\infty(\mathbb{M})$ a neighbourhood of ϕ, a $k \in \mathbb{N}_0$ and a smooth function $f : O \subset J^k\mathbb{M} \to \mathbb{C}$ such that, for all $\psi \in \mathcal{C}^\infty(\mathbb{M})$ satisfying $\phi + \psi \in N$, the map $x \in \mathbb{M} \mapsto (f \circ j^k_x)(\psi)$, where $j^k_x\psi$ denotes the k-jet of ψ at x, is compactly supported and

$$F(\phi + \psi) = F(\phi) + \int dx\, f \circ j^k_x(\psi).$$

Though at this level the above classification of smooth functional sounds like nothing but a few examples, in the sections to follow these will be used in the construction of the algebra of observables.

I.3 The algebraic description of the free quantum scalar field theory

In this section we discuss the basic aspects of Algebraic Quantum Field Theory (AQFT), focusing on the analysis of a real, free scalar quantum field theory. The construction of the algebra of observables will be presented in two steps. First we address the fundamental observable Φ_f, the field itself described by a linear functional as in equation (I.17). Subsequently, we shall discuss more delicate observables involving non-linear functionals. The latter step involves the use of microlocal techniques applied to quantum field theory, which will be addressed in the last part of this section, after discussing states in AQFT.

Throughout this section we shall be interested in field theories described by a Lagrangian functional of the form

$$\mathcal{L}_0(\phi) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2, \quad \phi \in \mathcal{C}^\infty(\mathbb{M}), \tag{I.20}$$

for some $m > 0$. From the free Lagrangian $\mathcal{L}_0$, one obtains the Klein-Gordon equation of motion

$$\left(\Box + m^2\right)\phi = 0, \tag{I.21}$$

where $\Box$ is the d'Alembertian operator described in section I.1. Effects of non null source term $j \neq 0$ in the right hand side of (I.21), as per equation (I.6), will be discussed in the next section.

Considering the field as the fundamental object of the theory corresponds, in a first approach, to considering the algebra of observables $\mathscr{A}$ as being generated by linear functionals Φ_f in (I.17), for different smearing functions $f \in \mathscr{D}(\mathbb{M})$ and a unity $\mathbf{1}$. In addition, at the algebraic level the physical characteristics of ϕ are manifested in the following properties of the elements of this algebra. First, the functional character of the field, which translates the physical requirement of considering smeared fields as meaningful objects instead of pointwise observables, is already incorporated within the algebra of observables $\mathscr{A}$ in the functional formalism. Second, in order to construct an algebra for the quantum theory, the canonical commutation relations (CCR) must also be implemented within $\mathscr{A}$. Moreover, as in the long run we might be interested in considering a representation of $\mathscr{A}$ over some Hilbert space, the algebra $\mathscr{A}$ must be endowed with an involution. Finally, Φ should satisfy the dynamical equation for the field, i.e. the Klein-Gordon equation (I.21). However, since we shall be interested in perturbative interacting theories, we shall not implement this condition over the algebras of observables. This will be placed upon states instead, as we shall see further below.

We start this section with the gradual construction of an algebra structure over the space of field configurations, which shall incorporate the physical requirements upon the field of above.

The algebra of observables of the classical theory, or simply the classical algebra of observables, is conceived as the algebra constructed upon the subset $\mathscr{F}_{reg}(\mathbb{M})$, with the pointwise product and unity $\mathbf{1} : \phi \mapsto 1 \in \mathbb{C}$, for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$. The set $\mathscr{F}(\mathbb{M})$ is endowed with a vector space structure by pointwise operations. We define

$$(F+G)(\phi) := F(\phi) + G(\phi), \quad (\alpha F)(\phi) := \alpha F(\phi) \quad \forall F, G \in \mathscr{F}(\mathbb{M}),\, \forall \phi \in \mathcal{C}^\infty(\mathbb{M}),\, \forall \alpha \in \mathbb{C}.$$

Next,the algebra structure over $\mathscr{F}_{reg}(\mathbb{M})$ is implemented via

$$(F \cdot G)(\phi) := F(\phi)G(\phi)\; \forall F, G \in \mathscr{F}_{reg}(\mathbb{M}),\, \forall \phi \in \mathcal{C}^\infty(\mathbb{M}),$$

as in $\mathscr{F}_{reg}(\mathbb{M})$ the pointwise product of functionals is well defined. At the level of classical theories, the above algebraic structure will suffice for us, and thus we define the following.

Definition 19. *Consider the algebra $(\mathscr{F}_{reg}(\mathbb{M}), \cdot)$, endowed with an involution $*$ defined as $F^*(\phi) := \overline{F(\phi)}$ for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$, for all $F \in \mathscr{F}_{reg}(\mathbb{M})$. In addition, consider over this algebra a topology such that for all sequence $(F_j)_{j\in\mathbb{N}} \subset \mathscr{F}_{reg}(\mathbb{M})$, $F_j \to F \in \mathscr{F}_{reg(\mathbb{M})}$ if and only if $F_j^{(k)} \to F^{(k)}$ for all $k \in \mathbb{N}$, where $F^{(k)}$ denotes the k-th functional derivative of F, and the pointwise product is continuous. Then, the unital, topological $*$-algebra $\mathscr{A}^{CLS} := (\mathscr{F}_{reg}(\mathbb{M}), \cdot, *)$ is called the* ***off-shell algebra of classical observables***.

One may notice that the above algebraic structure $\mathscr{A}^{CLS}$ encompasses, at the level of observables, all but one essential aspect of the the field discussed above, since there is no requirement for the elements of $\mathscr{A}^{CLS}$ to be solutions of the equation of motion. The algebra of on-shell observables may be obtained as the quotient of off-shell observables with solutions to the equation of motion as follows.

Definition 20. *We define the* ***on-shell algebra of classical observables*** *as the algebra obtained from $\mathscr{A}^{CLS}$ by replacing $\mathscr{F}_{reg}(\mathbb{M})$ with $\mathscr{F}_{reg}(\mathbb{M})/I_P$ with the induced product, where I_P is the closed ideal generated by the differential operator P, as discussed section I.1.*

I.3.1 Quantum Algebra of Regular Observables

As a matter of fact, we shall not be as interested in the on-shell as in the off-shell algebra of observables. This will be the case since we shall later on be interested in interacting quantum field theories, and as interaction changes the dynamics, the quotient presented in the above definition will no longer be preserved. Therefore, in order to discuss the perturbative construction of an algebra of interacting observables in the next section, we shall consider only off-shell functionals. The dynamical information will then be transferred upon state, as we shall see further ahead.

Moving now to the algebra of observables of the quantum theory, it will be constructed via deformation of the algebraic product of $\mathscr{A}^{CLS}$, in order to produce a non commutative product which implements the canonical commutation relations. This procedure, called **deformation quantization**, involves the formal construction of a product in terms of the deformation parameter $\hbar$. We hence would like to construct a product over $\mathscr{F}_{reg}(\mathbb{M})$, denoted by $\star$, as

$$(F \star G)(\phi) := \sum_{n \geq 0} \hbar^n a_n(F, G)(\phi), \quad \forall \phi \in \mathcal{C}^\infty(\mathbb{M}), \, \forall F, G \in \mathscr{F}_{reg}(\mathbb{M}),$$

where the symbols $a_n(F, G)$ should be such that *(i)* $a_0(F, G) = F \cdot G$; *(ii)* if $F, G \in \mathscr{F}_{reg}(\mathbb{M})$ are linear functionals respectively induced by $f, g \in \mathcal{C}_0^\infty(\mathbb{M})$, then $a_1(F, G) - a_1(G, F) = i\hbar\Delta(f, g)\mathbf{1}$ is proportional to the causal propagator Δ associated to the Klein-Gordon equation of motion (I.21), given in equation (I.12). This construction will therefore make sense as a formal power series of $\hbar$, with finitely-many terms for $F, G \in \mathscr{F}_{reg}(\mathbb{M})$. These requirements are fulfilled by constructing the $\star$-product as follows.

Definition 21. *Let $\mathscr{F}_{reg}[\![\hbar]\!]$ denote the space of formal power series in $\hbar$ with coefficients in $\mathscr{F}_{reg}(\mathbb{M})$. We define the product $\star_{i\Delta/2} : \mathscr{F}_{reg}[\![\hbar]\!] \times \mathscr{F}_{reg}[\![\hbar]\!] \to \mathscr{F}_{reg}[\![\hbar]\!]$ as*

$$(F \star_{i\Delta/2} G)(\phi) := \sum_{n \geq 0} \frac{\hbar^n}{n!} \Big\langle F^{(n)}(\phi), \Big(\frac{i}{2}\Delta\Big)^{\otimes n} G^{(n)}(\phi) \Big\rangle = M \circ e^{\hbar \Gamma_{i\Delta/2}} (F \otimes G)(\phi) \quad \text{(I.22)}$$

for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$, where $M : (A \otimes B) \mapsto AB$ is the pointwise multiplication operator, $\Delta = \Delta_R - \Delta_A$ is the causal propagator of Klein-Gordon equation (I.21)*, and*

$$\Gamma_{i\Delta/2} : \mathscr{F}_{reg}[\![\hbar]\!] \otimes \mathscr{F}_{reg}[\![\hbar]\!] \to \mathscr{D}(\mathbb{M}), \quad \Gamma_{i\Delta/2} := \frac{i}{2} \int dx dy \, \Delta(x - y) \frac{\delta}{\delta\phi(x)} \otimes \frac{\delta}{\delta\phi(y)}. \quad \text{(I.23)}$$

The above definition produces an associative product over the space $\mathscr{F}_{reg}[\![\hbar]\!]$ which fulfills the requirements described in the previous paragraph. In fact, we are constrained to define $\star_{i\Delta/2}$ in terms of an infinite series of powers of $\hbar$ in order for associativity to hold. Nevertheles, by restricting to polynomial functionals, the product of observables will reduce to finitely-many terms. We are then in position to present a first step toward the general algebra of observables of the quantum theory, which is analogous to the Borchers-Uhlmann algebra of test functions for Wightman fields – see [Bor62].

Definition 22. *The topological unital $*$-algebra $\mathscr{A}^0_{reg} := (\mathscr{F}_{reg}[\![\hbar]\!], \star_{i\Delta/2}, *)$, where $\star_{i\Delta/2}$ is the product defined in* (I.22) *and $*$ and $\mathbf{1}$ are as in definition 19, is called the **off-shell quantum algebra of regular observables**. Its topology is the one induced by smooth, compactly supported functions.*

We refer to [KM15] for details. Again, in the above definition there is no requirement for the observables to fulfill the dynamical equation for the fields. For completeness, however, we define the on-shell regular algebra of observables by considering the quotient of the off-shell algebra with respect to the ideal generated by the differential operator P, as in definition 20.

Selecting observables only among regular functionals would exclude others of physical interest, such as ϕ^2 of ϕ^4, for instance. However, while for elements of $\mathscr{F}_{reg}(\mathbb{M})$ the product is easily defined, extending the quantum product to more general observables is a delicate task. It will be at this point that the microcausal observables $\mathscr{F}_{\mu C}(\mathbb{M})$ will become particularly important in our discussion. In addition, we notice that $\mathscr{F}_{reg}(\mathbb{M}), \mathscr{F}_{loc}(\mathbb{M}) \subset \mathscr{F}_{\mu C}(\mathbb{M})$. Moreover, though we have considered the topology on $\mathscr{A}^{CLS}$ as the topology induced by the pointwise product, as discussed in [Hör90, chapter 8], we see that such a topology supplies no information about the wave front sets of the derivatives of elements of $\mathscr{F}_{\mu C}(\mathbb{M})$. Since we would like to be able to define the multiplication of functionals via the continuous extension of the product in smooth cases, we first consider in the algebra of obervables the Hörmander pseudotopology.

Let $\Gamma \subset \mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$ a closed cone. We define the subset $\mathscr{D}'_\Gamma(\mathbb{M}) \subset \mathscr{D}'(\mathbb{M})$ of elements of $\mathscr{D}'(\mathbb{M})$ whose wave front set are contained in Γ,

$$\mathscr{D}'_\Gamma(\mathbb{M}) := \{u \in \mathscr{D}(\mathbb{M}) : WF(u) \subset \Gamma\}.$$

The elements of $\mathscr{D}'_\Gamma(\mathbb{M})$ are the distributions u such that, for any cone $V \subset \mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\})$ of directions around an arbitrary localization $f \in \mathcal{C}^\infty_0(\mathbb{M})$ of u such that $V \cap \Gamma = \emptyset$, the distribution is such that $\sup_{k \in V} |k|^N |\widehat{fu}(k)| < +\infty$ for all $N \in \mathbb{N}$ – see [Hör90, lemma 8.2.1]. We say $(u_j)_{j\in\mathbb{N}} \in \mathscr{D}'_\Gamma(\mathbb{M})$ converges to $u \in \mathscr{D}'_\Gamma(\mathbb{M})$ if and only if both

(i). $u_j \to u$ weakly in $\mathscr{D}'(\mathbb{M})$; and

(ii). $\sup_{k\in V} |k|^N |\widehat{fu}(k) - \widehat{fu_j}(k)| \to 0$ as $j \to +\infty$ for all $f \in C^\infty_0(\mathbb{M})$, for all $N \in \mathbb{N}$ and for all closed cone $V \subset \mathbb{R}^n \backslash \{0\}$ satisfying $V \cap \Gamma = \emptyset$.

This defines the Hörmander pseudo topology. We now consider a sequence

$$(\Gamma_j)_{j\in\mathbb{N}} \in T^*\mathbb{M}^j, \quad \Gamma_j := \left(\overline{V_+}^j \cup \overline{V_-}^j\right)^c$$

and define

$$\mathscr{F}_{\Gamma_j} := \{F \in \mathscr{F}_{\mu C}(\mathbb{M}) : WF(F^{(j)}(\phi)) \subset \Gamma_j, \ \forall \phi \in \mathcal{C}^\infty(\mathbb{M}), \ \forall j \in \mathbb{N}\},$$

We now set the Hörmander pseudo topology for functional in the following manner. We refer to [BF00] for details.

Definition 23. *We say $(F_n)_{n\in\mathbb{N}} \in \mathscr{F}_{\mu C}(\mathbb{M})$ converges to $F \in \mathscr{F}_{\mu C}(\mathbb{M})$ if and only if $F_n^{(j)}(\phi) \to F^{(j)}(\phi)$ in $\mathscr{D}'_{\Gamma_j}(\mathbb{M})$ for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$, for all $j, n \in \mathbb{N}$, with respect to the Hörmander pseudo topology for distributions. This defines the Hörmander pseudo topology in $\mathscr{F}_{\mu C}(\mathbb{M})$.*

The above will suffice for the topological description of the algebra of observables yet to be presented. As for its algebraic aspects, since the above definition of algebra of observables $\mathscr{A}^0_{reg}$ is restrictive, it is necessary to extend its product, introduced in definition 22, in order to include more singular objects. First, we notice that the wave front set of the causal propagator has the form

$$WF(\Delta) = \{(x, y, k_x, k_y) \in T^*\mathbb{M}^2\backslash\{0\} : (x, k_x) \sim (y, -k_y)\},$$

where again $(x, k_x) \sim (y, k_y)$ means there exists a null geodesics in $\mathbb{M}$ connecting x to y, to which the covector k_x is cotangent at x, and with k_x parallel-transported to k_y along this geodesics, as in section I.2. See [Bro+18] for details. Then, on the one hand, as the $\star_{i\Delta/2}$-product above encompasses the product between distributions $F^{(n)}$ and Δ, it is not always well defined for $F \in \mathscr{F}_{\mu C}(\mathbb{M})$. In the particular case of regular observables, this is not a problem, since, for $F \in \mathscr{F}_{reg}(\mathbb{M})$, each $F^{(n)}$ has empty wave front set. In contrast, the pointwise powers of Δ, which appear if we consider the $\star_{i\Delta/2}$-product of polynomial local fields, are themselves ill-defined. On the other hand, the presence of the causal propagator is necessary in order for $\star_{i\Delta/2}$ to produce the canonical commutation relations. We then see that a procedure of extension of $\mathscr{A}^0_{reg}$ requires the substitution of Δ in (I.22) by another bidistribution, which at the same time respects such commutation rules and the Hörmander criterion for the product of distributions. Formally, the extension product may me presented as below, at the level of expectation values. We shall first present an heuristic discussion on this topic, in order to connect the product deformation and algebra extension procedure to the common approach to regularization in physics literature [as per PS95, for instance]. We shall then move to a precise formulation of deformation quantization so to discuss the extension of $\mathscr{A}^0_{reg}$.

I.3.2 States, product deformation the algebra extension

It is possible to notice that the desired extension of the algebra of observables onto more singular, polynomial observables is the algebraic equivalent to the construction of Wick polynomials, which hence requires an algebraic implementation of normal ordering. For instance, one may attempt to construct the squared-field functional from linear functionals, by setting its integral kernel as

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

in some sense for this limit. This however results in divergent expectation values, due to the singular behaviour of states in the coinciding points limit. The subtraction of singular terms from the above limit corresponds to the algebraic normal ordering. Considering the vacuum state two-point function Δ_0^+ (all this will become clearer later in this section), this translates into the subtraction

$$\text{“} :\phi^2(x):_{\Delta_0^+} = \lim_{y\to x} \frac{\phi(x)\star\phi(y)+\phi(y)\star\phi(x)}{2} - \Delta_{0,S}^+(x,y)\text{”}, \tag{I.24}$$

again in some sense. We denote $\star \equiv \star_{i\Delta/2}$, and $\Delta_{0,S}^+$ is the vacuum state two-point function symmetric part, such that

$$\Delta_{0,S}^+ = \Delta_0^+ - \frac{i}{2}\Delta.$$

By evaluating $:\phi^2(x):_{\Delta_0^+}$ on states close to the vacuum (Hadamard states), we obtain meaningful expectation values. This will be made precise later in this section. I.e., only when the above limit is taken after subtracting the symmetric part of a state close to the vacuum, we would obtain finite expectation values, heuristically speaking, although the observable within the limit above is itself divergent

The implementation of the formal limit above depends hence upon explicitly removing such divergence. As presented in the orthodox literature of quantum field theory (e.g. [PS95]), in Minkowski spacetime this procedure corresponds to the subtraction of vacuum expectation values, or normal ordering. We then construct the regularized expectation value of the squared field, with respect to some state ω, as

$$\omega\Big(:\phi^2(x):_{\Delta_0^+} \Big) := \lim_{y\to x} \left[\omega\left(\frac{\phi(x)\star\phi(y)+\phi(y)\star\phi(x)}{2}\right) - \Delta_{0,S}^+(x,y)\right], \tag{I.25}$$

where the product of fields in the right hand side corresponds to the quantum product, and Δ_0^+ is the two-point function of Minkowski vacuum, provided the above limit is meaningful.

Equation (I.24) is a formal representation of the squared-field. Although the above expectation value (I.25) is well defined since we consider the subtraction of $\Delta_{0,S}^+$ prior to the limit of coinciding points, $:\phi^2:_{\Delta_0^+}$ itself is not an observable in $\mathscr{A}_{reg}^0$. In order to include this kind of object into the algebra, it is necessary to deform the product $\star_{i\Delta/2}$, in order to regularize pointwise products of fields. This corresponds to the algebraic version of normal ordering. As we shall see below, this algebra extension is isomorphic to the algebra $\mathscr{A}_{reg}^0$ in definition 21.

The above procedure contains two limitations, though. First, in the spirit of AQFT, we would like to be able to introduce normal ordering in a state-independent manner. I.e., we would like to obtain an algebra of observables which does not depend on the choice of the state, whereas the extension described in the last paragraph is state dependent. Second, although the subtraction above may be meaningful in Minkowski spacetime, it may not be the case in a more general situation with curved background, which lacks for a preferred vacuum state. We see that the divergent behaviour of the expectation values of field polynomials are caused by the high frequency part of the state[3], which corresponds to measurements performed in small regions of spacetime, isomorphic to $\mathbb{M}$. Therefore, we may expect a more general subtraction of singularities mechanism to involve a state with the same divergent behaviour of the Minkowski vacuum, which motivates the definition of Hadamard state below. The algebraic extension might thus be seen as the algebraic equivalent of Wick polynomials construction, and requires a discussion about states on the algebra of quantum observables.

Definition 24. *Let $\mathscr{A}$ be a topological, unital $*$-algebra. A **state** $\omega : \mathscr{A} \to \mathbb{C}$ is a positive, normalized and continuous linear functional over $\mathscr{A}$. This means that $\omega(A^*A) \geq 0$ for all $A \in \mathscr{A}$ (positivity), and $\omega(\mathbf{1}) = 1$ (normalization), where $\mathbf{1}$ is the unity in $\mathscr{A}$ (normalization).*

Though we first discuss states over $\mathscr{A}^0_{reg}$, since this is the unique quantum algebraic structure we have constructed up to the present moment, much of the discussion below may be naturally extended to the algebras we shall obtain at the end of this section.

A state over the regular algebra $\mathscr{A}^0_{reg}$ is completely defined by its n-point functions. Namely, if $\Phi_f \in \mathscr{A}^0_{reg}$ represents the linear operator introduced in equation (I.17), then ω is completely characterized by the set of (generalized) n-point functions

$$\omega_n(f_1, \ldots, f_n) := \omega\left(\Phi_{f_1} \star_{i\Delta/2} \cdots \star_{i\Delta/2} \Phi_{f_n}\right),$$

which are distributions over $\mathcal{C}^\infty_0(\mathbb{M})^n$. A **Gaussian**, or **quasi-free** state, in particular, is such that for all $n \in 2\mathbb{N}$ its n-point function is characterized by its two-point function as

$$\omega_n(f_1, \ldots, f_n) = \sum_{\sigma_n \in S_n} \prod_{j=1}^{n/2} \omega_2\left(f_{\sigma_n(2j-1)}, f_{\sigma_n(2j)}\right),$$

and it is zero if $n \in \mathbb{N}$ is odd. Here, S_n denotes the set of all ordered permutations of n elements: if $\sigma_n \in S_n$, then

$$\sigma_n(2j-1) < \begin{cases} \sigma_n(2j), & 1 \leq j \leq n/2 \\ \sigma_n(2j+1), & 1 \leq j < n/2. \end{cases}$$

The definition of the $\star_{i\Delta/2}$-product over $\mathscr{A}^0_{reg}$ then implies that the anti-symmetric part of the two-point function of a state is

$$\omega_2(f, g) - \omega_2(g, f) = i\hbar\Delta(f, g).$$

This corresponds to the canonical commutation relations at the level of states. Finally, the equation of motion is implemented over the states $\omega : \mathscr{A}^0_{reg} \to \mathbb{C}$ by requiring them to be bisolutions to the dynamical equation, in the sense of

$$\omega_2(Pf, g) = \omega_2(f, Pg) = 0,$$

[3]This is analogous to normal ordering as introduced in the physics literature, reinterpreted as the removal of high frequencies, instead of merely the "placement of creation operator at left".

thus justifying our previous excuses for effectively ignoring the on-shell algebras of observables. In addition, we shall use the term two-point function to refer to both the bidistribution and its formal integral kernel.

Definition 25. *A state $\omega : \mathscr{A}^0_{reg} \to \mathbb{C}$ is called a **Hadamard state** if its truncated functions at all orders n with $n \neq 2$ are smooth, and, in addition, if one, and hence both the equivalent conditions below regarding its two-point function are satisfied:*

(i). its wave front set has the form

$$WF(\omega_2) = \{(x, y, k_x, k_y) \in T^*\mathbb{M}^2 \backslash \{0\} : (x, k_x) \sim (y, -k_y),\ k_x \rhd 0\},$$

where $(x, k_x) \sim (y, k_y)$ means there exists a null geodesics in $\mathbb{M}$ connecting x to y, to which the covector k_x is cotangent at x, and with k_x parallel-transported to k_y along this geodesics; in addition, $k_x \rhd 0$ means k_x future directed.

(ii). if for every $x_0 \in \mathbb{M}$ there exists a geodesically convex neighbourhood $N \subset \mathbb{M}$ of x_0 such that the formal integral kernel of ω_2 on $N \times N$, which we denote with the same symbol, has the form

$$\omega_2(x, y) = H(x, y) + W(x, y),$$

where

$$H(x, y) := \lim_{\varepsilon \to 0+} \left[\frac{U(x, y)}{\sigma_\varepsilon(x, y)} + V(x, y) \log \frac{\sigma_\varepsilon(x, y)}{l^2} \right], \tag{I.26}$$

with $\sigma_\varepsilon(x, y) := \sigma(x, y) + i2(x_0 - y_0)\varepsilon - \varepsilon^2$, σ half the square of the geodesic distance between x and y, and l is an arbitrary length scale which assures the logarithm's argument to be dimensionless. In addition, $U, V : N \times N \to \mathbb{R}$ are known, fixed smooth functions, called Hadamard coefficients, and $W : \mathbb{M} \times \mathbb{M} \to \mathbb{C}$ is a smooth function which characterizes the state.

We hence notice that, in order to classify a quasi-free Hadamrd state, it suffices to consider its two-point function.

We recall that a subset $O \subset M$ of a Lorentzian manifold M is geodesically convex if, for each pair of points $x, y \in O$, there exists a unique geodescis $\gamma : I \subset [0, 1] \to O$ connecting x to y. The coefficients U and V are entirely determined by the dynamical equation and the geometry of spacetime, and are both such that $PV = 0$ at each argument, whereas U satisfies

$$\partial_\mu U \partial^\mu \sigma - \frac{1}{2}\big(\Box_x \sigma - 4\big)U = 0.$$

Moreover, the coefficient V may be written as a series

$$V(x, y) = \sum_{n=0}^{+\infty} v_n \sigma^n(x, y)$$

with smooth coefficients v_n. In Minkowski spacetime, this series converges for all $x, y \in \mathbb{M}$ and gives a suitable Bessel function $K_1(m\sqrt{\sigma})$, see [BDF09], appendix A for details. The local expression for the two-point function of a particular Hadamard state in *(ii)* may be generalized to globally hyperbolic spacetimes. We refer to [KM15] for the details and a discussion on the existence of Hadamard states in globally hyperbolic spacetimes. The smooth function W, however, is characteristic of the state itself. For a given state ω, the difference $H = \omega_2 - W$ is called **Hadamard parametrix**.

The equivalence between conditions *(i)* and *(ii)* in the above definition 25 was established and explored in [Rad96b; Rad96a], a series of works which allowed the introduction of microlocal analysis into algebraic quantum field theory.

We now return to the problem of extending the algebra $\mathscr{A}^0_{reg}$ in order that we might consider more singular observables. Our main problem is the fact that definition 22 is too restrictive to contain physically interesting observables in the context of interacting theories, which would be found in $\mathscr{F}_{loc}(\mathbb{M})$ rather than $\mathscr{F}_{reg}(\mathbb{M})$. This extension procedure is preceded by a deformation of $\star_{i\Delta/2}$ which applies to microcausal observables in $\mathscr{F}_{\mu C}(\mathbb{M})$.

Looking back at the wave front set of Δ, we notice that, with the removal of $\{0\}$ from $T^*\mathbb{M}^2$, it is formed by two connected components. We hence decompose the causal propagator as the difference between two bidistributions,

$$\frac{i}{2}\Delta = \Delta^+ - \Delta^-, \tag{I.27}$$

with the requirements

$$WF(\Delta^\pm) = \{(x, y, k_x, k_y) \in WF(\Delta) : \pm k_x^0 \triangleright 0\}.$$

We observe that this is nothing but an asymptotic version of frequency decomposition for the causal propagator. I.e., this corresponds to decomposing the propagator into components which, asymptotically, present the same spectral decomposition as the Minkowski vacuum Δ_0^+, which is supported within the positive cone $k^0 \triangleright 0$. Such a decomposition always exists for globally hyperbolic spacetimes, though it is not unique. In fact, comparing the present situation with the definition 25 of Hadamard states, we realize that such decomposition may be obtained by means of a Hadamard state ω, using ω_2 instead of Δ^+. Given $\omega : \mathscr{A}^0_{reg} \to \mathbb{C}$ a Hadamard state, we define the alternative product $\star_\omega$ as, for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$ and for all $F, G \in \mathscr{F}_{reg}(\mathbb{M})$,

$$(F \star_\omega G)(\phi) := \sum_{n \geq 0} \frac{\hbar^n}{n!} \left\langle F^{(n)}(\phi), \omega_2^{\otimes n} G^{(n)}(\phi) \right\rangle = M \circ e^{\hbar \Gamma_\omega} (F \otimes G)(\phi) \tag{I.28}$$

where M is the multiplication operator as before and $\Gamma_\omega : \mathscr{F}_{reg}(\mathbb{M}) \otimes \mathscr{F}_{reg}(\mathbb{M}) \to \mathscr{D}(\mathbb{M})$ is given as in equation (I.23), with the replacement of $i\Delta/2$ by the two-point function of ω,

$$\Gamma_\omega := \int dxdy\, \omega_2(x, y) \frac{\delta}{\delta\phi(x)} \otimes \frac{\delta}{\delta\phi(y)}. \tag{I.29}$$

Considering instead the operator Γ_H constructed in a similar manner with the parametrix H instead of the two-point function ω_2, we define the map

$$\alpha_H := e^{\frac{\hbar}{2}\left\langle H, \frac{\delta^2}{\delta\phi^2}\right\rangle} : \mathscr{F}_{reg}(\mathbb{M}) \to \mathscr{F}_{reg}(\mathbb{M}) \tag{I.30}$$

such that for $F, G \in \mathscr{F}_{reg}(\mathbb{M})$, we obtain

$$F \star_\omega G = \alpha_H\big(\alpha_H^{-1} F \star_{i\Delta/2} \alpha_H^{-1} G\big).$$

This substantially concludes the algebraic implementation of normal ordering, as the $\star_\omega$-product in (I.28) has been constructed by removing the singular part from the propagator. In addition, the maps α_H in equation (I.30) allow for a precise representation of the formal expression (I.25), such that the regularized square field $:\phi^2:_{\Delta_0^+}$ above is associated to ϕ^2 itself via $\alpha_{\Delta_0^+}(:\phi^2:_{\Delta_0^+}) = \phi^2$. That is, the maps α reduce to the identity when applied to regularized polynomials with respect to the same parametrix. This analogy between the formal limit and exact objects may be concretely seen from the following example.

As presented in [FR15a], consider the sequence of functionals $(F_n)_{n\in\mathbb{N}}$, with

$$F_n(\phi) := \int dxdy\, f(x) g_n(x-y)\phi(x)\phi(y), \quad g_n, f \in \mathcal{C}_0^\infty(\mathbb{M}),$$

such that the sequence $(g_n)_{n\in\mathbb{N}}$ is an approximation to the δ-function. Denoting by H_S the symmetric part of the function H from equation (I.26), we then have for each $n \in \mathbb{N}$

$$\begin{aligned}\alpha_H^{-1} F_n &= \int dxdy \left[f(x)g_n(x-y)\phi(x)\phi(y) - H_S(x,y) f(x) g_n(x-y)\right] \\ &= \int dxdy \left[\phi(x)\phi(y) - H_S(x,y)\right] f(x) g_n(x-y).\end{aligned}$$

We hence denote $:\phi^2(x):_H \doteq \lim_{y\to x} \phi(x)\phi(y) - H_S(x,y)$, in the sense of $\alpha_H^{-1}(\phi^2)$, where the limit corresponds to the limit $n\to\infty$ in the previous expression, in the sense of distributions. At the level of expectation values, the procedure of explicitly subtraction of a Hadamard parametrix is called **point splitting regularization**, which, in light of what has just been discussed, may be understood in the sense of algebraic regularization. This will be of particular importance in chapter IV of this thesis. Last, we may also notice that α_H^{-1} contains Wick's theorem by computing, in terms of formal integral kernels,

$$\begin{aligned}:\phi^2(x):_H :\phi^2(y):_H =: \alpha_H^{-1}\Big(\phi^2(x) \star_\omega \phi^2(y)\Big) &= (\alpha_H^{-1}\phi^2) \star_{i\Delta/2} (\alpha_H^{-1}\phi^2) \\ &=: \phi^2(x)\phi^2(y):_H + i2 :\phi(x)\phi(y):_H H(x,y) - \frac{1}{2} H^2(x,y),\end{aligned}$$

which agrees with the calculation in [PS95], for instance, regarding Wick's theorem. An explicit calculation may be found in [FR15a].

As a result, not only the map α_H allows for a deformation of $\star_{i\Delta/2}$ over regular functionals into $\star_\omega$, but it also may be employed in order to extend the algebra of observables. With this product we may extend definition 21 to $\mathscr{F}_{\mu C}(\mathbb{M})$ as follows, cf. [FR15a; FR15b].

Definition 26. *For any given Hadamard state $\omega : \mathscr{F}_{reg}(\mathbb{M}) \to \mathbb{C}$, the topological unital $*$-algebra $\mathscr{A}^0_{\mu C} := (\mathscr{F}_{\mu C}[\![\hbar]\!], \star_\omega, *)$, $\mathscr{A}^0_{\mu C} \equiv \mathscr{A}^0$, endowed with the Hörmander pseudo topology, where $\star_\omega$ is the product defined in* (I.28) *and $*$ is as in definition 19, is called the off-shell **quantum free algebra of observables**, or **algebra of free observable**, for shortness.*

Considering the set of microcausal functionals supported in a relatively compact region $O \subset \mathbb{M}$, denoted as $\mathscr{F}_{\mu C}(O)$, we obtain the algebra of local observables of O, denoted $\mathscr{A}^0(O)$, cf. discussed in the introduction of this thesis in the context of Haag-Kastler axioms. Therefore, with the family of maps α in (I.30), labeled by the choice of parametrix H, we obtain an algebra structure which is independent of the state ω. In fact, at this point we have an abstract structure $\mathfrak{U}$, given as the family $\{(\mathscr{F}_{reg}(\mathbb{M}), \star_\omega)\}_\omega$, labeled by different choices of ω_2 in definition (I.28). Then, to each possible choice of state corresponds a concrete algebra. The state independence to which we refer here corresponds to the fact that all these concrete algebras are $*$-isomorphic. In order to present this algebra isomorphism, let $\mathscr{A}^0_1$ and $\mathscr{A}^0_2$ be as in definition 26, with the product $\star_{\omega_i}$ of $\mathscr{A}^0_i$ being given in terms of a Hadamard state ω_i, $i = 1, 2$ and $\omega_1 \neq \omega_2$. Then $\omega_1 - \omega_2$ is a smooth function and $\mu : \mathscr{A}^0_1 \to \mathscr{A}^0_2$,

$$\mu := \alpha_{\omega_2 - \omega_1}, \tag{I.31}$$

is a $*$-isomorphism, as may be seen by composing the map μ with the right hand side of equation (I.28).

When calculating expectation values of observables, a convenient choice of the $\star$-product will be the one constructed upon the state with respect to which the expectation values are calculated, since this choice produces

$$\omega(F \star_\omega G) = F \star_\omega G\Big|_{\phi=0}. \tag{I.32}$$

This follows from the fact that for linear observables Φ_f, Φ_g,

$$\omega\left(\Phi_f \star_\omega \Phi_g\right) = \omega\left(\Phi_f \cdot \Phi_g\right) + \hbar\omega_2(f, g),$$

and as the left hand side equals the two-point function of ω, the expectation value of the pointwise product $\Phi_f \cdot \Phi_g$ is zero. This may be iterated to arbitrary polynomial functionals in $\mathscr{F}_{\mu C}[\![\hbar]\!]$ to justify (I.32). The gaussian state $\omega : \mathscr{F}_{reg}(\mathbb{M}) \to \mathbb{C}$ may then be extended to microcausal observables via its n-point function as

$$\omega(F_1 \star_\omega \cdots \star_\omega F_n) = F_1(\phi) \star_\omega \cdots \star_\omega F_n(\phi)|_{\phi=0}, \quad \forall F_j \in \mathscr{A}^0 = (\mathscr{F}_{\mu C}[\![\hbar]\!], \star_\omega), j = 1, \ldots, n,$$

for all $n \in \mathbb{N}$. A general expression may be obtained by means of the $*$-isomorphism (I.31). From now on, we shall denote the non commutative product simply as $\star$, omitting the state or the propagator in the subscript whenever its choice is implicit.

One should not understand the $*$-isomorphism between two algebras $(\mathscr{F}_\mu C, \star_{\omega_i})$, which differ by the choice of Hadamard state in the construction of the product, with invariance of expectation values under this algebra isomorphism. The change $\star_{i\Delta/2} \to \star_\omega$, in the sense of the extension from definition 21 to definition 26, corresponds to the algebraic version of the Wick theorem, thus differences are to be expected in expectation values computations $\omega(F \star_1 G)$, $\omega(F \star_2 G)$, with respect to different regularizations. This difference is illustrated, for instance, when considering the expectation values of the squared-field with respect to a thermal equilibrium state, when normal ordering is implemented by means of the vacuum state. This example consists of the emergence of a thermal mass, a phenomenon which will be presented in the next chapter, when we shall introduce thermal aspects of quantum field theory.

At this point we close the circle which we started at the end of previous section. We presented microcausal functionals in definition 18 as a particular, abstract generalization of regular and local functionals, which contains physically meaningful observables not in $\mathscr{F}_{reg}(\mathbb{M})$. Among regular functionals, we then defined a non-commutative product $\star_{i\Delta/2}$, which produces the quantum algebra of regular observables $\mathscr{A}^0_{reg}$. However, as we have argued that this algebra is far too restrictive, we presented an extension of $\star_{i\Delta/2}$ to observables in $\mathscr{F}_{\mu C}(\mathbb{M})$. This has been performed in two steps: first we considered the deformation of $\star_{i\Delta/2}$ into $\star_\omega$ via the map α_H. Then, we argued that the $\star$-product may be extended to microcausal observables, and used such extension to define the algebra $\mathscr{A}^0$. As such extension is performed by using Hadamard states, we observe, first, that it may be both locally and globally characterized in equivalent manners; second, when comparing $WF(\omega)$ for a Hadamard state with $WF(F)$ for any $F \in \mathscr{F}_{\mu C}(\mathbb{M})$, the product is a well-defined extension of the product between regular observables. This whole procedure may be depicted in the diagram below,

$$\begin{array}{ccc} \mathscr{A}^{CLS}_{reg} = (\mathscr{F}_{reg}(\mathbb{M}), \cdot) & \xrightarrow{\;Quantization\;} & \mathscr{A}^0_{reg} = (\mathscr{F}_{reg}[\![\hbar]\!], \star_{i\Delta/2}, *) \\ & & \alpha_\omega \updownarrow \star\ deformation \\ \mathfrak{A}^0 \ni \mathscr{A}^0 = (\mathscr{F}_{\mu C}[\![\hbar]\!], \star_\omega, *) & \xleftarrow[Extension]{} & (\mathscr{F}_{reg}[\![\hbar]\!], \star_\omega, *) \in \mathfrak{A}_{reg} \end{array}$$

where each $\mathfrak{A}$ denotes the abstract algebra of formal power series of $\hbar$ with coefficients in the respective space of functional, labeled by different choices of $\star$-product.

We have generally defined states as continuous, positive and normalized complex-valued linear functionals over a $*$-algebra, and used gaussian states in the extension procedure for the algebra of formal power series of $\hbar$ with coefficients in $\mathscr{F}_{\mu C}(\mathbb{M})$. Therefore, although the conditions of normalization and continuity remain unchanged in the context of algebras of formal power series, the positivity of ω will be considered in the following sense: if A denotes a formal power series in $\hbar$, then we require $\omega(A \star A^*) \geq 0$.

Finally, dynamics is introduced into the algebra of free observables $\mathscr{A}^0$ by means of a particular one-parameter group of automorphism $(\alpha_t)_{t\in\mathbb{R}}$.

Definition 27. *The pair* $\big(\mathscr{A}, (\alpha_t)_{t\in\mathbb{R}}\big)$ *where* $\mathscr{A}$ *is some unital* $*$*-algebra and* $(\alpha_t)_{t\in\mathbb{R}}$ *is a one-parameter group of* $*$*-automorphism is called a* ***dynamical system****.*

In the particular case of the algebra $\mathscr{A}^0$, we consider the **free dynamics** given by the maps $\alpha_t : \mathscr{A}^0 \to \mathscr{A}^0$ as

$$\alpha_t F(\phi) := F(\phi_t), \quad \phi_t(x_0, \mathbf{x}) := \phi(x_0 + t, \mathbf{x}) \quad \forall x \in \mathbb{M}, \forall t \in \mathbb{R}, \tag{I.33}$$

for all $F \in \mathscr{A}^0$ and for all $\phi \in \mathcal{C}^\infty(\mathbb{M})$. More generally, the action of Poincaré group $\mathscr{P}$ over the algebra $\mathscr{A}^0$ is given by the group of automorphisms

$$\mathscr{P} \ni (\Lambda, \tau) \mapsto \alpha_{(\Lambda,\tau)} : \mathscr{A}^0 \to \mathscr{A}^0, \quad \alpha_{(\Lambda,\tau)} F(\phi) := F(\phi_{(\Lambda,\tau)}).$$

I.4 Algebraic structure of interacting theories

So far we have considered only observables of the free theory. These have been built upon field configurations which satisfy the linear equation of motion (I.21), with the two fundamental solutions Δ_R and Δ_A as in equation (I.10), completely characterized by their supports. Though the dynamical equation has not been explicitly implemented at the algebraic level, in the sense that we have focused on the off-shell algebra of observables, the construction of $\mathscr{A}^0_{reg}$ depends on the existence and uniqueness of the causal propagator $\Delta = \Delta_R - \Delta_A$, as in equation (I.22) the algebraic product was built upon Δ. In addition, when extending the algebra of observables, any $\star_\omega$-product is built from the two-point function of a bisolution of (I.21), whose antisymmetric part is again proportional to Δ. Therefore, even when considering only the off-shell algebra of observables, each construction is based on the dynamical equation (I.21), through its fundamental solutions $\Delta_{R/A}$.

Nevertheless, in practical situations we are usually interested in considering a system described by the lagrangian funcional

$$\mathcal{L}(\phi) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \mathcal{L}_I(\phi), \tag{I.34}$$

corresponding to a real scalar field propagating over Minkowski space according to the dynamical equation

$$\big(\Box + m^2\big)\phi = V'(\phi), \quad V \in \mathscr{F}_{loc}[\![\hbar]\!],\ V(\phi) = \int dx\, f(x)\mathcal{L}_I(x), \quad f \in \mathscr{D}(\mathbb{M}) \tag{I.35}$$

and where $\mathcal{L}_I$ is a local interaction term, which contains pointwise products of the field. Therefore, for non-linear polynomial interactions, the potential V requires normal ordering, resulting in the functional $:V:_H$ such as discussed previously. In these situations, we are usually left with perturbation theory for the algebraic description of the physical system. In the above expression, the smooth and compactly supported function f is a cutoff for the interaction term, which prevents the appearance of infrared interactions in the theory. In the long run, we are often interest in the so called

adiabatic or **thermodynamic** limit. Heuristically, this consists of an extension in the support of f, $f \to 1$, onto the whole space, and which we shall precisely consider in the following sense. Suppose the cutoff function is given in terms of separate functions as

$$\mathbb{M} \ni x \mapsto f(x) = \chi(x_0)h(\mathbf{x}), \quad \chi \in \mathcal{C}_0^\infty(\mathbb{R}),\ h \in \mathcal{C}_0^\infty(\mathbb{R}^3), \tag{I.36}$$

where χ is such that, for some arbitrary but fixed $\varepsilon > 0$,

$$\operatorname{supp} \chi \subset [-2\varepsilon, +2\varepsilon], \quad \chi|_{[-\varepsilon,+\varepsilon]} \equiv 1. \tag{I.37}$$

This choice may be interpreted as corresponding to the interaction term being turned on at $x_0 = -2\varepsilon$, smoothly increasing until $x_0 = -\varepsilon$, when it stabilizes and remains on until it is smoothly turned off. In order to be absolutely precise, we should consider both χ and h as functions on Minkowski space, but throughout this text we shall regard both as functions on the given coordinates. Thus, the adiabatic limit consists of an inductive limit $h \to 1$, the so-called van Hove limit that we shall discuss in this section, while χ is held fixed. The resulting functional hence describes an interaction term supported everywhere in space, but with a time cutoff given by χ. The particular form of the function χ will be further addressed at the end of this section, in view of the Fredenhagen and Lindner's description of a thermal equilibrium state for the perturbative theory [FL14], to be discussed in the next chapter. Finally, we should clarify that, although in the physics literature it is often the limit $\chi \to 1$ that is called adiabatic limit, whereas the previously considered limit $h \to 1$ is frequently referred to as thermodynamical limit, we shall use both the terminologies "adiabatic" or "thermodynamic" always to refer to the inductive limit $h \to 1$, for fixed χ.

Our approach towards perturbative theories mimics the Bogoliubov's analysis presented in [BS80], which is based on representing interacting observables as the functional derivative of a formal S-matrix, the exponential of the interacting lagrangian with respect to the time-order product. Therefore, in this section we first briefly introduce time-ordered products of local observables, which will allow us to define the formal S-matrix and the Bogoliubov map. In this way we end up with a formal representation of interacting observables within the free algebra $\mathscr{A}^0$. Finally, we shall briefly discuss the principle of perturbative agreement presented in [HW05; DHP17], which concerns the equivalence between the perturbative and the exact approach to ressummable theories. We also briefly discuss regularization methods for the time-ordered product, but we shall focus on the regularization of diagrams appearing in the estimations in the chapters III and IV.

I.4.1 The time-ordered product for regular observables

Once a $\star$-product has been fixed for the algebra $\mathscr{A}^0$, we may construct the time-ordered product of functionals. This is defined for local observables, and should satisfy the causal factorization property

$$T(F,G) = \begin{cases} F \star G, & \text{if } F \succ G; \\ G \star F, & \text{if } G \succ F, \end{cases} \tag{I.38}$$

where the notion of succession is established as $F \succ G$ if and only if there exists a Cauchy surface $\Sigma \subset \mathbb{M}$ such that $\operatorname{supp} F \subset J_+(\Sigma)$, $\operatorname{supp} G \subset J_-(\Sigma)$. In the particular case of regular functional $F, G \in \mathscr{F}_{reg}(\mathbb{M})$, equation (I.38), along with bilinearity, completely characterizes the map T. It is then possible to notice that the obtained map $T : \mathscr{F}_{reg}[\![\hbar]\!] \otimes \mathscr{F}_{reg}[\![\hbar]\!] \to \mathscr{F}_{reg}[\![\hbar]\!]$ is unambiguously defined over regular functionals as

$$T(F,G) := \sum_{n\geq 0} \frac{\hbar^n}{n!} \Big\langle F^{(n)}(\phi), \Delta_F^{\otimes n} G^{(n)}(\phi) \Big\rangle = M \circ e^{\hbar \Gamma_F} (F \otimes G)(\phi) \quad \forall \phi \in \mathcal{C}^\infty(\mathbb{M}), \tag{I.39}$$

where $\Gamma_F : \mathscr{F}_{reg}[\![\hbar]\!] \otimes \mathscr{F}_{reg}[\![\hbar]\!] \to \mathscr{D}(\mathbb{M})$ is given as in equation (I.29). In addition, if Δ^+ denotes the two-point function of a quasi-free Hadamard state, which is employed in the $\star$-product, then Δ_F is the Feynman propagator associated to Δ^+, which is given by

$$\Delta_F := \Delta^+ + i\Delta^A, \tag{I.40}$$

with Δ_A the advanced propagator of the free Klein-Gordon equation (I.21), as in equation (I.10). In the particular case $\Delta^+ = \Delta_0^+$, the vacuum state two-point function, Δ_F is the usual Feynman propagator. The properties of Δ_F stated below follow directly from its definition and the properties of the propagators presented so far.

Proposition 10. *The Feynman propagator* (I.40) *is a bidistribution which may be written in the equivalent ways*

$$\begin{aligned} \Delta_F(x) &= \Delta^+(x) + i\Delta_A(x) = \Delta^-(x) + i\Delta_R(x) \\ &= \frac{1}{2}\Big\{ \Delta^+(x) + \Delta^-(x) + i\Big[\Delta_R(x) + \Delta_A(x)\Big] \Big\} \end{aligned}$$

In addition, if Δ^+ is translation invariant, then so is the Feynman propagator. Its formal integral kernel then $\Delta_F(x,y)$ reduces to $\Delta_F(x)$, denoted with the same symbol.

Equation (I.39) above may be constructed for regular functionals by writing the time-ordered product of arbitrary regular observables as

$$T(F,G)(\phi) = \sum_{n\geq 0} \hbar^n b_n(F,G)(\phi),$$

and comparing this expansion with condition (I.38). From the first order term, by using the properties of the retarded and advanced propagators and the given conditions on the supports of the functionals, we obtain

$$b_1(\Phi_f, \Phi_g) = \begin{cases} \Delta^+(f,g), & \text{if } \operatorname{supp} f \succ \operatorname{supp} g; \\ \Delta^-(f,g), & \text{if } \operatorname{supp} g \succ \operatorname{supp} f. \end{cases}$$

The two conditions above are combined in $b_1(F,G) = \Delta_F(f,g)$ by using the Feynman propagator, whose wave front set is

$$WF(\Delta_F) = WF(\delta) \cup C_F, \tag{I.41}$$

with $C_F := \{(x,y,k,-k) \in T^*\mathbb{M}^2 \backslash \{0\} : (x_0 - y_0)^2 - |\mathbf{x} - \mathbf{y}|^2 = 0,\, x_0 - y_0 \neq 0, k^0 = \lambda(x_0 - y_0),\, k^i = -\lambda(x_i - y_i),\, \lambda > 0\}$ – see [BDH14] and references there mentioned. We thus conclude that the map T may be defined at all orders as in (I.39), provided $\text{supp}\, f \cap \text{supp}\, g \neq \{0\}$. In fact, considering the translation invariance of the propagators, for regular functionals the causal factorization property (I.38) defines the time-ordered product up to the origin $0 \in \mathbb{M}$, or, equivalently, up to the thin diagonal $diag(\mathbb{M}^2)$. The map T then may be uniquely extended by continuity to the whole of $\mathbb{M}$, and therefore we may affirm that equation (I.38) or (I.39) both completely and equivalently define T for regular functionals. In conclusion, we obtain over $\mathscr{A}^0_{reg}$ an additional product, which satisfies the following properties.

Proposition 11. *The map $T : \mathscr{F}_{reg}[\![\hbar]\!] \times \mathscr{F}_{reg}[\![\hbar]\!] \to \mathscr{F}_{reg}[\![\hbar]\!]$ as defined in* (I.39) *is an associative, commutative product between regular functionals, which, in addition, is $*$-isomorphism to the pointwise product.*

Proof. Associativity is explicitly verified as for the $\star$-product in (I.22). Commutativity follows from the symmetry of the Feynman propagator Δ_F. The map

$$T = e^{\hbar \Gamma_F} : \mathscr{F}_{reg}[\![\hbar]\!] \to \mathscr{F}_{reg}[\![\hbar]\!], \quad G \mapsto \sum_{n \geq 1} \frac{\hbar^n}{n!} \big\langle G^{(2n)}, \frac{1}{2}\Delta_F^{\otimes n} \big\rangle$$

is invertible and may be seen as an extension, or completion of the map defined in (I.39), equivalent to taking the time-ordered product of some observable with $\mathbf{1}$. It produces the algebra $*$-isomorphism in the sense of $T(F,G) = T(T^{-1}F \cdot T^{-1}G)$. □

Throughout the text, we shall intertwine two equivalent notations for the time-ordered product, $T(F,G) \equiv F \cdot_T G$. The time-ordered product T may be extended from regular to local functionals, but in this case the construction is not unique. Besides, along the thin diagonal of $\mathbb{M}^2$, where the product with local functional could be not well defined, an extension for powers of the Feynman propagator would be required. The extension of T onto $\mathscr{F}_{loc}$ is a fundamental part in the treatment of interacting theories, which we briefly discuss next.

In order to extend the T-product to local functionals of a real scalar theory, we consider for each $n \in \mathbb{N}_0$ maps

$$T_n : \mathscr{F}_{loc}[\![\hbar]\!]^n \to \mathscr{A}^0, \quad T_n(F_1, \ldots, F_n) := F_1 \cdot_T \cdots \cdot_T F_n.$$

Each map T_n is required to fulfill the following conditions.

I. $T_0 \equiv \mathbf{1} \in \mathscr{A}^0_{loc}$, $T_1 = id : \mathscr{F}_{loc}[\![\hbar]\!] \hookrightarrow \mathscr{A}^0_{loc}$;

II. (Causal factorization property) if $(\cup_{j=1}^{n-k}\mathrm{supp}\, F_j) \cap (\cup_{l=n-k+1}^{n} J_{-}\mathrm{supp}\, F_l)$, then $T_n(F_1, \ldots, F_n) = T_{n-k}(F_1, \ldots, F_{n-k}) \star_\omega T_k(F_{n-k+1}, \ldots, F_n)$ – an extension of property (I.38);

III. The map $T_n(F_1, \ldots, F_n) : \mathcal{C}^\infty(\mathbb{M}) \to \mathbb{C}$ depends on $\phi \in \mathcal{C}^\infty(\mathbb{M})$ only via the functional derivatives the functionals F_j at ϕ, $j = 1, \ldots, n$, for all $n \in \mathbb{N}_0$, thus extending the form of expression (I.39);

IV. for all $n \in \mathbb{N}_0$, T_n is symmetric;

V. (Unitarity) $T^*(F_1, \ldots F_n) = \overline{T}(F_1^*, \ldots, F_n^*)$, where $\overline{T}$ is the anti-time ordering

$$\overline{T}_n(F_1, \ldots, F_n) := n! \sum_{\sigma \in \mathbb{P}_n} (-1)^{n+|\sigma|} \prod_{I \in \sigma} \frac{1}{\#I!} T_{\#I}\Big(F_1, \ldots, F_{\#I}\Big),$$

where $\mathbb{P}_n$ is the set of pairwise disjoint partitions of the set $\{1, \ldots, n\}$, $\#I$ denotes the cardinality of the partition, and $\prod$ refers to the $\star$-product.

VI. (Covariance) Let $\alpha_{(\Lambda,\tau)}$ denote the action of Poincaré group $\mathscr{P}$ on $\mathscr{F}_{loc}(\mathbb{M})$, then $\alpha_{(\Lambda,\tau)} \circ T_n = T_n \circ \alpha_{(\Lambda,\tau)}$

In [EG73], Epstein and Glaser proved that such maps T_n, satisfying conditions I-IV, may be recursively constructed for quantum field theories in Minkowski space. In order to construct time-ordered products of local observables and extend this product to the whole space $\mathbb{M}$, the authors proceed by induction. In this way, the map T_n in the above is obtained from all the precedent maps T_l, $l \leq n-1$. This procedure is not unique, however, as there is a freedom in the extension of each T_n onto the thin diagonal $diag(\mathbb{M}^n)$. At each recursive step, the causal factorization property II above fixes the map T_n up to the thin diagonal $diag(\mathbb{M}^n)$, and T_n may be extended onto the diagonal by means of some scaling limit. In particular, we shall later briefly describe an extension procedure which mimics the extension of homogeneous distributions, based on the Steinmann scaling degree.

The time-ordered product of local-functionals is then understood in the sense of a properly constructed family $\{T_n\}_{n\in\mathbb{N}_0}$. This recursive construction, however, is not unique, and two time-ordered products T, T', constructed as families $\{T_n\}_{n\in\mathbb{N}_0}$ and $\{T'_n\}_{n\in\mathbb{N}_0}$, may differ by a family $\{Z_n\}_{n\in\mathbb{N}_0}$ of multilocal maps $Z_n : \mathscr{F}_{loc}^{\otimes n}[\![\hbar]\!] \to \mathscr{F}_{loc}[\![\hbar]\!]$, each one supported in a thin diagonal $diag(\mathbb{M}^n)$. At each recursive step, the map Z_n depends only on a finite number of constants, the so-called **renormalization constats**. The freedom in fixing these constants is known in physics as renormalization freedom. From the family $\{Z_n\}_{n\in\mathbb{N}_0}$ we obtain the so-called Stückelberg-Peterman renormalization group, which we shall not discuss in this thesis. Moreover, though we have restricted our discussion to he construction of the time-ordered product on Minkowski spacetime, on curved background a similar construction was presented in [HW02].

We shall not enter formal aspects of the renormalization group. As a matter of fact, for the purpose of this thesis it will suffice to to say that the T-product of local functionals satisfying conditions I-VI exists, and that the ambiguities in its definition manifests via the presence of finitely many terms at each recursive step, which depend on arbitrary renormalization constants. For further details, we refer to [EG73; Rej16; FR15b; HW01; HW02; BDF09; BF00; Kel10]. However, a brief discussion about the Epstein-Glaser analysis and the extension of distributions is appropriate. We first illustrate the problem from a computational oriented perspective.

Consider for instance the squared-field functionals

$$\Phi^2_f(\phi) = \int dx\, f(x)\phi^2(x), \quad f \in \mathcal{C}^\infty_0(\mathbb{M}),$$

and Φ^2_g, $g \in \mathcal{C}^\infty_0(\mathbb{M})$ constructed in the analogous way. If $\operatorname{supp} f \cap \operatorname{supp} g = \emptyset$, then, according to equation (I.39)we would have

$$\Phi^2_f \cdot_T \Phi^2_g(\phi) = \Phi^2_f \cdot \Phi^2_g(\phi) + 4\hbar \int dxdy\, f(x)g(y)\phi(x)\phi(y)\Delta_F(x,y) + \\ + 2\hbar^2 \int dxdy\, f(x)g(y)\Delta^2_F(x,y).$$

The last term contains the pointwise product of Δ_F with itself, which, given the form of its wave front set in equation (I.41) and the Hörmander criterion for the product of distributions in proposition 8, is well defined only within $\mathbb{M}^2 \backslash diag(\mathbb{M}^2)$. The task of defining the time-ordered product at second order T_2 therefore heuristically assumes the form of extending powers Δ^2_F to a everywhere well-defined distribution. As we work on Minkowski space and due to the translation invariance of the Feynman propagator, this is equivalent to extending these powers to the origin. In addition, due to the recursive construction of the time-orderes product, this task generalizes, in the sense that at order *n* one is left with extending the map T_{n-1}, well defined over the subdiagonals of $\mathbb{M}^{n-1}$, onto the subdiagonals of $\mathbb{M}^n$, which correspond to the subset

$$D(\mathbb{M}^n) := \{(x_1, \dots, x_n) \in \mathbb{M}^n : x_i = x_j \text{ for some } i, j = 1, \dots, n\}.$$

The construction of T_n is then performed in two steps. First, the causal factorization property allows for the construction of a map $\tilde{T}_n$ over $\mathbb{M}^n \backslash diag(\mathbb{M}^n)$, which is subsequently extended in order produce T_n itself.

In fact, the above example only partially illustrates the problem, since in practical computations we often have to consider coinciding point limits of higher order products of distributions. I.e., though in the previous example we encountered the problem of meaningfully treating the square $\Delta^2_F(x-y)$ in the limit $x - y \to 0$, important expectation values involve similar coinciding points limiting procedures with far more points involved. This may be seen, for instance, from extending the previous example and considering $\Phi^2_f \cdot_T \Phi^2_f \cdot_T \Phi^2_g$. We shall return to this problem at the end of the next section.

I.4.2 Extension of $\cdot_T$ and aspects of renormalization.

The above discussion, in the context of quantum field theories over Minkowski space, may be properly stated based on the following.

Definition 28. *Let $u \in \mathscr{D}'(\mathbb{M}\backslash\{0\})$ be a distribution over test functions supported in $\mathbb{M}\backslash\{0\}$. A distribution $\tilde{u} \in \mathscr{D}'(\mathbb{M})$ is called an* ***extension*** *of u if, for all $\phi \in \mathscr{D}(\mathbb{M}\backslash\{0\})$, $\tilde{u}(\phi) = u(\phi)$.*

If there exists an extension of $u \in \mathscr{D}'(\mathbb{M}\backslash\{0\})$, u is called **extendable**. Notice that not all distributions may be extended, and that if u is extendable, its extension may not be unique[4]. However, cf. [Hör90, see thms. 2.3.3 and 2.3.4],

Proposition 12. *A distribution $u' \in \mathscr{D}'(\mathbb{M})$ with support equal to $\operatorname{supp} u' = \{y\} \subset \mathbb{M}$ is a polynomial in the derivatives of the Dirac δ-function δ_y.*

Consequently, two different extensions to some distribution differ by a distribution supported in the origin. The freedom which arises from proposition 12 above is called **renormalization freedom**.

There are a few important methods employed in the extension of Feynman propagator and the explicit construction of renormalized time-ordered product. For instance, we may allude to the dimensional regularization method by C. G. Bollini and J. J. Giambiagi, presented in [BG72], which is beyond the scope of this thesis. An alternative method consists of the regularization scheme used in [EG73], which, for a broader class of distributions, mimics the methods of homogeneous distributions extension described in [Hör90]. In this analysis, which we briefly introduce, the homogeneous degree is replaced by the Steinmann scaling degree. We refer to [Ste71; BF00; Kel10] for the details.

Consider the action of the positive real numbers over $\mathscr{D}(\mathbb{M})$ as

$$\mathbb{R}_+ \times \mathscr{D}(\mathbb{M}) \to \mathscr{D}(\mathbb{M}), \quad (a, f) \mapsto f_a,\ f_a(x) := \frac{1}{a^n} f\left(\frac{x}{a}\right),$$

the composition of a translation and a dilatation on the support of f. This induces a similar action of $\mathbb{R}_+$ over $\mathscr{D}'(\mathbb{M})$ via pullback,

$$\mathbb{R}_+ \times \mathscr{D}'(\mathbb{M}) \to \mathscr{D}'(\mathbb{M}), \quad (a, F) \mapsto F_a,\ F_a(f) := F(f_a).$$

The **scaling degree** of a distribution $F \in \mathscr{D}'(\mathbb{M})$ provides a measure of the divergent behaviour of F around the origin. It is defined as

$$\text{sd } F := \inf\left\{t \in \mathbb{R} : \lim_{a \to 0^+} a^t F_a = 0 \in \mathscr{D}'(\mathbb{M})\right\} \in \mathbb{R} \cup \{\pm\infty\},$$

the limit within the definition meant in the sense of distributions. Hence, as in the limit $a \to 0^+$ the region over which the distribution is estimated is shrunk, the scaling degree provides a comparison of the localized behaviour of F around 0 with respect to a polynomial decrease. It will be appropriate to introduce a complementary quantity: in $\mathbb{M}$, the **divergence degree** of $F \in \mathscr{D}'$ is the number

$$\text{div } F := \text{sd } F - 4.$$

[4] An example of a non-extendable distribution is, for instance, $\mathcal{C}_0^\infty(\mathbb{M}) \ni f \mapsto \int dx\, f(x) e^{1/x}$, see [Kel10].

where 4 corresponds to the dimension of Minkowski spacetime. In particular, if F is a homogeneous distribution of degree $a \in \mathbb{R}_+$, sd $F = a$. More generally, a homogeneous distribution of degree $z \in \mathbb{C}$ has scaling degree $\Re z$. In addition, in arbitrary dimension n the δ-distribution is such that its scalling degree equals n, since

$$\lim_{a\to 0^+} a^t \delta_a(f) = \lim_{a\to 0^+} a^t a^{-n} \delta\left(f\left(\frac{\cdot}{a}\right)\right) = \lim_{a\to 0^+} a^{t-n} f(0).$$

For our discussions, it will be particularly important to notice that $sd\,\Delta_F = 2$, and hence $sd\,\Delta_F^2 = 4$, where Δ_F is the Feynman propagator in Minkowski spacetime in equation (I.40).

The scalling degree of a distribution has the following properties, see [Kel10] and references there mentioned.

Proposition 13. *Let $F, G \in \mathscr{D}'(\mathbb{R}^n)$, and let $\alpha \in \mathbb{N}^n$ be a multiindex. Then*

(i). the scaling degree cannot decrease buy differentiation: sd $(\partial^\alpha F) \leq$ sd $F + |\alpha|$;

(ii). $sd\,(x^\alpha F) \leq sd\ F - |\alpha|$;

(iii). $sd\,fF \leq sd\,F, \forall f \in C^\infty(\mathbb{R}^n)$;

(iv). $sd\,F \otimes G = sd\,F + sd\,G$;

(v). $F \cdot G =$ sd $F +$ sd G, whenever the left hand side is well defined.

The Steinmann scalling degree permits a classification of extension procedures of distributions as follows.

Proposition 14. *Let $u \in \mathscr{D}'(\mathbb{R}^n\backslash\{0\})$. If sd $u < n$, then there exists a unique extension $\tilde{u} \in \mathscr{D}'(\mathbb{R}^d)$ of u such that sd $\tilde{u} =$ sd u. If $n \leq$ sd $u < +\infty$, then there are several extensions of u with the same scaling degree, equals to sd u. Finally, if sd $u = \infty$, the disctribution is not extensible.*

For a proof of this theorem, see [BF00; Kel10]. Although we are mainly interested in theories on Minkowski spacetime, in the present we keep the dimension of the $\mathbb{R}^n$ space implicit, in order to highlight the role of n in this analysis. For the case $sd\,u < n$, let $f : \mathbb{R} \to \mathbb{R}$ be a smooth function such that $f|_{|x|<1} \equiv 0$ and $f|_{|x|\geq 2} \equiv 1$ and set now $f_{*p}(x) := f(px)$ for arbitrary $p \in \mathbb{R}$. In [BF00], the authors show that the limit $\tilde{u} := \lim_{p\to+\infty} f_{*p}u$ produces a distribution on $\mathbb{R}^n$ given by

$$\tilde{u}(g) := \lim_{p\to 0} u(f_{*p}g) \in \mathbb{R}$$

with the same scaling degree of u. The uniqueness of such extension then follows from the fact that two extensions $\tilde{u}, \tilde{u}'$ would differ by a polynomial in the derivative of Dirac's delta function, which however has scaling degree grater or equal n.

In order to examine the case $n \leq \text{sd}\, u < +\infty$, we consider the space $\mathscr{D}_\lambda(\mathbb{R}^n)$ of smooth, compactly supported functions which, together with its derivatives, vanish up to order $\lambda > 0$ at the origin. I.e.

$$\mathscr{D}_\lambda(\mathbb{R}^n) := \{f \in \mathscr{D}(\mathbb{R}^n) : \forall \alpha \in \mathbb{N}_0^n,\ |\alpha| < \lambda, (\partial^\alpha f)(0) = 0\}.$$

Let W denote the projector $\mathcal{C}_0^\infty(\mathbb{R}^n) \hookrightarrow \mathscr{D}_\lambda(\mathbb{R}^n)$, given by

$$\mathcal{C}_0^\infty(\mathbb{R}^n) \ni f \mapsto W(f) := f - \sum_{|\alpha| \leq \lambda} m_\alpha f^{(\alpha)}(0)$$

with smooth, compactly supported functions m_α such that $\partial^\beta m_\alpha(0) = \delta_{\alpha\beta}$ equals a suitable product of Kronecker deltas. In theorem 5.3 of [BF00], the authors construct the extension of u from the projectors W, and also show that the above projection completely characterize the extension of u, in the sense that each $\tilde{u}$ is given from the values of $\tilde{u}(m_\alpha)$. The existing freedom underneath the possible choices of family m_α corresponds to the renormalization freedom, and the difference between two choices $(m_\alpha)_\alpha$, (m'_α) is supported in the origin. We then end up with several extensions with the same scaling degree, all which coincide up to terms localized in the origin $0 \in \mathbb{R}^n$.

A different renormalization method which we shall employ in future sections of this thesis is the Källén-Lehmann procedure, which consists of writing the squared Feynman propagator as an integral over the mass term of Δ_F. From the definition $\Delta_F := \Delta_0^+ + i\Delta_A$, it is possible to see the Feynman propagator is a distribution with scaling degree $sd\, \Delta_F = 2$, and hence its extension to the origin is straightforward, as described above. On the other hand, its square is such that $sd\, \Delta_F^2 = 4$, and hence though it may be extended to the origin, such extension is not unique. See [Fre], for instance. Due to the Lorentz invariance of the propagator on Minkowski space, we may write

$$\Delta_F^2(x) = (-\Box + a^2) \int_{(2m)^2}^{+\infty} dM^2\, \frac{\rho_2(M^2)}{M^2 + a^2} i\Delta_F(x; M), \quad \rho_2(M^2) := \frac{1}{16\pi^2}\sqrt{1 - \frac{4m^2}{M^2}}, \tag{I.42}$$

where $\Delta_F(x, M)$ is the Feynman propagator for the scalar theory with mass M. The above construction may be iterated in order to obtain higher order powers of Δ_F. In the above expression, the real parameter a accounts for the renormalization freedom, and two different choices of parameters, say a and b, imply a difference

$$\begin{aligned}\frac{\left(-\Box + a^2\right)\Delta_F(x)}{M^2 + a^2} - \frac{\left(-\Box + b^2\right)\Delta_F(x)}{M^2 + b^2} &= \frac{(a^2 - b^2)}{(M^2 + a^2)(M^2 + b^2)} \left(\Box + M^2\right)\Delta_F(x) \\ &= \frac{(a^2 - b^2)}{(M^2 + a^2)(M^2 + b^2)}\delta(x),\end{aligned}$$

as stated in proposition 12 above.

This concludes our discussion about renormalization and the extension if the time-ordered product. We once again affirm that, for the scope of this thesis, it will be enough to say that a time-ordered product of local observables always exists, and, although it is not unique, it may be constructed recursively, in such a way that at each step the ambiguity in its definition is represented in finitely many constants to be fixed from additional requirements.

I.4.3 The S-matrix and the Bogoliubov map

We examine now how the time-ordered map explicitly enters the analysis of interacting field theories. Consider an interaction term $\lambda V \in \mathscr{F}_{loc}(\mathbb{M})$, with λ a perturbation parameter which we eventually consider equal to one. We shall first consider a compactly supported, smooth interaction term such as in equation (I.35), and later address the so called adiabatic limit, briefly discussed at the begining of this section. We then define the abstract S-matrix as the time-ordered exponential of the interaction term,

$$\mathcal{S}(f) = \mathbf{1} + \sum_{n\geq 1} \frac{i^n}{\hbar^n} \int dx_1 \dots dx_n \, f(x_1) \dots f(x_n) T(\mathcal{L}_I(x_1), \dots \mathcal{L}_I(x_n)), \tag{I.43}$$

with $f \in \mathcal{C}_0^\infty(\mathbb{M})$ the interaction cutoff as in equation (I.35). The S-matrix is then a unitary operator, in the sense of formal power series in the parameters λ and $\hbar$. In the spirit of eventually setting $\lambda = 1$, we shall from now on frequently omit this interaction parameter from the notation. Next, we also consider the **relative S-matrix**

$$\mathcal{S}_g(f) := \mathcal{S}(g)^{-1} \star \mathcal{S}(g+f), \tag{I.44}$$

where $\mathcal{S}^{-1}$ corresponds to the inverse $\mathcal{S}$-matrix with respect to the $\star$-product. The following is directly obtained.

Proposition 15. *Let $f, g, h \in \mathcal{C}_0^\infty(\mathbb{M})$ such that supp $f \cap J_-$supp $h = \emptyset$. Let $\mathcal{S}^{-1}$ denote the inverse of the S-matrix with respect to the $\star$-product in $\mathscr{A}^0 = (\mathscr{F}_{\mu C}(\mathbb{M}), \star)$, with $\star$ constructed with the two-point function of some Hadamard state ω as in the previous section. Then, regardless of further assumptions on supp g,*

(i). $\mathcal{S}_g(f+h) = \mathcal{S}_g(f) \star \mathcal{S}_g(h)$;

(ii). $\mathcal{S}_{g+f}(h) = \mathcal{S}_g(h)$;

(iii). if, in addition the interacting lagrangian $\mathcal{L}_I$ in equation (I.43) *is a local field, then* $\mathcal{S}_{g+h}(f) = \mathcal{S}_g(h)^{-1} \star \mathcal{S}_g(f) \star \mathcal{S}_g(h)$.

In addition, under the same hypothesis of item (iii) we have

$$\mathcal{S}(f+g+h) = \mathcal{S}(f+g) \star \mathcal{S}(g)^{-1} \star \mathcal{S}(g+h) \tag{I.45}$$

It is often convenient to represent the S-matrix or the relative S-matrix in a different, but equivalent manner. Considering the maps $\{T_n\}_{n\in\mathbb{N}_0}, T_n : \mathscr{F}_{loc}^{\otimes n}[\![\hbar]\!] \to \mathscr{A}^0_{\mu C}$ discussed in the previous subsection, we may represent the formal S-matrix as

$$S : \mathscr{F}_{loc}[\![\hbar]\!] \to \mathscr{A}^0, \quad S(V) := \sum_{n\geq 0} \frac{i^n}{\hbar^n} T_n(V^{\otimes n}) = e_T^{iV/\hbar}. \tag{I.46}$$

In the above equation, V is given cf. in equation (I.35) as

$$V(\phi) = \int dx\, f(x)\mathcal{L}_I(x), \quad f \in \mathscr{D}(\mathbb{M}),$$

such that the formal integral kernel $\mathcal{L}_I$ is the one present in (I.43). We hence employed the same terminology as employed in equation (I.43). In fact, throughout this thesis we shall refer to both the maps in equations (I.43) and (I.46) as the S-matrix, and denote them both with the same symbol S, since the two are equivalent, in a certain sense. While in equation (I.43) we define the map acting on the cutoff of the interaction term V, in equation (I.46) the S-matrix is represented in terms of the local functional V itself.

Following the ideas of Bogoliubov [BS80], we then define the **Bogoliubov map** $\mathcal{R}_V$

$$\mathcal{R}_V : T\mathscr{F}_{loc}[\![\hbar]\!] \to \mathscr{A}^0 = (\mathscr{F}_{\mu C}[\![\hbar]\!], \star_\omega, \cdot_T),$$

as

$$\mathcal{R}_V(F) := -i\frac{d}{d\lambda}S(V)^{-1} \star S(V+\lambda F)\big|_{\lambda=0} = S^{-1}(V) \star_\omega \Big[S(V) \cdot_T F\Big], \tag{I.47}$$

where we included the time-ordered product in $\mathscr{A}^0$, $\cdot_T$ to be understood among local functionals only. The Bogoliubov map provides a representation of local interacting observables into the algebra the free theory, in the sense of formal perturbation series. The interacting observables fulfill the interacting equation of motion, in a formal sense. Let Φ_f be an linear observable in $\mathscr{F}_{reg}(\mathbb{M})$, with $f \in \mathcal{C}_0^\infty(\mathbb{M})$, and let, in addition, $f = Pg$ for some $g \in \mathcal{C}_0^\infty(\mathbb{M})$, where P denotes the Klein-Gordon operator. Then, with a local interaction term $V \in \mathscr{F}_{loc}(\mathbb{M})$, we obtain

$$\Phi_{Pg} = \mathcal{R}_V\big(\Phi_{Pg} + V'(g)\big),$$

which is a particular form of the Schwinger-Dyson equation, see [IZ80] for details. In conclusion, we shall consider the interacting observables in the following sense.

Definition 29. *Let $V \in \mathscr{F}_{loc}(\mathbb{M})$ and let $\lambda \in \mathbb{R}$ a perturbation parameter. The $*$-subalgebra $\mathscr{A}^I := \big(\mathcal{R}_V(\mathscr{F}_{loc}[\![\hbar]\!]), \star, \cdot_T\big)$ given by the image of $\mathcal{R}_V : \mathscr{F}_{loc} \hookrightarrow \mathscr{A}^0 = (\mathscr{F}_{\mu C}[\![\hbar, \lambda]\!], *, \star_\omega, \cdot_T)$ is called **algebra of interacting observables**.*

For future use, we write the up to second order expansion of $\mathcal{R}_V A$ as

$$\begin{aligned}\mathcal{R}_V A = A + iV \cdot_T A - iV \star A + \frac{1}{2}(V \cdot_T V) \star A - V \star V \star A - \frac{1}{2}V \cdot_T V \cdot_T A + \\ + V \star (V \cdot_T A) + O(\lambda^3)\end{aligned} \tag{I.48}$$

I.4.4 The adiabatic limit.

Throughout this section, we have considered interacting theories for compactly supported local interaction terms, as in equation (I.35). In the present subsection, we discuss the adiabatic limit mentioned at the beginning of this chapter, which consists of an indutive limit for the cutoff of V. The result of this limit should formally correspond to a local functional supported on the whole space $\mathbb{R}^3$, obtained as an inductive limit $f \to 1$. In [BF00], the adiabatic limit is presented as $f \to 1$ in the S-matrix (I.43). In this thesis, we shall consider a cutoff function of the form $f(x) = \chi(x_0)h(\mathbf{x})$ as in (I.36), and examine the limit $h \to 1$, for fixed $\chi \in \mathcal{C}_0^\infty(\mathbb{M})$, and from the discussion below we shall see that this choice is not excecively restrictive. As we shall se below, by restricting to the algebra of observables of some connected, relatively compact region $O \subset \mathbb{M}$, it suffices to have $\chi = 1$ in a neighbourhood $I \times \mathbb{R}^3$ of O, for some $I \subset \mathbb{R}$ compact. This hence justifies keeping the time cutoff χ fixed. The analysis of this adiabatic limit plays a substantial part in the construction of the interacting KMS state in [FL14], to be discussed in the next chapter.

Often, mostly in the physical literature, we encounter a description of an interacting system which was initially free, until an interaction term was turned on and so left henceforth. This would correspond to a time cutoff of the form

$$\tilde{\chi} \in C^\infty(\mathbb{R}), \quad \tilde{\chi}|_{t<t_i} \equiv 0,\ \tilde{\chi}|_{t>t_i+\delta} \equiv 1, \tag{I.49}$$

for some $t_i, \delta \in \mathbb{R}$. Moreover, it is also possible to find descriptions of interaction terms abruptly turned on. In this case, the cutoff $\tilde{\chi}$ would not be a smooth function, but rather it would be given as the Heaviside step function shifted according to t_i. In the present section we shall also discuss the behaviour of the time cutoff, in particular the equivalence between a compactly supported $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ and an everlasting $\tilde{\chi}$ as in (I.49). The way the interaction is turned on will be also considered in chapter three, where we shall present examples of expectation values which diverge if the interaction is abruptly turned on.

Let then $O \subset \mathbb{M}$ be a relatively compact subregion, and let $\mathscr{F}_{loc}(O)$ denote the subset of local functionals $F \in \mathscr{F}_{loc}(\mathbb{M})$ with $\operatorname{supp} F \subset O$. We thus consider a compactly supported interaction term $V \in \mathscr{F}_{loc}(\mathbb{M})$, in the sense of equation (I.35), with $f \in \mathscr{D}(\mathbb{M})$ a compactly supported cutoff, and the formal kernel $\mathcal{L}_I$ polynomial in the field $\phi(x)$. Moreover, let f be such that $O \subset \operatorname{supp} f$, and $f|_O \equiv 1$. In this way, we consider observables supported in a compact region O of $\mathbb{M}$, and an interaction term supported only in a compact neighbourhood of O. We hence construct the algebra $\mathscr{A}^I(O)$ of interacting observables supported in O by means of the relative S-matrices $S_{V_f}(F)$, given in equation (I.44) and whose functional derivatives produce the Bogolubov map $\mathcal{R}_V$ in (I.47), since

$$\mathcal{R}_{V_f}(F) = -i\frac{d}{d\lambda} S_{V_f}(\lambda F)\big|_{\lambda=0}.$$

We introduced the subindex f in order to highlight the interaction term cutoff. This is roughly what we have presented up to this subsection.

In this situation, the time-slice property, which we briefly discussed in the introduction when discussing the Haag-Kastler axioms, implies that the algebra of observables supported in certain larger regions $O' \supset O$ coincide with $\mathscr{A}^I(O)$, up to terms which vanish on-shell. The validity of the time-slice property for perturbative interacting theories was proved in [CF09].

Proposition 16. (Time-slice property) *Let $O, O' \subset M$ be relatively compact and globally hyperbolic regions of a globally hyperbolic manifold M. Let $V_f \in \mathscr{F}_{\mu C}$ as in* (I.35)*, with* $\operatorname{supp} f \supset O$*, and let $\mathscr{A}^I(O)$, $\mathscr{A}^I(O')$ be the algebras of interacting observables supported in the respective region . Let in addition $\Sigma_O \subset O$ be a Cauchy surface of O. Then, if $O' \subset O$ is a neighbourhood of Σ_O, there exists an algebra isomorphism between $\mathscr{A}^I_{on-shell}(O) \to \mathscr{A}^I_{on-shell}(O')$, where for each region, $\mathscr{A}^I_{on-shell}$ denotes the on-shell algebra constructed as the quotient of $\mathscr{A}^I$ with the ideal obtained from the Klein-Gordon equation* (I.21)*.*

The time-slice condition is a particular specification of the isotony condition, discussed in the introduction of this thesis, and it may be regarded as a weak, algebraic version of determinism by initial conditions. By using this property, we may hence extend the algebra of observables $\mathscr{A}^I(O)$. Consider $O \subset \mathbb{M}$ as before, and let $\varepsilon > 0$ and the strip

$$\Sigma_\varepsilon := [-\varepsilon, +\varepsilon] \times \mathbb{R}^3, \tag{I.50}$$

such that $O \subset \Sigma_\varepsilon$. Suppose also that V is supported within Σ_ε, with cutoff $f(x) = \chi(x_0)h(\mathbf{x})$ as in (I.36), $h \in \mathscr{D}(\mathbb{R}^3)$, $\chi \in \mathcal{C}^\infty_0(\mathbb{R})$, such that $O \subset \operatorname{supp} f$. In this way, due to the time-slice property 16 above, the interacting algebra of local observables relative to each bounded region O coincides, up to terms vanishing on-shell, to that of region $O \cap \Sigma_\varepsilon$. Hence, with the strip Σ_ε a neighbourhood of the Cauchy surface $\Sigma_0 = \{0\} \times \mathbb{R}^3$, the analysis of $\mathscr{A}^I(\Sigma_\varepsilon) = (\mathcal{R}_V \mathscr{F}_{loc}(\Sigma_\varepsilon), \star)$ completely describes the algebra $\mathscr{A}^I(\mathbb{M})$ up to terms which vanish on-shell. We shall see below that, in addition, due to the causal factorization property the local algebra $\mathscr{A}^I(\Sigma_\varepsilon)$ is independent of cutoff function particular form in the outside of Σ_ε.

Notice also that we first considered V compactly supported in a neighbourhood $\operatorname{supp} f \supset O$, and then discussed the implications of the time-slice property, supposing V may be extended to the some neighbourhood of Σ_ε, in order to obtain the algebra of interacting observables $\mathscr{A}^I(\mathbb{M})$. I.e., we assumed an extension of V and used the time-slice property to construct an algebra of observables supported on $\mathbb{M}$. In fact, this extension of the interaction term V is well defined at the algebraic level, and it employs the causal factorization property (I.45) for the S-matrix. As may be seen from [IS78], given the time-ordered product and the S-matrix properties, the effect of V over the observables in $\mathscr{A}^I(O)$ supported in O depends only on the form of V in the past of O, in the sense of the next proposition.

Proposition 17. *Let $O \subset \mathbb{M}$ be a relatively compact region, and let V_f, V_g be two local interaction functional as in* (I.35)*, differing only by the choice of cutoffs $f, g \in \mathscr{D}(\mathbb{M})$. Moreover,*

(i). if $\operatorname{supp}(f-g) \cap J_-(O) = \emptyset$, then $S_{V_g}(F) = S_{V_f}(F)$ for all $F \in \mathscr{F}_{loc}(O)$;

(ii). if $\operatorname{supp}(f-g) \subset J_-(O)\backslash O$, then there exists a unitary map $Z : \mathscr{A}^I(O) \to \mathscr{A}^I(O)$ such that

$$S_{V_f}(F) = Z \star S_{V_g}(F) \star Z^{-1}, \quad \forall F \in \mathscr{F}_{loc}(O).$$

The map Z is given as $Z = S_{V_g}(V_g - V_f)$.

See also comments in [BF00]. Hence, due to the above result and the form of the Bogoliubov map (I.47), the algebra of interacting observables $\mathscr{A}^I(O)$ is, up to isomorphisms, completely determined by interaction terms within the past of O for fixed V. In the next chapter we will use this result and the time-slice property in the construction of KMS states for the interacting theory. The result in proposition 17 is shown explicitly in [FL14], in the context of perturbative AQFT. Consider now the strip

$$\Sigma_{2\varepsilon} := [-2\varepsilon, +2\varepsilon] \times \mathbb{R}^3, \tag{I.51}$$

and a cutoff $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ such that $\operatorname{supp}\chi \in \Sigma_{2\varepsilon}$, $\chi|_{[-\varepsilon,+\varepsilon]} \equiv 1$, as in equation (I.37). Set a smooth partition of unity formed by χ and $\chi_+, \chi_- \in C^\infty(\mathbb{R})$ defined as

$$\chi_+(t) := \begin{cases} 1-\chi(t), & t \geq 0 \\ 0, & \text{otherwise}, \end{cases} \qquad \chi_-(t) := \begin{cases} 1-\chi(t), & t \leq 0 \\ 0, & \text{otherwise}. \end{cases}$$

Then, due to proposition 15 and the causal factorization property (I.45), the relative S-matrix $S_V(A)$ is such that, for all $A \in \mathscr{F}_{loc}(O)$ and for arbitrary potential V,

$$\begin{aligned} S_V(A) &= S(V)^{-1} \star S(V+A) = S_{\chi V + \chi_+ V + \chi_- V}(A) = S_{\chi V + \chi_- V}(A) \\ &= S_{\chi V}(\chi_- V)^{-1} S_{\chi V}(A) S_{\chi V}(\chi_- V). \end{aligned}$$

We conclude that $S_V(A)$ is independent of the choice of the support of V, but within the past of O, as in above. We may hence regard the algebra $\mathscr{A}^I(O)$ not as depending on V itself, but rather on an equivalence class $[f]$ of cutoffs, with $g \sim f$ if and only if $g|_{J(O)} = f|_{J(O)}$, for fixed $\mathcal{L}_I$.

Therefore, the thermodynamic limit corresponding to a everywhere defined interaction term V is finally performed in the sense of an inductive limit in the space support h as $h \to 1$. In fact, the content of this subsection results in the following statement.

Proposition 18. *Let $O \subset \mathbb{M}$ be a relatively compact region, and let $\varepsilon > 0$ be such that $O \subset \Sigma_\varepsilon := [-\varepsilon, +\varepsilon] \times \mathbb{R}^3$. In addition, let $f \in C^\infty(\mathbb{M})$ be given as $f(x) = \chi(x_0)h(\mathbf{x})$ for some χ as in* (I.37), *and for some $h \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ such that $h|_{O_{sp}} \equiv 1$, where*

$$O_{sp} := \{\mathbf{x} \in \mathbb{R}^3 : \exists t \in \mathbb{R} \text{ s.t. } (t, \mathbf{x}) \in O\}.$$

Consider a sequence $(h_n)_{n\in\mathbb{N}_0} \in \mathcal{C}_0^\infty(\mathbb{R}^3)$, $h_0 = h$, such that $\operatorname{supp} h_n \subset \operatorname{supp} h_{n+1}$ for all $n \in \mathbb{N}$, and with $\{\operatorname{supp} h_n\}_{n\in\mathbb{N}} \subset \mathbb{R}^3$ a covering of $\mathbb{R}^3$. Suppose also that $h_{n+1}|_{\operatorname{supp} h_n} \equiv h_n$, and so that $h_n \to 1$ converges to unity. For each $n \in \mathbb{N}$, consider also $V_n \in \mathscr{F}_{loc}(\mathbb{M})$ given by

$$V_n(\phi) = \int dx\, \chi(x_0) h_n(\mathbf{x}) \mathcal{L}_I(x),$$

with $\mathcal{L}_I$ as in (I.35). *Finally, consider $\mathscr{A}^I(O)$ the algebra of formal power series in $\lambda, \hbar$ with coefficients in $\mathscr{F}_{loc}(O)$, as per definition 29. Then, the algebra of interacting observables obtained in the the inductive limit $h \to 1$, as $\lim_{n\to\infty} \mathscr{A}^I(\Sigma_{2\varepsilon} \times \operatorname{supp} h_n)$, is well defined, in the sense of formal power series of the parameters $\lambda, \hbar$ with coefficients in $\mathscr{F}_{loc}(\mathbb{M})$.*

The above proposition considers the inductive limit at the algebraic level, which up to the isomorphism Z in proposition 17 is the algebraic adiabatic limit $f \to 1$ of [BF00]. It thus addresses the extension of an algebra $\mathscr{A}^I(O)$ of observables supported in O, O within the support of V, to the algebra $\mathscr{A}^I(\Sigma_{2\varepsilon})$ of microcausal observables with support in the strip $\Sigma_{2\varepsilon}$, where V is supported. By means of the time-slice condition in proposition 16, it is possible then to obtain the algebra $\mathscr{A}^I(\mathbb{M})$ up to the unitary maps Z. However, the latter proposition does not encompass the particular behaviour of states over $\mathscr{A}^I$. Given the way the adiabatic limit is implemented, via an inductive limit for compactly supported cutoffs, infrared divergences are not present in the algebra of interacting observables. However, when considering expectation values of interacting observables, one has to consider possible divergences due to the particular state, and thus a complete analysis regarding the infrared divergences of the expectation value has to be discussed case by case. In the next chapter, we shall examine a particular case, regarding the thermal equilibrium state for the perturbative theory, by Fredenhagen and Lindner [FL14].

Therefore, although the sequence of cutoffs $(h_n)_{n\in\mathbb{N}}$ in proposition 18 suffices for the adiabatic limit, in the chapters to follow we shall be particularly interested in the adiabatic limit in the sense of van Hove, which we shall define below. When discussing the adiabatic limit for expectation values, one has to consider also the behaviour of particular states in this limit. Considering a van Hove sequence will permit to restrict the analysis of this limit to a region whose contribution tends to zero as $h \to 1$.

Definition 30. *A sequence $(h_n)_{n\in\mathbb{N}} \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ is called a van Hove sequence if and only if , for all $n \in \mathbb{N}$ and for all $\mathbf{x} \in \mathbb{R}^3$,*

$$0 \leq h_n(\mathbf{x}) \leq 1, \quad h_n(\mathbf{x}) = \begin{cases} 1, & |\mathbf{x}| \leq n \\ 0, & |\mathbf{x}| \geq n+1. \end{cases}$$

*The inductive limit $\lim_{n\to\infty} h_n$ is called **van Hove limit** and will be denoted $h \to 1$ for any sequence $(h_n)_{n\in\mathbb{N}} \ni h$.*

Finally, we observe that this treatment towards the adiabatic limit has firm physical motivations. Consider an experimentalist performing a measurement, or collecting data from a quantum real scalar field, arranged in a certain state. If the physical system has a self-interacting component, one is often interested in considering this interaction homogeneously distributed throughout space. In addition, any change in the field self-interaction term occurring in the future of the measurement may not be detected by the experimentalist, in accordance with the causality principle. Therefore, considering an interaction time cutoff $\tilde{\chi} \in \mathcal{C}^\infty(\mathbb{R})$ as in (I.49), at the level of observables algebras, has no actual physical meaning, and should be seen as a formal representation of a cutoff (I.37), in the light of propositions 17 and 18. Since states present non local behaviour, on the other hand, the adiabatic limit for expectation values has to be discussed case by case.

I.4.5 The Principle of Perturbative Agreement (PPA).

at the beginning of this section, we argued that perturbation theory is the usual approach towards interacting scalar theories. In some particular cases, though, the dynamical equation may be exactly solved. This is the case of a field-quadratic interaction term,. In this case the interaction may be treated as a mass correction. Hence, this naturally raises the question about the relation between the exact and the perturbative description of a quantum system, if both of them are possible.

Consider the free Klein-Gordon Lagrangian

$$\mathcal{L}_0 = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2.$$

At this point one is left with two choices to approach the free system at the algebraic level. The first, as we have seen, consists of exactly solving the equation of motion, obtaining the causal propagator in terms of its fundamental solutions and constructing the free algebra $\mathscr{A}^0$ as described in section I.3. An alternative approach, however, would be to consider $\mathcal{L}_0$ as the Lagrangian of an interacting theory, thus considering the kinematic term $1/2\partial_\mu\phi\partial^\mu\phi$ itself as the free Lagragian of a massless Klein-Gordon theory, and the mass term proportional to $m^2\phi^2$ as an interaction term, to be treated perturbatively. One would then expect the two approaches to coincide, in the sense of being algebraic equivalent. This example illustrates one of the axioms discussed in the latter of a series of works on quantum field theory on curved spacetimes by Hollands and Wald [HW05], a requisite described and proved to hold in [HW05; DHP17] as the **principle of perturbative agreement**.

Let then $\mathcal{L}_1$ and $\mathcal{L}_2$ be two real scalar fields Lagrangians such that $\mathcal{L}_1 - \mathcal{L}_2 \equiv \mathcal{L}_I$ is a local functional proportional to the square field, i.e. a mass-like term, with the respective equations of motion for individuals $\mathcal{L}_1$ and $\mathcal{L}_2$ exactly solvable. So far we have considered compactly supported interaction terms when addressing the interacting theory, and we may suppose $\mathcal{L}_I$ to be smooth and compactly supported. Let then $\mathscr{A}_i^0$ be the free quantum algebra of observables of the i-theory, $i = 1, 2$, and let $\tilde{\mathscr{A}_1}$ be the abstract algebra of interacting observables of the theory 2 seen as $\mathcal{L}_1 - \mathcal{L}_I$, which is represented into $\mathscr{A}_1^0$ via the Bogoliubov map $\mathcal{R}_V$, with V given in terms of the formal kernel $\mathcal{L}_I$. The equivalence between the algebraic descriptions may be described as the existence of a $*$-isomorphism $\xi : \tilde{\mathscr{A}_1} \to \mathscr{A}_2$ between the algebras $\mathscr{A}_1^I = \mathcal{R}_V(\tilde{\mathscr{A}_1})$ and the exact theory $\mathscr{A}_2^0$, such that the following diagram commutes:

$$\begin{tikzcd}
\mathscr{A}_1 \arrow[d, "R_{12}"'] & \widetilde{\mathscr{A}_1} \arrow[l, dashed, "\mathcal{R}_V"'] \arrow[dl, dashed, "\xi"'] \\
\mathscr{A}_2 &
\end{tikzcd} \tag{I.52}$$

In this diagram, R_{12} represents the classical Møller map, which may be regarded as the limit $\hbar \to 0$ of $\mathcal{R}_V$. In addition, ξ corresponds to $\xi = R_{12} \circ \mathcal{R}_V$.

More precisely, we state the following condition on the algebraic description and renormalization procedure for quantum field theories

Definition 31. *Let $\mathcal{L}_1$, $\mathcal{L}_2$ and $\mathcal{L}_I$ be as in the previous paragraph, and let $\mathscr{A}_i^0$ be the free quantum algebra of observables with product $\star_i$, induced by the respective Lagrangian, $i = 1, 2$. The time-ordered maps defined for the local functionals of each algebra are said to fulfill the* ***Principle of Perturbative Agreement (PPA)*** *if there exists $\xi : \tilde{\mathscr{A}_1} \to \mathscr{A}_2$ a $*$-isomorphism such that, for all $n \in \mathbb{N}_0$ and for all $F_0, \ldots, F_n \in \mathscr{F}_{loc}(\mathbb{M})$,*

$$T_2 F_0 = (\xi \circ T_1)(F_0), \quad F_1 \cdot_{T_2} \ldots, \cdot_{T_2} F_n = \xi\big(\xi^{-1} F_1 \cdot_{T_1} \cdots \cdot_{T_1} \xi^{-1} F_n\big)$$

where T_i denotes the time-ordered product in $\mathscr{A}_i^0$, and if, in addition, the map ξ preserves the interacting Lagrangian $\mathcal{L}_I$ up to renormalization terms.

Since general local observables are described as Wick products of local fields, as discussed earlier in this thesis, the PPA implies that T_2 acts as the identity on local observables, thus mapping Wick powers into Wick powers. In addition, the map ξ is supposed to preserve the interacting Lagrangian, up to the introduction of terms which may be compensated with a proper choice of renormalization constants. In other words, ξ is such that one may not distinguish its effect from possible choices of renormalization. We again refer to [DHP17] for details. This simpler version of the PPA will suffice for the scope of this thesis. A more general statement of this property, as well as a more detailed discussion upon it, is presented in the already quoted references [HW05] and [DHP17].

I.5 Graphic representation of products

In the past few sections we have discussed how products $\star$ or the $\cdot_T$ are obtained from a particular set of propagators, bidistributions which we often formally realized as functions. Now, when considering e.g. the product

$$\Phi_f \star \Phi_g = \int dx\, f(x)\phi(x) \star \int dy\, g(y)\phi(y) = \Phi_f \Phi_g + \int dxdy\, f(x)g(y)\Delta^\sharp(x,y),$$

where $\Delta^\sharp$ corresponds to the two-point function of some Hadamard state, we may picture the integral kernel $f(x)g(y)\Delta^\sharp(x,y)$ as the function f at $x \in \mathbb{M}$, connected to the function g at $y \in \mathbb{M}$ via a line representing the propagator $\Delta^\sharp$. In fact, in some situations the object $\Delta^\sharp(x,y)$ may be interpreted as the correlation between the two points via a particle created at y propagating to x – see [PS95; Haa96]. The above expression may then be pictorially represented as

$$\int dxdy\, f(x)g(y)\Delta^\sharp(x,y) = \; f \; \bullet\!\!\xrightarrow{\;\Delta^\sharp\;}\!\!\bullet \; g \; .$$

The time-ordered product could also be represented in a similar way, with the Feynman propagator instead of $\Delta^\sharp$. In addition, when considering higher order products, $\Delta^\sharp$ could as well be replaced by Δ_R, Δ_A or Δ, or products of propagators whenever such are well-defined

This diagrammatic representations of expectation values is an important representation in quantum field theory, and even when such expansion is not explicitly presented, it is useful to conceive products of field in terms of graphs. Moreover, the formulation of a set of Feynman rules associated to a given theory is an important technology whenever it exists, and, as we shall briefly see further below, it may guide the formalization of a quantum theory. To this end, in this section we briefly discuss graphs. Later, we shall understand a Feynman diagram as a set of graphs to which are assigned a set of Feynman rules, a set of rules which allow for a computational estimation of a given graph.

Definition 32. *A **graph** G is a set $V(G) \neq \emptyset$ of vertices and a set $E(G)$ of edges, both of them countable, with maps $\mathtt{s}, \mathtt{t} : E(G) \to V(G)$. The map $\mathtt{s}$ assigns a **source** to each edge, whereas $\mathtt{t}$ assigns a **target**. An **orientation** over a graph G with $E(G) \neq \emptyset$ is an association $\mathtt{O} : E(G) \times V(G) \to \{0, \pm 1\}$ defined as*

$$\mathtt{O}(e, v) := \begin{cases} +1, & \text{if } \mathtt{t}(e) = v; \\ -1, & \text{if } \mathtt{s}(e) = v; \\ 0 & \text{otherwise.} \end{cases}$$

*A graph endowed with an orientation is called an **oriented graph**.*

If for given $e \in E(G)$ and $v \in V(G)$ we have $\mathtt{s}(e) = \mathtt{t}(e) = v$, the pair (e, v) is called a **tadpole**. If G is a graph, a subgraph G' is a pair of subsets $E(G') \subset E(G)$, $V(G') \subset V(G)$, $V(G') \neq \emptyset$, endowed with maps $\mathtt{s}', \mathtt{t}' : E(G') \to V(G')$ given by the restrictions of the maps $\mathtt{s}, \mathtt{t}$ of G. An orientation is given over the subgraph by the restriction of $\mathtt{O}$ to $E(G') \times V(G')$ whenever $E(G'), V(G') \neq \emptyset$. If G' is an oriented graph and if G' is an oriented subgraph with an orientation given as the restriction of that of G, we denote $G' \subset G$.

In a graph G, a **path** from some $v_1 \in V(G)$ to some $v_2 \in V(G)$ with $v_1 \neq v_2$ is sequence $(e_j)_{j \in I} \subset E(G)$ for some $I \subset \mathbb{N}_0$, which connects v_1 and v_2, in the sense that there are $e_k, e_l \in (e_j)_{j \in I}$ such that $\mathtt{t}(e_l) = v_1$, $\mathtt{s}(e_k) = v_2$ or vice-versa. A graph is called connected if each pair of vertices is connected by a path. A connected subgraph is a connected graph on its own. A graph with $E(G) = \emptyset$ is not connected by definition.

Let G be a finite oriented graph, i.e. such that $\#V(G), \#E(G) < +\infty$[5]. If in addition G is connected and such that $V(G) \neq \emptyset$, $\#V(G) = n < +\infty$ and $\#E(G) = n - 1$, it is called a **tree**. A disjoint union of trees defines what is usually called a forest. Let $V(G)$ as just stated and consider a indexing of the vertices. I.e., to each $v \in V(G)$ we associate a unique number $k \in \{1, \ldots, n\} \subset \mathbb{N}$, so that $V(G) \simeq \{1, \ldots, n\}$. Consider then the sequence of edges $(e_k)_{k \in \{1, \ldots, n\}} \in E(G)$, where the indexing of each edge corresponds to the indexing of its source. Consider now the sequences of vertices $u \equiv (u_k)_{k \in \{1, \ldots, n\}}$ and $v \equiv (v_k)_{k \in \{1, \ldots, n\}}$, $u_k = \mathtt{s}(e_k)$ and $v_k = \mathtt{t}(e_k)$. If there exists a permutation of the indexing set $\{1, \ldots, n\}$ such that either: *(i).* the only repeated elements in u or v correspond to either vertex 1 or n; or *(ii).* the only common elements in u and v are

[5] For an arbitrary set A, we denote by $\#A$ its cardinality.

vertices 1 or n; then G is called a **cycle**. If an indexed graph may be turned into a connected cycle via the subtraction of a finite number of edges, then it is called a **loop**. We refer to [Die05] to aspects of graph theory, though the nomenclature employed in the mathematics literature often differs from the one adopted in physics, and which we have been using.

We then associate a sum of graphs to the expectation value of a product of observables by writing $\omega(F \star G) = F \star G|_{\phi=0}$ for some gaussian state ω as in equation (I.32), and describing each term $\langle F^{(n)}, \omega_2^{\otimes n} G^{(n)} \rangle$ as a graph as follows. We assign vertices to the integral kernels of each $F^{(n)}$ and $G^{(n)}$, and regard the propagators $\omega_2^{\otimes n}$ connecting these kernels as n edges connecting the vertices, with sources $F^{(n)}$ and targets $G^{(n)}$. We then see that in the computation of expectation values by means of equation (I.32), i.e. with respect to the same state used to define the $\star$-product, there corresponds a sum of loops only. In addition, in the diagrammatic representation of products of regular or local functionals, we may establish a one to one correspondence between vertices and points of the spacetime. The same is not true for microcausal observables, nor for observables given by formal power series with coefficients in $\mathscr{F}_{\mu C}(\mathbb{M})$. In these cases, as will become evident in chapter three, vertices may be given as more complex structures as subdiagrams themselves.

In future sections, when representing products of observables with graphs we shall represent time-ordered products as simple, non oriented lines, since these are symmetric; two-point functions will be represented as arrows, with orientation established as follows: when representing $\omega_2(x, y)$ as an edge, it corresponds to an arrow from x to y. In resume, we shall adopt the following representation for the formal integral kernels of propagators.

$$\omega_2(x,y) \equiv \; x \;\bullet\!\!\longrightarrow\!\!\bullet\; y \tag{I.53}$$

$$\Delta(x,y) \equiv \; x \;\bullet\!\!-\!\!\times\!\!-\!\!\bullet\; y \tag{I.54}$$

$$\Delta_F(x,y) \equiv \; x \;\bullet\!\!-\!\!\!-\!\!\!-\!\!\bullet\; y \tag{I.55}$$

$$\Delta_R(x,y) \equiv \; x \;\bullet\!\!-\!\!<\!\!-\!\!\bullet\; y \tag{I.56}$$

$$\Delta_A(x,y) \equiv \; x \;\bullet\!\!>\!\!-\!\!-\!\!\bullet\; y \tag{I.57}$$

In addition, from the construction of $\cdot_T$ we see that graphs for time-ordered products contain no tadpoles. The conventions adopted in this thesis are such that we have the following properties for the propagators for a real Klein-Gordon field. All these follow from what has been discussed so far, and we recollect these expressions in order to proper clarify conventions and transformations which will be particularly used in chapter III. Hence,

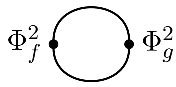
$$\Delta^-(x) = \overline{\Delta^+}(x) = \Delta^+(-x) \tag{I.58}$$

$$\Delta(x) = \Delta_R(x) - \Delta_A(x) = -i\Big(\Delta^+(x) - \Delta^-(x)\Big) \tag{I.59}$$

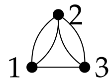
$$\Delta_{R/A}(x) = \pm\theta(\pm x_0)\Delta(x) \tag{I.60}$$

$$\Delta_F(x) = \Delta^+(x) + i\Delta_A(x) = \Delta^-(x) + i\Delta_R(x)$$
$$= \frac{1}{2}\left\{\Delta^+(x) + \Delta^-(x) + i\Big[\Delta_R(x) + \Delta_A(x)\Big]\right\} \tag{I.61}$$

Before closing this chapter, we return to a topic discussed in the previous section. In a diagrammatic representation, renormalization may be seen as a coincide points limit in a graph. For instance, when considering the time-ordered product $\Phi_f^2 \cdot_T \Phi_g^2$, represented as



equation (I.42) corresponds to the limit of coinciding vertices. Regularization of higher order diagrams are generaly seen as an interactive limit of this form. As an illustrative example, consider the three points diagram below,



$$\equiv \Delta_F(1,2)^2 \Delta_F(2,3)^2 \Delta_F(1,3). \tag{I.62}$$

The regularization procedure via extension to the origin, presented in equation (I.42), is not enough to remove all the singularities contained in (I.62). For instance, by means of extending the squared Feynman propagator Δ_F^2 to a distribution well defined at zero, the singularity corresponding to the limit $1 \to 3$ may be removed, and similarly the singularities in the propagators connecting vertices 1 to 2 and 2 to 3 separately may be dealt with, once we have properly extended Δ_F^2. However, the above diagram contains also a singularity in the limit $1 = 2 = 3$, which is not removed by the single extension of Δ_F^2. The removal of such singularity corresponds to the next iterative step in the construction of maps T_n for the time-ordered product, as previously discussed.

Taking into consideration the analysis and estimations in the third chapter, we shall strongly limit our discussion upon renormalization of higher order diagrams. As we did for the construction of the time-ordered product, we affirm the singularities in such diagrams may be recursively removed at all orders, by means of employing the so-called forest formula. We refer to [Kel10] for details.

II. Descriptions of thermal equilibrium in Perturbative Quantum Field Theory

In the previous chapter we presented the algebraic description of quantum field theory, and discussed the perturbative approach to interacting theories mainly at the level of the algebra of observables. Little has been said about states, though. In particular, we have discussed the adiabatic limit within the algebra of observables by means of an inductive limit, defined via a sequence of compactly supported, local interaction terms, thus avoiding infrared divergences for the observables. On the other hand, we have also argued that there is no reason why this construction should eliminate such divergences from expectation values, since states may still present such divergent behaviour. Due to its rather non-local aspect, divergences at the level of states may have to be discussed case by case. If we restrict our analysis to an interacting state given as $\omega^I := \omega \circ \mathcal{R}_V$ for some fixed state ω over the free algebra $\mathscr{A}^0$, then the removal of infrared divergences discussed in proposition 18 suffices for the regularization of expectation values. However, this may not be the case in more general situations, for instance if the interacting state of our interest depends itself on the interaction cutoff. In addition, from the physical perspective, states of the form $\omega \circ \mathcal{R}_V$ may not suffices for an appropriate description of a system.

In quantum field theory, the characterization of thermal equilibrium is performed at the level of states. In the case of interacting scalar theories, as it has been recently shown by Fredenhagen and Lindner in [FL14] (see also [Lin13]), this analysis is based on a state which has both the characteristics described in the previous paragraph, in the sense that it may not be written as the composition of a free state with the Bogoliubov map over observables. Notwithstanding, often in the physical literature we encounter descriptions of thermal equilibrium states for the interacting theory as given by a thermal equilibrium state of the free theory, composed with the Bogoliubov map as before. Corroborating a series of papers addressing the properties and characterization of thermal equilibrium for perturbative algebraic quantum field theories ([FL14; DFP18; Dra19] among others to be mentioned throughout the text), we shall present, later in chapter III, further arguments which shall permit to conclude that a general and precise characterization of thermal equilibrium may not be given in these terms.

The aim of this chapter is to properly introduce this discussion on perturbative systems at finite temperature. We shall consider interacting states over $\mathscr{A}^I$, focusing particularly on thermal equilibrium states, which prove to be of a different form than

$\omega \circ \mathcal{R}_V$. In order to do so, we shall first properly define thermal equilibrium states in the sense of the KMS condition. We shall not extensively discuss the motivation behind this definition, nor shall we discuss any further aspects in quantum statistical mechanics employed in our analysis. For the latter topic we refer to [Gal99; BR81]. In the next chapter we shall discuss exact relations between two different descriptions of thermal equilibrium in quantum field theory. Namely, the one often called *thermal field theory* (TFT), as described, for instance, in [LW87; Bel00]; and the recent analysis by Fredenhagen and Lindner presented in [FL14; Lin13]. Therefore, in this chapter we also briefly introduce these two descriptions, and later indicate the conflicts and connections between them. In the next chapter, we shall see that the problem preventing the exact equivalence between the two descriptions lies, to a great degree, on aiming at a completely characterization of an interacting state through the composition of a free state with the Bogoliubov map. We shall discuss also in which cases the interacting thermal state reduces to such a form.

In addition, since the state constructed by Fredenhagen and Lindner dependends on the interaction cutoff, as will be seen in section II.2, in this chapter we shall also discuss aspects of the large time limit of expectation values in thermal equilibrium, for perturbative theories. Much of this discussion was established in [DFP18] already. We shall return to this topic later in chapter III.

Apart from particular details to be discussed in sections II.2 and II.3, the main structure of the physical system discussed in this chapter has been adapted from [Bel00]. We shall initially consider a free, real scalar system, prepared in a unique thermal equilibrium state at a given inverse temperature $\beta > 0$. Then, at time $t = t_i$, a self-interaction term is switched on. We then suppose the system returns to thermal equilibrium after a long enough time has passed, and thus we modify the initial state accoringly. In these conditions, we then analyze expectation values estimations. This thermalization hypothesis, as showed in [DFP18], is fulfilled in certain conditions, which we shall later discuss. Therefore, the kind of system we shall be considering is described by a particular form of (I.34), i.e. a time-dependent Lagrangian

$$\mathcal{L}(t) = \mathcal{L}_0 - \mathcal{L}_I(t) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \mathcal{L}_I(t), \quad \mathcal{L}_I(t) \equiv 0 \text{ if } t < t_i, \tag{II.1}$$

where we highlight the explicit time-dependence of $V \in \mathscr{F}_{loc}(\mathbb{M})$, whose formal integral kernel $\mathcal{L}_I(x)$ is supposed polynomial in the field configurations. In other words, we shall be mainly interested in terms V as per (I.35) of the form

$$V = \int dtd\mathbf{x}\,\chi(t)h(\mathbf{x})\mathcal{L}_I(t,\mathbf{x}) = \lambda \int dtd\mathbf{x}\,\chi(t)h(\mathbf{x})\frac{\phi^n(t,\mathbf{x})}{n}, \quad n \in \mathbb{N}, \tag{II.2}$$

where from now on we shall often denote $t \equiv x_0$. In the above expression, $h \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ correspond to the space cutoff functions of V, as in equations (I.35), whereas the time cutoff $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ is given as in (I.37). Considering the perturbative interaction acting both upon the state and the dynamics, at a later time $t_f > t_i$ we evaluate expectation values of some observables. In particular, we shall be interested in the evaluation of the n-point functions at later times, and in their large time behaviours. Further details concerning the description of the physical system and, in particular, the form of the interaction term will be given in the forthcoming sections.

Finally, before properly starting this chapter we should strongly emphasize that our discussion concerning aspects of thermal field theory in section II.3 will be absolutely formal. Our purpose there will merely be to present the basic concepts of the so-called real- and imaginary time formalisms involved in the later discussion of chapter III, in order to establish a proper relation between thermal field theory and the Fredenhagen and Lindner analysis. Therefore, section II.3 should be seen as an heuristic discussion on thermal systems. The relation between this heuristic discussion and the Fredenhagen and Lindner analysis will be completed in the next chapter.

II.1 KMS-states in non-interacting QFT.

In quantum statistical mechanics, the description of thermal equilibrium for an ideal Bose gas in a finite volume is performed upon the so-called Gibbs states. In this context, the algebra of observables $\mathfrak{A}$ reduces to a C^*-algebra of bounded operators over a Hilbert space $\mathcal{H}$, and the Hamiltonian H_0 consists of a selfadjoint operator over $\mathcal{H}$. The Gibbs state is then given in terms of the density matrix $\rho = Z^{-1}\exp(-\beta H_0)$, supposing $\exp(-\beta H_0)$ is a trace-class operator and thus $Z = Tr(\rho) \in \mathbb{C}$ is a finite normalization constant, as

$$\rho(A) = \frac{1}{Z} Tr\big(\rho A\big), \quad A \in \mathfrak{A}$$

denoting both the state and the operator with the same symbol. Considering the one-parameter group of automorphism $(\tau_t)_{t\in\mathbb{R}}$ given as

$$\mathfrak{A} \ni A \mapsto \tau_t(A) := e^{iH_0 t} A e^{-iH_0 t}, \tag{II.3}$$

the pair $(\mathfrak{A}, (\tau_t)_{t\in\mathbb{R}})$ forms a dynamical system as in definition 27. We notice that Gibbs states are completely characterized by the following property. Consider the function

$$\mathbb{R} \ni t \mapsto \rho\big(A\tau_t B\big),$$

for arbitrary $A, B \in \mathfrak{A}$. It may be analytically extended to complex arguments $z \in \mathbb{C}$ with $\Im z \in (0, \beta)$, being continuous at the boundaries of such a region, and satisfies the formal relation

$$\rho(A\tau_t B)\big|_{t=i\beta} = \rho(BA), \tag{II.4}$$

where the left hand side is understood as the analytic extension of a function onto $\mathcal{S} := \{z \in \mathbb{C} : \Im z \in (0, \beta)\}$, which for real values reduces to $\rho(A\tau_t B)$. We refer to [BR81] for further details.

In the analysis of a finite system in quantum statistichal mechanis, thus restricting to a finite volume $V \subset \mathbb{R}^3$, Gibbs states are interpreted as describing a system in thermal equilibrium with a thermal reservoir at inverse temperature $\beta > 0$. Hence, due to the above characterization of Gibbs states in terms of its analytic properties, following [HHW67] thermal equilibrium states in more general situations are characterized by an extension of property II.4. This is the so-called KMS condition, usually stated as below. It requires the notion of dynamical invariance for states.

Definition 33. *Let $\big(\mathscr{A}, (\alpha_t)_{t\in\mathbb{R}}\big)$ be a dynamical system as per definition 27 and let $\omega : \mathscr{A} \to \mathbb{C}$ be a state over the $*$-algebra $\mathscr{A}$. The state is called α_t-invariant if and only if $\omega \circ \alpha_t = \omega$ for all $t \in \mathbb{R}$.*

The next definition provides a precise meaning to equation (II.4).

Definition 34. *Let $\big(\mathscr{A}, (\alpha_t)_{t\in\mathbb{R}}\big)$ be a dynamical system, let ω be an α_t-invariant state and let $0 < \beta < +\infty$. For arbitrary but fixed $A, B \in \mathscr{A}$, set the functions $F, G : \mathbb{R} \to \mathbb{C}$ as*

$$\mathbb{R} \ni t \mapsto F(t) := \omega(A\alpha_t(B))$$
$$\mathbb{R} \ni t \mapsto G(t) := \omega(\alpha_t(B)A).$$

If both F, G have analytic extensions into the domain $\mathcal{S} := \{z \in \mathbb{C} : \Im z \in (0, \beta)\}$ which are also continuous in $\partial\mathcal{S}$, and if for all $t \in \mathbb{R}$

$$G(t) = F(t + i\beta), \tag{II.5}$$

then the state ω is called a KMS state at inverse temperature $\beta > 0$, with respect to the dynamics $(\alpha_t)_{t\in\mathbb{R}}$.

Gibbs states are particular examples of KMS states, thus there are states which satisfy the above definition, in the context of quantum statistical dynamics. In addition, we shall see other examples further below. In the context of perturbative AQFT, following [FL14], the definition of KMS state may be written in the following form.

Definition 35. *Let $\mathscr{A}^0$ be as in definition 26, let $(\mathscr{A}^0, (\alpha_t)_{t\in\mathbb{R}})$ be a dynamical system, and let ω a α_t-invariant state as per definition 33. For any $n \in \mathbb{N}$ and for arbitrary but fixed $A_1, \ldots, A_n \in \mathscr{A}$, let the function*

$$F : \mathbb{R}^n \to \mathbb{C}, \quad (t_1, \ldots, t_n) \mapsto F(t_1, \ldots, t_n) := \omega\big(\alpha_{t_1}A_1 \star \cdots \star \alpha_{t_n}A_n\big).$$

If F is analytically extendable onto the strip

$$\mathcal{S} := \{(z_1, \ldots, z_n) \in \mathbb{C}^n : 0 < \Im z_j - \Im z_i < \beta, \forall i, j = 1, \ldots, n,\ i < j\}. \tag{II.6}$$

for some $0 < \beta < +\infty$ and if, in addition, F is continuous along $\partial\mathcal{S}$ and satisfies the condition

$$F(t_1, \ldots, t_{k-1}, t_{k+i\beta}, \ldots, t_{n+i\beta}) = F(t_k, \ldots, t_n, t_1, \ldots, t_{k-1}) \quad \forall k = 1, \ldots, n, \tag{II.7}$$

*then ω is called a KMS state at inverse temperature β with respect to the dynamics $(\alpha_t)_{t\in\mathbb{R}}$.For shortness, we shall call it simply **KMS-state** or **β-KMS state** whenever we want to highlight the particular value of β. A β-KMS will be denoted ω^β.*

We observe that definition 35 extends the previous definition 34 in the sense that, for a Gaussian KMS-state as per def. 35, the content of definition 34 is automatically fulfilled. In other words, the latter characterization of thermal equilibrium states extends the former one to non Gaussian states.

We emphasize the importance of the dynamics for the above definitions: a state may be a β-KMS state with respect to a one-parameter group of automorphisms $(\alpha_t)_{t\in\mathbb{R}}$, and at the same time may not be β-KMS state with respect to a different dynamics $(\alpha'_t)_{t\in\mathbb{R}}$. This comment concerns an important aspect of the analysis to be presented in the next sections. This may be seen also in light of the fact that thermal equilibrium states are defined among dynamical invariant states, and hence a change in the dynamics itself is expected to affect the notion of thermal equilibrium. As definition 35 reduces to definition 34 if we set $n = 2$, in this case we shall frequently use the notation

$$\omega_\beta(A \star \alpha_{t+i\beta}B) \equiv F(t + i\beta).$$

This should be understood only in the formal sense of equation (II.7), since the action of the dynamics α_t is defined only for real parameters $t \in \mathbb{R}$, whereas the KMS condition provides a meaningful continuation to the expectation value $F(t)$ at time t.

We now consider the form of a KMS state for real, free scalar field theory, as represented by the Lagrangian I.20. By combining the KMS condition with the requirement that any state over the algebra of observables should be a solution of the Klein-Gordon equation of motion, we conclude the following characterization of a quasifree KMS-state for a massive free scalar field.

Proposition 19. *The two-point function of a β-KMS state for the dynamical system $(\mathscr{A}^0, \alpha_t)_{t\in\mathbb{R}}$, with $\mathscr{A}^0$ as in definition 26 and $(\alpha_t)_{t\in\mathbb{R}}$ as per equation* (I.33)*, has the form*

$$\Delta^+_\beta(x) = \frac{1}{(2\pi)^3}\int \frac{d^3\mathbf{p}}{2w_\mathbf{p}}\left(b_+(\mathbf{p})e^{-iw_\mathbf{p}x^0} + b_-(\mathbf{p})e^{iw_\mathbf{p}x^0}\right)e^{i\mathbf{p}\cdot\mathbf{x}}, \quad x \in \mathbb{M}, \tag{II.8}$$

where $w_\mathbf{p} := \sqrt{\mathbf{p}^2 + m^2}$, $m > 0$ is the mass term from the Klein-Gordon equation and

$$b_+(\mathbf{p}) := \frac{1}{1 - e^{-\beta w_\mathbf{p}}}, \quad b_-(\mathbf{p}) := \frac{1}{e^{\beta w_\mathbf{p}} - 1}. \tag{II.9}$$

Proof. As the antisymmetric part of any state is proportional to the causal propagator,

$$\Delta^+_\beta(x, y) - \Delta^+_\beta(y, x) = i\Delta(x, y),$$

using the translation invariance of ω^β and Δ and the KMS condition we have

$$\Delta^+_\beta(x_0, \mathbf{x}) - \Delta^+_\beta(-x_0, \mathbf{x}) = \Delta^+_\beta(x_0, \mathbf{x}) - \Delta^+_\beta(x_0 + i\beta, \mathbf{x}) = i\Delta(x_0, \mathbf{x}),$$

where we denoted $\Delta^+_\beta(x) \equiv \Delta^+_\beta(x_0, \mathbf{x})$. In frequency space, the above expression assumes the form

$$\widehat{\Delta}^+_\beta(p_0, \mathbf{p}) - \mathcal{F}\left(T^0_{-i\beta}\Delta^+_\beta\right)(p_0, \mathbf{p}) = i\widehat{\Delta}(p_0, \mathbf{p})$$

where T_a^0 denotes the translation operator acting on the zeroth coordinate by $a \in \mathbb{C}$. We use both $\mathcal{F}$ and $\widehat{\cdot}$ to denote the Fourier transform in all four coordinates. We therefore obtain, using the form of the causal propagator in frequency space presented in (I.12),

$$\widehat{\Delta}_\beta^+(p) = \frac{i\widehat{\Delta}(p)}{1 - e^{-\beta p_0}} \Rightarrow \Delta_\beta^+(x) = \frac{1}{(2\pi)^3} \int dp \, \frac{\varepsilon(p_0)\delta(p_0^2 - w_{\mathbf{p}}^2)}{1 - e^{-\beta p_0}} e^{ipx}. \tag{II.10}$$

The two point function of a KMS state with $m = 0$ is analogous, up to terms proportional to $\delta(p_0)$ which cannot appear in the massive case. Performing the integration with respect to dp_0 over $\mathbb{R}$ then results in (II.8). □

A comparison between the two-point function of a β-KMS state and condition *(i)* in definition 25 , which provides a global characterization of Hadamard states from the wave front set of its two-point function, shows that ω^β is itself a Hadamard state, since the wave front set of (II.8) coincides with that of the vacuum two-point function Δ_0^+.

Corroborating the interpretation of a β-KMS state as a thermal equilibrium state, the evaluation of particular observables in the free algebra $\mathscr{A}^0$ with respect to a β-KMS state ω^β provides direct information about the thermal aspects of system. For instance, if we consider the expectation value $\omega^\beta(:\phi^2:_{\Delta_0^+})$, with regularization implemented via the Minkowski vacuum two-point function Δ_0^+, it provides a thermometer for the field theory, as, for massless theories,

$$\omega_\beta\left(:\phi^2:_{\Delta_0^+}\right) = \frac{1}{12\beta^2}. \tag{II.11}$$

A similar result may be obtained for massive theories. Therefore, the evaluation of particular observables in the β-KMS state ω^β permits also the characterization of macroscopical thermal properties of the system. We therefore see the effect of the interaction between the field and a thermal reservoir at temperature $\beta > 0$ manifested via the observable $:\phi^2:$, where regularization is understood with respect to the vacuum two-point function Δ_0^+. A further discussion and examples may be found in [BOR02; Buc03].

As a matter of fact, denoting as $\star_0$ the product constructed with respect to the Minkowski vacuum, the result of equation (II.11) corresponds exactly to the coinciding point limit of $\omega^\beta(\Phi_f\Phi_g)$. This contribution appears when we consider expectation values of some field polynomials such as ϕ^2 and ϕ^4 in the algebra $(\mathscr{F}_{\mu C}, \star_0)$, with respect to the β-KMS state. The emergence of this contribution may be seen as the acquisition of a mass-like term in the dynamical equation for the field propagation. It is this effect, mentioned already in the previous chapter, named **thermal mass**. We refer to [DHP17; Dra19] for details.

The following property concerning the decay along time directions of a β-KMS state are extracted from [BB02] and [DFP18]. It will be important also in the analysis presented in both chapters III and IV. From now on, we shall refer to a β-KMS state for the dynamical system described in proposition 19 as a **free KMS state**, or a **KMS state for the free theory**, recalling that we restrict our analysis to real, massive scalar field theories.

Proposition 20. *Let ω^β be a free KMS state. Then, denoting its two-point function as in* (II.8) *by Δ^+_β, there exists a constants $C \in \mathbb{R}$ such that, for all $x, y \in \mathbb{M}$ with $y - x$ a timelike, future pointing vector and $|x^0 - y^0| > 1$,*

$$|\Delta^+_\beta(x,y)| \leq \frac{C}{|x^0 - y^0|^{3/2}}. \tag{II.12}$$

Proof. We present a sketch of the proof presented in [BB02], similar to the schematic discussion presented in [DFP18].[1] As ω^β is a Hadamard state, then $\omega^\beta - \omega_0$, with ω_0 the Minkowski vacuum state of the free theory, is a smooth function. In addition, considering the same hypothesis, if y and x are such that $y - x$ is a timelike, future-directed vector, then $(x,y) \notin \operatorname{singsupp} \Delta^+_\beta,\ \operatorname{singsupp} \Delta^+_0$, and thus both two-point functions are given by smooth functions in a neighbourhood of (x,y). In particular, the vacuum two-point function assumes the form

$$\Delta^+_0(\sigma) = \frac{4\pi m K_1(im\sqrt{\sigma^2})}{i\sqrt{\sigma^2}},$$

with $\sigma^2 \equiv (x_0 - y_0)^2 - (\mathbf{x} - \mathbf{y})^2$, and K_1 the first modified Bessel function of the second kind, which present the same decayind property as the one presented in (II.12) – see [GR07, sec. 8.432, 8.451]. Therefore, by considering

$$|\Delta^+_a(x,y)| = |\Delta^+_\beta(x,y) - \Delta^+_0(x,y)| + |\Delta^+_0(x,y)|,$$

we are left with the decaying behaviour of $|\Delta^+_\beta(x,y) - \Delta^+_0(x,y)|$. From the latter difference, consider the function

$$x \mapsto \int dp \left[\frac{\varepsilon(p_0)}{1 - e^{-\beta p_0}} - \theta(p_0)\right] \delta(p^2 - m^2) e^{ipx} = \sum_{s=\pm 1} \int \frac{d\mathbf{p}}{2w_{\mathbf{p}}} \frac{e^{isw_{|p|}x_0} e^{-i\mathbf{p}\cdot\mathbf{x}}}{e^{\beta w_{\mathbf{p}}} - 1},$$

with $\mathbf{x}$ in a compact domain and for positive x_0. In spherical coordinates, the latter integration becomes

$$\sum_{s=\pm 1} \int_0^{+\infty} dr \int_{\mathbb{S}^2} d\Omega \frac{r^2}{2w_r} \frac{e^{isw_r x_0} e^{-ir\mathbf{e}\cdot\mathbf{x}}}{e^{\beta w_r} - 1},$$

with $d\Omega \equiv d\Omega(\mathbf{e})$ the solid angle measure relative to the sphere of radius $|\mathbf{e}| = 1$. We now perform a change of variables $v := (w - m)x_0$ and obtain

$$\sum_{s=\pm 1} e^{ismx_0} x_0^{-3/2} \int_0^{+\infty} dv\, v^{1/2} e^{isv} k_s\left(v x_0^{-1}\right),$$

[1] There is a small mistake in the proof presented in [BB02] regarding a substitution of variables, which is absent in [DFP18], though.

with

$$k_s(z) := \frac{\sqrt{z+2m}}{2} \int_{\mathbb{S}^2} d\Omega \frac{e^{-i\sqrt{z(z+2m)}\mathbf{e}\cdot\mathbf{x}}}{e^{\beta(z+m)}-1}.$$

Noticing the decaying factor $x_0^{-3/2}$ in the previous equation, in order to conclude we prove that the integration in dv is uniformly bounded in x_0. The functions k_s are rapidly decaying functions and we may conclude that, for some $\delta \in \mathbb{R}$, there are constants C_N such that

$$\sup_{0<z,\,\mathbf{x}\in K} |z^{-\delta}\partial_z k_s(z)| \leq C_N(1+m)^{-N}$$

for any $N \in \mathbb{N}$ and for $K \subset \mathbb{R}^3$ compact. The above inequality implies $|k_s(z) - k_s(0)| \leq c_N(1+m)^{-N}$, see [BB02]. We now write

$$\int_0^{+\infty} dv\, v^{1/2} e^{isv} k_s\left(vx_0^{-1}\right) = \lim_{\varepsilon\to 0^+} \left\{ k_s(0) \int_0^{+\infty} dv\, v^{1/2} e^{isv-\varepsilon v} + \right.$$
$$\left. + \int_0^{+\infty} dv\, v^{1/2} e^{isv-\varepsilon v} \Big[k_s\left(vx_0^{-1}\right) - k_s(0) \Big] \right\}.$$

By using the above inequality and twice integrating by parts the second integral in the limit above, thus writing $e^{isv-\varepsilon v} = (is-\varepsilon)^{-2}\partial_v^2(e^{ivs-\varepsilon v}-1)$, we may observe that the integration in dv converges and is bounded in x_0. Hence, $|\Delta_\beta^+(x,y) - \Delta_0^+(x,y)| \leq C|x_0 - y_0|^{-3/2}$.

□

In the next section we shall address a result by Fredenhagen and Lindner which concerns the behaviour of KMS states two-point functions along spacelike direction. A result similar to the above holds also for derivatives of the field. We shall only state the proposition, whose proof may again be found in [DFP18].

Proposition 21. *Let $F, G \in \mathscr{A}^0$. Then, under the hypothesis of proposition 20, there exist constants $C, d \in \mathbb{R}$ which may depend on F, G and such that*

$$\left| \left\langle \frac{\delta}{\delta\phi}\alpha_t F,\, \Delta_\beta^+ \frac{\delta}{\delta\phi'}\alpha_{t'} G \right\rangle \right| \leq \frac{C}{(|t-t'|+d)^{3/2}}.$$

II.2 The Fredenhagen and Lindner construction.

In the last few paragraphs we have presented the characterization of thermal equilibrium for free, scalar field systems, made possible with the KMS condition introduced in definition 35, and we have also discussed some properties satisfied by the KMS state. The question of how to describe thermal equilibrium for interacting theories is however much more complex. In this context, a common approach in the physics literature frequently starts with a "change to interaction picture". Heuristically, one starts with a free, real scalar field system, described by a Klein-Gordon Lagrangian $\mathcal{L}_0$, or equivalently by the free Hamiltonian H_0 obtained from $\mathcal{L}_0$ via a Legendre transform. As of instant $t_i = 0$, for instance, an interaction term is turned on, and so at later times the total Hamiltonian becomes $H_0 + H_I$. We then consider the dynamics given by the adjoin action of $\exp(itH_0)$, as in equation (II.3), to be deformed accordingly into the calculation of expectation values. I.e., let

$$R \ni t \mapsto U(t) = e^{i(H_0+H_I)t}e^{-iH_0t},$$

and consider the interacting dynamics introduced via the adjoint action of U as

$$\mathscr{A}^I \ni A \mapsto Ad\Big(U(t)\Big)(A) := U(t)AU^*(t).$$

More precisely, we consider the free part $e^{iH_0t}\,(\cdot)\,e^{iH_0t}$ acting upon observables, whereas the composition $\omega \circ Ad\big(U(t)\big)$ in the above sense, where ω corresponds to the initial free state of the system, would define the interacting state. This is what one finds in traditional physics literature for quantum field theory at zero temperature, see [PS95], for instance.

There are, however, problems concerning this approach in a generic framework. For instance, the very definition of a interacting Hamiltonian over each time surface as

$$H_I(t) = \int d^3\mathbf{x}\,\mathcal{H}_I(t,\mathbf{x}) \tag{II.13}$$

is generally not well posed, and one is left with Haag's theorem stating the impossibility of a interaction picture representation – see [Haa96; EF06]. In addition to the fact that the integration over $\mathbb{M}$ in (II.13) in general does not converge, even with the introduction of a cutoff $h \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ in its integral kernel, the interacting Hamiltonian is problematic. At first, the formal kernel $\mathcal{H}_I$ usually involves poitwise products of field configurations – as mentioned in the previous chapter, physically relevant systems contain quadractic, cubic or quartic iteraction terms, for instance (see [CM05] for intersting recent applications and a list of further references). These products are implemented in the algebraic level via normal ordering, as presented in the previous chapter. However, still the restriction of the Hamiltonian interaction to a constant time surface of $\mathbb{M}$ is ill defined, as mentioned in [FL14]. Besides that, for what concerns in particular the characterization of thermal equilibrium states, the perturbative formulation of the KMS-condition represents a difficulty on its own. Even if $\omega \circ Ad\big(U(t)\big)$ is a well-defined state, one must assure it satisfies the KMS condition with respect to the perturbed dynamics in order to interpret it as a thermal equilibrium state at some finite temperature. This particular situation was examined in [FL14], as we shall discuss next.

These difficulties in a perturbative approach to quantum field theory at finite temperature have been overcome in the context of algebraic quantum field theory, following the work of H. Araki in the early 1970s in [Ara73], in the context of quantum statistical mechanics.

Araki considered a C^*-dynamical system $(\mathfrak{A}, (\tau_t)_{t\in\mathbb{R}})$, with $\mathfrak{A}$ an algebra of bounded operators acting over some Hilbert space $\mathcal{H}$, and the one-parameter group of $*$ automorphisms $(\tau_t)_{t\in\mathbb{R}}$ generated by some self-adjoint operator H_0 on $\mathcal{H}$, as $\tau_t = Ad(\exp(itH_0))$. Considering then a self-adjoint, bounded perturbation H_I to the generator H_0, such that $H_0 \to H_0 + H_I$ and $\tau_t \to \tau_t^I = Ad(\exp(it(H_0 + H_I))$, according to [Ara73] a KMS state Ω^I, with respect to the perturbed dynamics, may be obtained from the free KMS state Ω^0 through the limit

$$\lim_{t\to\infty} \Omega^0 \circ \tau_t^I(A) = \Omega^I(A).$$

The above property, describing the achievement of a thermal equilibrium after a long time since the perturbed dynamics has been turned on, is called **return to equilibrium**, and holds provided a certain clustering condition for Ω^I is satisfied. We shall return to this topic at the end of this section, in the context of AQFT. In addition, considering a C^*-dynamical system, Araki also constructed a family of operators $\mathbb{R} \ni t \mapsto U(t)$ intertwining the free and the perturbed dynamics as

$$u(t) = \sum_{n\geq 0} (-i)^n \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n \tau_{t_n}(H_I) \dots \tau_{t_1}(H_I),$$

where H_I is as in above. The operators $U(t)$ are hence such that

$$\tau_t^I(A) = u(t)\tau_t(A)u^{-1}(t), \quad \forall A \in \mathfrak{A}, \forall t \in \mathbb{R}.$$

The use of such operators permits to construct the function, for arbitrary but fixed $A \in \mathfrak{A}$,

$$\mathbb{R} \ni t \mapsto \frac{\Omega^0\big(Au(t)\big)}{\Omega^0\big(u(t)\big)}.$$

In addition, Araki showed that this function may be extended to an analytic function on $\mathcal{S}$ as in (II.6), and continuous along $\partial\mathcal{S}$. Taking advantage of this result, it was possible to define the interacting KMS state Ω^I as

$$\Omega^I(A) := \frac{\Omega^0\big(Au(i\beta)\big)}{\Omega^0\big(u(i\beta)\big)}, \tag{II.14}$$

which agrees with the return to equilibrium property but does not require a large time limit.

Due to the problems regarding a Hamiltonian interaction functional of the form (II.13) and the interaction picture evolution discussed in the first paragraphs of this section, the starting point of the Fredenhagen and Lindner analysis in [FL14; Lin13], which extends the Araki's construction (II.14) to the realm of AQFT, is the time-slice property of $\mathscr{A}^I$ in proposition 16. After the algebraic introduction of normal ordering and the recursive renormalization procedure implemented at each step in the construction of the time-ordered map, the main problems concerning the interacting Hamiltonian regard the support of the formal inetarcting Hamiltonian density $\mathcal{H}_I$ in (II.13). As mentioned before, the integration over the whole space results in infrared divergences if one does not introduce a cutoff for the interaction term, whereas the restriction $H_I(t)$ is not well defined. In order to construct a KMS state for the perturbative theory, adapting the Araki state (II.14) to AQFT, it is necessary to construct first a family of operators $t \mapsto U(t)$ which intertwine the interacting and the free dynamics.

The construction of the interacting KMS state is performed first prior to the adiabatic limit, in the context presented in section I.4.4, based in the construction of the operators U on a finite volume. I.e., we consider the algebra of interacting observables supported in a relatively compact region $O \subset \mathbb{M}$, with the interaction supported in a finite neighbourhood of O. The adiabatic limit for the state is then obtained via the limit $h \to 1$ in the sense of van Hove, for fixed χ supported in a neighbourhood $\Sigma_{2\varepsilon}$ of the Cauchy surface $\Sigma_0 - \{0\} \times \mathbb{R}^3$. The result of this limit represents a KMS state over the whole spacetime $\mathbb{M}$, which does not depend on the particular form of the time cutoff χ.

Therefore, in [FL14], from the causal factorization property the authors presented formal operators $t \mapsto U_V(t)$, in the sense of formal power series in $\hbar$, interchanging the interacting and the free dynamics. Considering the free dynamics as defined in equation (I.33), the interacting equivalent is defined via pullback as

$$\alpha_t^V \mathcal{R}_V(A) := \mathcal{R}_V(\alpha_t A), \quad \forall A \in \mathscr{F}_{loc}(\Sigma_{2\varepsilon}). \tag{II.15}$$

For positive values of t, the operators U are such that

$$U(t) := S_V(W_t), \quad W_t := \alpha_t V - V = \int^t dt' \alpha_{t'} \dot{V}, \quad \forall t > 0, \tag{II.16}$$

where

$$\dot{V} := \int dx \dot{\chi}(x_0) h(\mathbf{x}) \mathcal{L}_I(x), \quad \dot{\chi} := \begin{cases} \frac{d\chi}{dt}, \ t < 0; \\ 0 \text{ otherwise.} \end{cases} \tag{II.17}$$

They permit a correlation between the two dynamics as

$$\alpha_t^V \mathcal{R}_V A = U(t) \star \alpha_t \mathcal{R}_V A \star U(t)^{-1}. \tag{II.18}$$

Moreover, the following holds.

Definition 36. *The one-parameter family of formal operators* $(U(t))_{t>0}$ *in* (II.16) *fulfill the so-called* ***cocycle condition***

$$U(t+s) = U(t) \star \alpha_t U(s). \tag{II.19}$$

In addition, it is a solution to the formal differential equation

$$\frac{d}{dt} U(t) = iU(t) \star \alpha_t K, \quad K := -i \frac{d}{dt} U(t) \Big|_{t=0} = \mathcal{R}_V \dot{V}, \tag{II.20}$$

with $\dot{V}$ *as in* (II.17).

The equalities above may be found in [FL14; Lin13], and permit to write the cocycle U for arbitrary $t \in \mathbb{R}$ as a solution of (II.20) as the formal power series operator

$$U(t) = \mathbf{1} + \sum_{n \geq 1} i^n \int_{tS_n} dt_1 \dots dt_n \, \alpha_{t_1} K \star \dots \star \alpha_{t_n} K, \tag{II.21}$$

where the above integration is then performed in the n-dimensional, real symplex

$$tS_n := \{(t_1, \dots, t_n) \in \mathbb{R}^n : 0 < t_n < \dots < t_1 < t\}.$$

In addition, we state that fhe above equation permits to represent the interacting dynamics α_t^V perturbatively as

$$\alpha_t^V(A) = \alpha_t(A) + \sum_{n \geq 1} i^n \int_{tS_n} dt_1 \dots dt_n \left[\alpha_{t_1} K, \left[\dots [\alpha_{t_n} K, \alpha_t A]\right]\right], \quad A \in \mathscr{F}_{\mu C}(\mathbb{M}). \tag{II.22}$$

In [FL14; Lin13], the cocycle $U(t)$ explicitly enters the construction of a KMS-state for the interacting theory in the following result.

Proposition 22. *Let $O \subset \mathbb{M}$ be a relatively compact region of $\mathbb{M}$, and let $\varepsilon > 0$ such that $O \subset \Sigma_\varepsilon$, the time strip as in proposition 18. Let $V \in \mathscr{F}_{loc}[\![\hbar]\!]$ be a local, compactly supported interaction term as in* (I.35)*, for fixed $h \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ and $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ and χ as in* (I.37)*. Suppose also $h|_{O_{sp}} \equiv 1$. Last, let $\mathbb{R} \ni t \mapsto U(t)$ be as in* (II.16)*. Then, for any arbitrary but fixed $\mathcal{R}_V A \in \mathscr{A}^I(O)$, the map*

$$\mathbb{R} \ni t \mapsto \frac{\omega^\beta\big(\mathcal{R}_V A \star U(t)\big)}{\omega^\beta\big(U(t)\big)},$$

where ω^β is a β-KMS state with respect to the free dynamics $(\alpha_t)_{t\in\mathbb{R}}$, has an analytic extension onto the strip (II.6)*. In addition,*

$$\omega^{\beta,V}(\mathcal{R}_V A) := \frac{\omega^\beta\big(\mathcal{R}_V A \star U(i\beta)\big)}{\omega^\beta\big(U(i\beta)\big)}, \quad \mathcal{R}_V A \in A^I(O), \tag{II.23}$$

defines a β-KMS state for the interacting dynamics $(\alpha_t^V)_{t\in\mathbb{R}}$.

The analysis by Fredenhagen and Lindner presents another important result. Let $\chi, \chi' \in \mathcal{C}_0^\infty(\mathbb{R})$ represent two possible choices of time cutoff, hence both supported within $\Sigma_{2\varepsilon}$ and identically equal to 1 within Σ_ε. Then, according to [FL14, proposition 2], the cocycles U_χ and $U_{\chi'}$, constructed respectively from χ, χ', coincide up to unitary equivalence. In addition, in proposition 4 of the same reference, the authors show that, prior to the adiabatic limit, the difference in the cocycles does not manifest in the interacting KMS state $\omega^{\beta,V}$. I.e., the associated KMS states $\omega_\chi^{\beta,V}$ and $\omega_{\chi'}^{\beta,V}$ coincide, and for this reason we have omitted the cutoff from the notation $\omega^{\beta,V}$.

We shall often refer to the KMS state in (II.23) as FL-state, for simplicity. We observe that the interacting KMS state $\omega^{\beta,V}$ may also be written in an alternative form. For any state ω over $\mathscr{A}^0$ and for each $n \in \mathbb{N}$, consider the map $\omega_n^c : (\mathscr{A}^0)^{\otimes n}[\![\hbar]\!] \to \mathbb{C}$, recursively defined as

$$\omega_1^c(\mathbf{1}) = 0, \quad \omega^c(A_1 \otimes \cdots \otimes A_n) = \sum_{\sigma \in \mathbb{P}_n} \prod_{I \in \sigma} \omega_{\#I}^c\Big(\bigotimes_{i \in I} A_i\Big),$$

again where $\mathbb{P}_n$ is the set of pairwise disjoint, non-empty partitions of the set $\{1, \dots, n\}$, $\#I$ denotes the cardinality of the partition, and with $\omega_{\#I}$ the $(\#I)$-point function of ω. The maps ω_n^c are called nth **connected component** of ω and permits to write the interacting KMS state $\omega^{\beta,V}$ as

$$\omega^{\beta,V}(A) := \mathbf{1} + \sum_{n \geq 1} (-1)^n \int_{\beta S_n} dU_n \omega_{n+1}^{\beta,c}\Big(A \otimes \bigotimes_{j=1}^{n} \alpha_{iu_j} K\Big), \tag{II.24}$$

where

$$\beta S_n := \{(u_1, \dots, u_n) \in \mathbb{R}^n : 0 < u_1 < \cdots < u_n < \beta\} \tag{II.25}$$

is an n-dimensional symplex, and $\omega^{\beta,c}$ is the connected component of the free KMS state ω^β, cf. again [FL14; Lin13].

In addition to the result described in proposition 22, in section 4.2 of [FL14] the authors show that equation (II.23) may be extended to define a KMS state in the adiabatic limit. Fredenhagen and Lindner showed that the van Hove limit in definition 30 is well defined in this context, provided that the n connected functions of the free KMS state are $L^1(\beta S_n \times \mathbb{R}^{3n})$ for all $n \in \mathbb{N}$. In resume, since it has been shown that we may restrict to an interaction term supported within the strip $\Sigma_{2\varepsilon}$, the adiabatic limit has to be considered only in the sense of a van Hove sequence for the spacial cutoff $h \to 1$. The result showing that this limit is well defined, due to the fast decaying behaviour of the KMS state connected functions along spacelike directions, is presented below, cf. [FL14, prop. 5, see also appendix B].

Proposition 23. *Let ω^β be a β-KMS state of the free, real scalar theory with mass $m > 0$ and inverse temperature $0 < \beta < +\infty$, whose translation invariant two-point function is given as in proposition 19. Let $O \subset \mathbb{M}$ as before and let $R > 0$ finite, such that $O \subset B_R$, the ball of radius R in $\mathbb{R}^4$. For arbitrary $n \in \mathbb{N}$, consider also the symplex βS_n as in* (II.25). *Then, for all $A_0, \dots, A_n \in \mathscr{A}^I(O)$, the connected n-point functions*

$$F_n(u_1, x_1 \dots, u_n, x_n) := \omega^{\beta,c}\big(A \otimes \bigotimes_{k=1}^{n} \alpha_{iu_k} A_k(x_k)\big) \tag{II.26}$$

are such that, for some $C \in \mathbb{R}$,

$$|F_n(u_1, x_1 \dots, u_n, x_n)| \leq C \exp\left(-\frac{m}{\sqrt{n}} \sqrt{\sum_{j=1}^{n} |\mathbf{x}_j|^2}\right). \tag{II.27}$$

This permits to state the well-posedness of $\omega^{\beta,V}$ in the adiabatic limit $h \to 1$ as previously mentioned. It will also be used in chapter IV. In the end, considering the adiabatic limit in the sense of van Hove, due to proposition 23one is left with considering correlation functions in regions of R^3 whose contribution to the total limit tends to zero, given the exponential decay of the connected components.

After the analysis by Fredenhagen and Lindner and following the ideas establishe in [Ara73], in [DFP18] the authors addressed the return to equilibrium property of $\omega^{\beta,V}$. Two of their important results may be recalled as follows. See propositions 3.4 and 4.1 in [DFP18] for details.

Proposition 24. *Let $\mathscr{A}^I(O)$ be the algebra of interacting observables supported within a relatively compact region $O \subset \mathbb{M}$ and let $V \in \mathscr{A}^I$ be as in* (II.2) *with $h \in C_0^\infty(\mathbb{R}^3)$. Let also α_t^V and $\omega^{\beta,V}$ be as in the above* (II.15) *and* (II.23)*, respectively. Then, for any $A \in \mathscr{A}^I(O)$, return to equilibrium holds, i.e.*

$$\lim_{t\to\infty} \omega^\beta \circ \alpha_t^V(A) = \omega^{\beta,V}(A). \tag{II.28}$$

The above result, however, is valid only prior to the adiabatic limit $h \to 1$. Namely, considering a non space-compactly supported interaction term, the limit

$$\lim_{t\to\infty} \lim_{h\to 1} \omega^\beta \circ \alpha_t^V(A)$$

does not produce a thermal equilibrium state, as discussed in [DFP18]. At the core of return to equilibrium property (II.28) lies the decaying property of the free KMS state two-point function in proposition 20. In order to prove (II.28) holds, we observe the free KMS state satisfies the clustering property

$$\lim_{t\to\infty} \omega^\beta\big(A \star \alpha_t^V(B)\big) - \omega^\beta\big(A\big)\omega^\beta\big(\alpha_t^V B\big) = 0, \tag{II.29}$$

for all $A, B \in \mathscr{A}^0(O)$. Equality (II.29) follows from the fact that only connected components $\omega^{\beta,c}$ are present within the limit. If the adiabatic limit $h \to 1$ is considered prior to the large time $t \to +\infty$, property (II.12) does not provide the fast decaying necessary for result (II.29), and, therefore, (II.28) to hold. In resume, the return to equilibrium property (II.28) depends on the clustering condition (II.29), which is a consequence of the decaying behaviour of Δ_0^+ along timelike directions. This fact will be of especial importance in the discussion in chapter III.

II.3 Aspects of Thermal Field Theory.

In this section we intend to introduce the basic aspects of what is generally known in the physics literature as Thermal Field Theory (TFT). In particular, we shall describe the so-called real- and immaginary-time formalisms; the latter is often refered to as Matsubara formalism as well. Later in chapter III we shall describe the precise relations between TFT and the description of thermal equilibrium in perturbative AQFT, established by

Fredenhagen and Lindner and further explored in [DHP17; DFP18; Dra19]. We should again emphasize, however, that our discussion on the present topic will be, besides introductory, completely formal, and our only goal will be to lay down the basis for the comparison between different approaches. We refer to [LW87; Bel00] for the details on thermal field theory.

The physical system we shall consider is similar to the one presented in the previous sections, described by equation (II.1). Again, it is supposed to be initially free and in thermal equilibrium, characterized by a free β-KMS state. We shall eventually address systems initially prepared in the vacuum state, for comparison. At a certain instant, an interaction term is smoothly turned on and then becomes stable as of a certain latter instant. In order to obtain a thermal equilibrium state for the interacting theory at later stages, the free state is then modified accordingly. Following the physics literature, the interaction time cutoff is first supposed as in (I.49). We shall then be interested in expectation values of observables measured after the interaction has stabilized, and in particular in the large time limit of such expectation values.

II.3.1 Formal Thermal Field Theory (TFT).

Bearing in mind the system described in the previous paragraph, we consider the Fock space representation induced by the Minkowski vacuum state over a Hilbert space $\mathcal{H}$. The system description is based on the Hamiltonian operator over $\mathcal{H}$, given by

$$H = H_0 + H_I(t), \quad H_I|_{t<t_i} \equiv 0$$

where H_0 is a free Klein-Gordon Hamiltonian and $H_I(t)$ is a time dependent, local interaction term which does not contain derivatives of the fields. Supposing the exponentials $\exp(-\beta H_0), \exp(-\beta H)$ are traceclass, with this Hamiltonian we define an evolution operator

$$U_H(t,t_i) = U_{H_0}(t,t_i)U_I(t,t_i),$$

where U_I is often called evolution operator in the interacting picture. It satisfies the differential equation

$$i\frac{d}{dt}U_I(t,t_i) = H_I(t)U_I(t,t_i) \Rightarrow U_I(t,t_i) = T\bigg(\exp\bigg[-i\int_{t_i}^{t} H_I(t')dt'\bigg]\bigg), \tag{II.30}$$

where T is the time ordering map. Moreover, for any $t_1, t_2 > t_i$, it also fulfills the splitting property

$$U_I(t_2,t_1) = U_I(t_2,t_i)U_I(t_i,t_1) = U_I(t_2,t_i)U_I^*(t_1,t_i). \tag{II.31}$$

The family of operators U_I is a formal equivalent it the Fredenhagen and Lindner's cocycle U in equation (II.21).

We now define the thermal propagator via the generalized n-point functions

$$G(x_1,\ldots,x_n) := \langle T\phi(x_1)\cdots\phi(x_n)\rangle, \tag{II.32}$$

where T is the time-ordering operator. In order to highlight the different, formal spirit of the present discussion, we generally adopt in this section a notation usually employed in the physics literature. Therefore, the quantum product between observables A, B will be substituted by the common notation AB, and, in addition , we denote as $\langle A\rangle$ the expectation value of the observable A in some initial state of the free theory. This will correspond to either a β-KMS state, or the Minkowski vacuum. In the limit case of zero temperature, the thermal propagator reduces to the Feynman propagator related to the vacuum state. Let now Ψ be the state vector in $\mathcal{H}$, such that $G(x,y) = \langle\Psi, T\phi(x)\phi(y)\Psi\rangle$, and suppose also that $T\phi(x)\phi(y) = \phi(x)\phi(y)$. If we now redefine the field ϕ according to

$$\phi(x) \to \phi_I(x) := U_I(x_0,t_i)\phi(x)U_I^*(x_0,t_i),$$

what in the physics literature is called *interaction picture representation*, then the thermal two-point function G becomes, for $t_i < y_0 < x_0 < t_f$,

$$G(x,y) = \langle\Psi, U^{-1}(x_0,t_i)\phi_I(x)U(x_0,y_0)\phi_I(y)U(y_0,t_i)\Psi\rangle.$$

We now obtain

$$\begin{aligned} G(x_0,y_0) &= \langle\Psi, U(t_i,t_f)U(t_f,x_0)\phi_I(x_0)U(x_0,y_0)\phi_I(y)U(y_0,t_i)\Psi\rangle \\ &= \left\langle\Psi, T_C\left(\phi_I(x)\phi_I(y)e^{-i\int_C H_I(t)dt}\right)\Psi\right\rangle. \end{aligned}$$

In the above integral we introduced a time contour C from t_i to t_f and then back from t_f to t_i. The time-ordering operator T_C is therefore regarded as a time-ordering along such a contour, i.e., it consists of the time ordering operator in the first part of C, going from the initial to the final time, and of the anti-time ordering in the line from t_f to t_i. If C is parametrized by a $\tau \in (0,1)$, T_C then corresponds to time-ordering with respect to the parameter τ.

The analysis of n-point functions is often addressed after the introduction of the so-called **generating functioals**. The thermal Green function G may be obtained from

$$Z_I(j) := \left\langle T\exp i\int_C dx\,\left[\mathcal{L}_I(x) + j(x)\phi(x)\right]_{int}\right\rangle, \tag{II.33}$$

where all terms in the right hand side are written in the interaction picture. Besides that, $j \in C^\infty(\mathbb{M},\mathbb{C})$ is a complex-valued source term, and $\mathcal{L}$ is as in (II.1), thus containing no derivatives of the field. This produces

$$G_I(x,y) = \frac{1}{Z(0)}\frac{\delta^n}{\delta j(x)\delta j(y)}Z_I(j)\bigg|_{j=0} \tag{II.34}$$

Eventually we consider the limits $t_i \to -\infty$, $t_f \to +\infty$. In this context, if $|\Psi_I\rangle \to |0\rangle_{\text{free}}$ tends to the vacuum of the free theory, where we suppress any further discussion concerning in which sense this limit is performed, we end up with the Gell'Mann-Low formula

$$G(x,y)=\frac{\langle 0_{in}|T\Big(\phi_I(x)\phi_I(y)e^{-i\int_{-\infty}^{+\infty}H_I(t)dt}\Big)|0_{in}\rangle}{\langle 0_{in}|T\Big(e^{-i\int_{-\infty}^{+\infty}H_I(t)dt}\Big)|0_{in}\rangle}. \tag{II.35}$$

which permits to obtain expectation values for the interacting theory without modifying the initial state.

This result does not hold at finite temperature $\beta > 0$, however. As discussed in [Ste95], Gell'Mann-Low theorem depends on the spectral condition of the vacuum state. In the case of thermal equilibrium states, the free and the interacting situations present different assimptotic behaviours. In [FL14], the authors considered the time-slice condition and restricted to a time-finite region. In this situation, only the behaviour of the state along spacelike directions enters the analysis.

Returning now to the case in which the initial state in (II.32) correspond to a β-KMS state, the two point function is written as in the context of Quantum Statistical Mechanics in terms of the interacting density matrix instead. This formally corresponds to

$$G(x,y)=\frac{1}{Z(H)}\mathrm{Tr}\left(e^{-\beta H}T_C\big(\phi_I(x)\phi_I(y)e^{-i\int_C H_I(t)dt}\big)\right). \tag{II.36}$$

The exponential $e^{-\beta H}$, combined with the operator U in the previous analysis, may be seen as an "imaginary time evolution". We may combine the Hamiltonian exponentials in $G(x,y)$ in order to obtain the formal representation

$$G(x_1,x_2)=\frac{\mathrm{Tr}\left(e^{-\beta H_0}T\big(\phi_I(x_1)\phi_I(x_2)e^{-i\int_{C\cup C_v}H_I(t)dt}\big)\right)}{\mathrm{Tr}\left(e^{-\beta H_0}T\big(e^{-i\int_{C\cup C_v}H_I(t)dt}\big)\right)}, \tag{II.37}$$

which involves only the initial free state. Due to the KMS condition for Gibbs states as per 34, in the above expression the time contour C from $-\infty$ to $+\infty$ gained another part C_v, which corresponds to a vertical component in the complex plain. The complete contour $C\cup C_v$ then corresponds to a path in the complex plane covering the real line back and forth, and an imaginary component down to $-i\beta$, which formally corresponds to the contribution $U(i\beta)$ in the FL-state (II.23). This is the so-called **Keldysh-Schwinger contour** represented in figure II.1. Notice that the density matrix became the free density matrix $e^{-\beta H_0}$. The point here is precisely that the information about thermal aspects of the state, which previously was contained in $e^{-\beta H}$, drifted to the contour, which is telling us where (or when) to calculate fields expectation values. In this sense thermal field theory should perturbatively describe interacting thermal systems by means of the free thermal equilibrium state.

The analysis of expectation values by means of an integration along C, thus neglecting the C_v-contribution, is usually called **real-time formalism**.

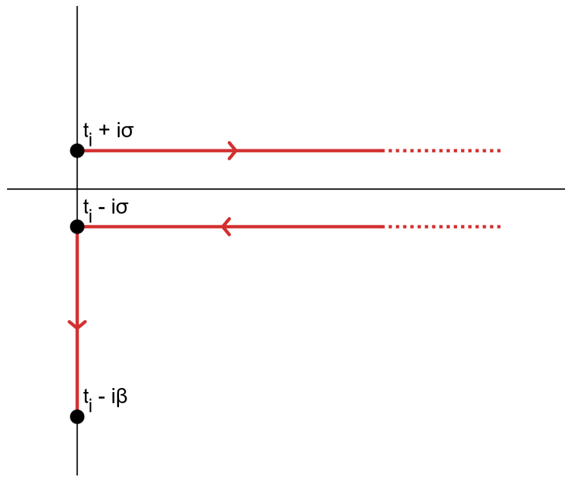


Figure II.1: Representation of the Keldysh-Schwinger contour. It consists of a path starting at $t_i + i\sigma$ and going up to $+\infty$ along the real line, and then returning to $t_i - i\sigma$. In addition, it contains a vertical component from $t_i - i\sigma$ to $-i\beta$. We consider the limit $\sigma \to 0^+$ in the imaginary parts $\pm i\sigma$ of the horizontal lines. In addition, one often considers the limit $t_i \to -\infty$.

II.3.2 Formal analogy with the Fredenhagen and Lindner construction.

At this point we have presented two different descriptions of thermal equilibrium systems in quantum field theory. On the one hand, we have formally discussed what has been presented under the general name of *thermal field theory*. On the other, we have considered the construction of a KMS state for the interacting theory in the context of perturbative AQFT, as performed in [FL14; Lin13]. We may then notice structural similarities between the two formalisms, which we intend to point out in this subsection. It should be emphasized, however, that the purpose of the present discussion is to show heuristic relations between the Fredenhagen and Lindner analysis and elements of TFT, while presenting obstacles for a proper equivalence between the formalisms. The exact relation between TFT and the FL construction will be the content of next chapter.

Hence, if we first translate the content of the above subsection into the language of AQFT, we first consider the equivalent generating functional in the form

$$\mathscr{Z}(J) := \omega^\beta\big(S_V(J)\big), \quad J(\phi) := \int dx\, j(x)\phi(x),$$

with $j \in \mathscr{D}(\mathbb{M})$ as before. We notice this is analogous to (II.33), and performing the second functional derivatives with respect to the source j we obtain what would be the analog of G in (II.34). In addition, by comparing the above discussion about TFT with the content of section II.2, in particular equations (II.20) and (II.30), we notice that the two objects denoted by U are formally analogous.

Considering the physical system described at the beginning of this chapter, we address the expectation value of some suitable observable $A \in \mathscr{A}^0$, performed at some instant later than $t_0 > -\varepsilon$, with the interaction term smoothly turned on at $t = -2\varepsilon$. Also considering the analogies described in the previous paragraph, the integration along the real time contour, from time $t = 0$ to $+\infty$ and back again, is then described by

$$\varsigma_\beta(t_0) := \frac{(\omega^\beta \circ \mathcal{R}_V)\big(A \cdot_T S(W_{t_0})\big)}{(\omega^\beta \circ \mathcal{R}_V)\big(S(W_{t_0})\big)} \tag{II.38}$$

with W_t, as per equation (II.16), given by

$$W_t = \int^t dt' \alpha_{t'} \dot{V}, \quad \forall t > 0.$$

The above expression has its origin justified in the theorem 1 above. We may anticipate that it may be obtained considering equation (II.23) prior to the analytic extension onto the strip $\{z \in \mathbb{C} : \Im z \in (0,\beta)\}$, and its interpretation as a description of the real-time formalism is justified according to the proof of theorem 1. In addition, we anticipate that the exact equivalent to the real-time formalism, in the language of AQFT, is not given by equation (II.38) nor by theorem 1 below, but rather by theorem 2 on page 98, chapter III. Both equation (II.38) and the following theorem 1 serve only to illustrate the problems that emerge when one tries to interpret the state $\omega^\beta \circ \mathcal{R}_V$, in the real of TFT, as a thermal equilibrium state.

Although the above expression has been constructed neglecting the imaginary contribution C_v to the time contour in equation (II.37), we may consider whether it describes a state which may be analytically extended onto the strip $\{z \in \mathbb{C} : \Im z \in (0,\beta)\}$. If this were the case, not only we might be able to re-obtain the contribution of C_v to the above expectation value, as we might perhaps interpret ς^β as the β-KMS state of the interacting theory. In this way, we would be able to establish an equivalence between TFT and the Fredenhagen-Lindner construction. Prior to any analytic continuation, for real times we have the result below. Expression (II.38) will then formally correspond to an expectation value estimated in the real-time formalism. As mentioned above, this is obtained supposing the imaginary time contribution to the Keldysh-Schwinger factorizes. In the proposition below, we see that this expectation value is equivalent to the FL-state prior to the required analytic continuation in the cocycle in (II.23).

Theorem 1. *Let $O \subset \mathbb{M}$, $O \subset \Sigma_{2\varepsilon}$ as in proposition 22. Let ω^β be a KMS state at inverse temperature $\beta > 0$ for the free theory, and let $V \in \mathscr{F}_{loc}(\mathbb{M})$ a compactly supported interaction term also as in proposition 22. Let in addition S be the S-matrix cf.* (I.46)*, $\mathcal{R}_V$ be the Bogoliubov map as in* (I.47)*, and U be the cocycle in* (II.16)*. Finally, let W_t as in* (II.16)*, for $t > -\varepsilon$. Then,*

$$\frac{\omega^\beta\big(\mathcal{R}_V(A) \star U(t)\big)}{\omega^\beta\big(U(t)\big)} = \frac{(\omega^\beta \circ \mathcal{R}_V)\big(A \cdot_T S(W_t)\big)}{(\omega^\beta \circ \mathcal{R}_V)\big(S(W_t)\big)}, \tag{II.39}$$

for all $\mathcal{R}_V A \in \mathscr{A}^I(O)$.

Proof. The argument within the expression in the left hand side may be rewritten as

$$\begin{aligned}
\mathcal{R}_V(A) \star U(t) &= \left[\frac{d}{d\lambda} S^{-1}(V) \star S(V+\lambda A)\right] \star S^{-1}(V) \star S(V_t)\Big|_{\lambda=0} \\
&= \frac{d}{d\lambda} S^{-1}(V) \star S(V+\lambda A) \star S^{-1}(V) \star S(V+W_t)\Big|_{\lambda=0} \\
&= \frac{d}{d\lambda} S^{-1}(V) \star S(V+\lambda A + W_t)\Big|_{\lambda=0} \\
&= S^{-1}(V) \star \{S(V+W_t) \cdot_T A\} = S^{-1}(V) \star \big[S(V) \cdot_T A \cdot_T S(W_t)\big] \\
&= \mathcal{R}_V\big(A \cdot_T S(W_t)\big).
\end{aligned}$$

The step from the first to the second line above follows from the causal factorization property fulfilled by the S-matrix, whereas the factorization $S(V+W_t) = S(V) \cdot_T S(W_t)$ is due to the time-ordered product commutativity and associativity. Equation (II.39) then follows after we consider the expectation value of the two terms in the equality above, together with the normalization factors.

The formal interpretation of the above equation (II.38) as the translation of real-time formalism into the language of AQFT may be finally justified from the equalities above. In particular, as we consider the expectation value of some observable A supported in a finite region in the future of $t = -\varepsilon$, the product

$$S^{-1}(V) \star \{S(V+W_t) \cdot_T A\}$$

contains the same information presented in the description of real-time formalism. It is possible to notice in the above the first real line forming the Keldysh-Schwinger contour, represented by the S-matrix $S(V+W_t)$ and causally related to the observable A via a time-ordered product. As for the anti-time ordered line, this is then described by the inverse matrix $S^{-1}(V)$, the last term to act in the products of fields within the expectation value estimation. We then observe that the Bogoliubov map implicitly contains the same doubling of the field as the real-time formalism. □

It is possible to recognize that the analytic continuation of the left hand side of (II.39) results in the FL-state. In addition, the same analytic continuation for the right hand side would be the continued formal thermal propagator. This latter analytic extension involves also the problem of constructing an holomorphic continuation of the Feynman propagator Δ_F^β in the time-ordered products. It happens that, as discussed in [FR87], such continuation for Δ_F^β is not well defined. In Minkowski spacetime, an extension of Feynman propagators corresponds to an extension of Heaviside functions which do not present a fast decreasing in Fourier space (see also [Hör90, th. 7.3.1]). Therefore, an analytic extension of (II.39) has to be understood in the sense of the FL-state. Furthermore, neglecting the C_v-contribution to the thermal propagator in $S(W_t)$ is formally equivalent to forgetting the factor $U(i\beta)$ in $\omega^{\beta,V}$.

An additional sign of incompleteness in the real-time formalism of perturbative thermal field theory is found in the case of a $\lambda\phi^2$ interacting theory. As discussed in the last chapter, the Principle of Perturbative Agreement states the equivalence between the perturbative and the exact approach to interacting theories, whenever the dynamical equation may be exactly solved, or whenever a ressumation of the perturbative series is possible. In this spirit, consider the particular Lagrangian

$$\mathcal{L}(\phi) = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \frac{\lambda}{2}\delta m^2(x)\chi(x_0)\phi^2$$

with $m > 0$ and $\mathcal{L}_I(x) = \lambda\delta m^2(x)\chi(x_0)\phi^2(x)$, where $\delta m^2(x)$ is a compactly supported, positive mass contribution term. Consider the large time limit addressed in [DHP17], regarded as a "thermalization limit",

$$\begin{aligned}&\lim_{t\to\infty}\omega^\beta\big(\alpha_t^V\mathcal{R}_V\phi(x)\star\mathcal{R}_V\phi(y)\big) = \\ &= \frac{1}{(2\pi)^3}\int\frac{d^3\mathbf{p}}{2\tilde{w}}\left[b_+(w_\mathbf{p})e^{i\tilde{w}(x_0-y_0)} + b_-(w_\mathbf{p})e^{-i\tilde{w}(x_0-y_0)}\right]e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})},\end{aligned}$$

where $w_\mathbf{p}$ is as before, and $\tilde{w} := \sqrt{\mathbf{p}^2 + m^2 + \delta m^2}$. We then see that the "interacting two-point function" ressembles that of a KMS state, Δ_β^+ in (II.8), except for the Boltzmann factors. I.e., the map $\mathcal{R}_V$ is capable of changing the modes in the above decomposition for the state, but not the terms $b_\pm(\mathbf{p})$ from equation (II.9). In other words, even in the large time limit $\omega^\beta\circ\mathcal{R}_V$ does not characterize a thermal equilibrium state. We shall return to this topic in chapters III and IV, and we refer to [DHP17; Dra19] for further discussion.

In addition, if $\omega^\beta\circ\mathcal{R}_V$ is to be a KMS state with respect to the interacting dynamics, considering the formal notation $\alpha_{i\beta}$ within the expectation value of ω^β discussed after definition 35, then we should have that

$$\omega^\beta\circ\mathcal{R}_V\big(A\star B\big) = \omega^\beta\big(\mathcal{R}_V B\star\alpha_{i\beta}^V\mathcal{R}_V A\big).$$

This is nothing but the KMS condition with respect to the interacting dynamics α_t^V. There are two problems regarding the equation above. First, in order to employ the KMS condition fulfilled by the free state ω^β with respect to the free dynamics, so to prove that the KMS condition for the interacting case holds as in the previous equation, we should use (II.18) to introduce the free dynamics into the right hand side. At this point, for generic $t\in\mathbb{R}$ we would obtain an expression in the form

$$\omega^\beta\left(\alpha_t^V\mathcal{R}_V A\star\mathcal{R}_V B\right) = \omega^\beta\left(\mathcal{R}_V B\star U(t+i\beta)\star\alpha_t\mathcal{R}_V A\star U(t+i\beta)^{-1}\right).$$

Due to the form of U in (II.21), we notice that already the analytic domain of ω^β is surpassed by the composition of dynamical operators α_t involved. This may be precisely observed by considering the analytic domain required in the KMS condition, alongside with the cocycle condition (II.19) in definition 36 and the form of U depicted in equation (II.21).

In addition, also the cyclic property in the KMS condition is not fulfilled. We notice the second statement by introducing the cocycle U of section II.2. We hence obtain

$$\begin{aligned}\omega^\beta\big(\mathcal{R}_V B \star \alpha^V_{i\beta}\mathcal{R}_V A\big) &= \omega^\beta\big(\mathcal{R}_V B \star U(i\beta) \star \alpha_{i\beta}\mathcal{R}_V A \star U^*(i\beta)\big)\\ &= \omega^\beta\big(U(i\beta) \star \alpha_{i\beta}\mathcal{R}_V A \star U^*(i\beta) \star \alpha_{i\beta}\mathcal{R}_V B\big)\\ &= \omega^\beta\big(\alpha^V_{i\beta}\mathcal{R}_V A \star \alpha_{i\beta}\mathcal{R}_V B\big).\end{aligned}$$

Comparing the left hand side of the previous equation with the right hand side of the latter, we conclude that

$$\omega^\beta\big(\alpha_{-i\beta} \circ \alpha^V_{i\beta}\mathcal{R}_V A \star \mathcal{R}_V B\big) = \omega^\beta \circ \mathcal{R}_V\big(A \star B\big),$$

which fails to fulfill the KMS condition.

II.3.3 Real-time and Matsubara formalisms.

In the physics literature of TFT, we often find arguments attesting the factorization of the imaginary contribution. I.e., the integration C_v, in the large time limit $t_f \to \infty$, should factorize, and thus only the integration along the real component of C would affect the expectation value, or the Green function. This is the so-called **real-time formalism**. We refer to [LW87] for a particularly detailed discussion about this topic. As we shall see in more details in the next chapter, however, this factorization may happen only in particular cases.

In thermal field theory one may adopt a different choice of the contour. If one considers expectation values of observables which are time independent, then the real component of the integration along $C \cup C_v$ does factorize, and we are left with the a path from $t_i = 0$ to $-i\beta$ in the complex plane only. This case, introduced in [Mat55b], originates the so called **Matsubara**, or **imaginary-time formalism**.

In this situation, it is convenient to work with the thermal propagator for imaginary times. In the next chapter, the Matsubara propagator will be treated in a precise way. For now, the idea, and roughly what we usually find in the physics literature, is the following. We obtain a Euclidean propagator by means of a Wick rotation of the Klein-Gordon dynamical operator by $t \to -i\tau$. Then, for $\tau \in (0, \beta)$ we seek for a fundamental solution $\Delta(\tau, \mathbf{x})$ of the Euclidean dynamical problem

$$(-\partial_\tau^2 - \nabla^2 + m^2)\Delta(\tau, \mathbf{x}) = \delta(\tau)\delta(\mathbf{x}). \tag{II.40}$$

The function $\tau \mapsto \Delta(\tau)$ may be expanded in a Fourier series, and it results in the expression

$$\Delta(\tau) = \sum_n \widehat{\Delta}(w_n)e^{i\omega_n\tau}, \quad \widehat{\Delta}(w_n) = \frac{1}{2\beta}\int_{-\beta}^{\beta} d\tau\widehat{\Delta}(\tau)e^{-i\omega_n\tau}.$$

Combining the above with equation (II.40) we then obtain

$$\widehat{\Delta}(w_n, \mathbf{p}) = \frac{1}{w_n^2 + w_{\mathbf{p}}^2}, \quad w_n := \frac{2\pi n}{\beta},\ n \in \mathbb{Z}, \tag{II.41}$$

again with $w_{\mathbf{p}}^2 = \mathbf{p}^2 + m^2$. These are respectively called the **Matsubara propagator** in momentum space, $\widehat{\Delta}(w_n, \mathbf{p})$, and w_n are the **Matsubara frequencies**. By the Fourier inversion theorem we obtain

$$\Delta(\tau, \mathbf{x}) = \frac{1}{2\beta} \sum_{n \in \mathbb{Z}} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{e^{-i\mathbf{p}\cdot\mathbf{x}} e^{iw_n\tau}}{w_n^2 + w_{\mathbf{p}}^2}, \tag{II.42}$$

which solves equation (II.40). From (II.41) we see that, due to the form of the differential operator, the Matsubara frequencies represent both the modes of the series expansion of $\Delta(\tau)$ and the singularities of the propagator in momentum space.

The Matsubara formalism is particularly employed for computations of time independent partition functions, and the thermodynamical quantities from it derived. We again refer to [LW87]. More details about the imaginary-time formalism and the Matsubara propagator will be given in the next chapter. Arguably, the great advantage of the Matsubara formalism lies in the fact that the Feynman rules for expectation values computations in this context are quite similar to those for the vacuum state. As briefly mentioned in the last section of chapter I, Feynman rules provide a straightforward method for the computations of expectation values. Therefore, it is convenient to work within Matsubara formalism, whenever possible. In addition, since the Matsubara frequencies correspond to singularities of the propagator in (II.41), expectation values may be obtained via residues theorem, in the sense of distributions. In this case, integration over configuration space is replaced by a summation over the Matsubara frequencies. Often one of the hardest tasks in this formalism is to prove the convergence of such summation, which is not a trivial task.

The Matsubara formalism has a particular disadvantage. Since the propagator is defined for imaginary times, its extension to real values require a continuation over the real line. For this reason, this formalism is particularly convenient for the analysis of time-independent expectation values. If, however, this is not the situation of one's interest, one frequently considers the real-time formalism. Whereas the former is obtained from (II.37) by neglecting the contribution C in the integration along $C \cup C_v$, the latter formalism comes from the factorization of the imaginary part, which corresponds to neglecting the imaginary line C_v in (II.37) instead.

One of the most important result presented in [BDP19], and reproduced in this thesis, corresponds to the fact that both the Matsubara and the real-time formalisms are obtained from the Fredenhagen and Lindner's construction in particular situations. Hence, as a matter of fact, a precise and general interpretation of physical system in thermal equilibrium should be based on the latter formalism, discussed in section II.2. For this reason, we limit our discussion about further aspects of TFT.

III. Graphic representation of thermal equilibrium interacting systems

In the previous chapter we briefly discussed the construction of a thermal equilibrium state $\omega^{\beta,V}$ for the perturbative theory given by Fredenhagen and Lindner in [FL14; Lin13]. In addition, we have also presented some properties of both the cocycle U, used in the construction of the state $\omega^{\beta,V}$, and the state itself, in relation to the return to equilibrium property (II.28). From now on, U will always denote the cocycle described in section II.2. Finally, in a rather formal way, in the last section we presented the general structure of both Matsubara and the real-time formalism, grouped in what has been called *thermal field theory* (TFT), and we also presented arguments stating incompleteness in this canonical treatment of thermal systems. Moreover, we have particularly indicated that both the real-time and the Matsubara formalism cannot separately provide general characterizations of thermal equilibrium, when one considers a system such as the one described at the beginning of the previous chapter and characterized by the Lagrangian (II.1). We have seen that establishing the equivalence between the FL-state and TFT would require an analytic extension process which, as a matter of fact, lacks mathematical precision. In addition, the real-time formalism of thermal field theory does not consider an important contribution to the interacting KMS state, and hence neglects aspects in the description of thermal equilibrium for perturbative theories which have been discussed in the context of AQFT framework – as seen in the references mentioned in the previous chapter. I.e., since the real-time formalism is based on considering the interacting state of the form $\omega^{\beta} \circ \mathcal{R}_V$, we have seen that this characterization does not contain important physical information, and it is not enough to characterize thermal equilibrium in general.

In this chapter we intend to analyze the relation between the two approaches to thermal theories. In particular, we shall show that the interacting KMS state $\omega^{\beta,V}$ given in [FL14; Lin13] reduces to either the Matsubara or to the real-time formalism in particular cases. At the same time, a complete and general description of thermal systems is obtained only when the two are altogether considered. That is, a complete and accurate description of thermal equilibrium for the interacting theory is obtained only by considering FL-state $\omega^{\beta,V}$, which reduces to the Matsubara or to the real-time formalism in particular situations. In this manner, we show also that Matsubara and real-time formalism are not only two particular (but partially incomplete) choices for describing the physical system, as described in the TFT literature, but are also part of a larger analysis corresponding to $\omega^{\beta,V}$. In establishing a proper correspondence between formalisms, we shall introduce a graphic representation scheme for the perturbation series of expectation values $\omega^{\beta,V} \circ \mathcal{R}_V(A)$. We shall conclude this chapter presenting two important examples of expectation value computations showing the importance of considering the cocycle U in (II.23).

The results presented in this chapter have been published in [BDP19].

III.1 Exact relations between the FL state and TFT

According to what we have discussed up to now, in particular to section I.5, a diagramatic representation of some expectation value of the form $\omega^{\beta,V} \circ \mathcal{R}_V(A)$ would involve a particular set of propagator representing different edges. Such propagators would be the fundamental solutions of the dynamical equation Δ_A and Δ_R and their difference Δ, the causal propagator; the two-point function of the free-KMS state Δ_β^+; the Feynman propagator related to Δ_β^+, denoted Δ_F^β. Therefore, in aiming at a description of thermal systems which connects with the content of section II.3, we first of all present the expansion of Δ_+^β in terms of the Matsubara frequencies, thus obtaining a thermal propagator formally equivalent to the one discussed in the previous chapter. We shall later see how this representation of the thermal Wightman function introduces the Matsubara formalism into the FL-analysis. Therefore, we recall the form of the translation invariant two-point function from equation (II.8),

$$\begin{aligned}\Delta_\beta^+(x) =& \frac{1}{(2\pi)^3} \int dp \, \frac{\varepsilon(p_0)\delta(p_0^2 - w_{\mathbf{p}}^2)}{1 - e^{-\beta p_0}} e^{ipx} \\ =& \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{p}}{2w_{\mathbf{p}}} \frac{1}{1 - e^{-\beta w_{\mathbf{p}}}} \left(e^{-iw_{\mathbf{p}}x_0} + e^{-\beta w_{\mathbf{p}}} e^{iw_{\mathbf{p}}x_0} \right) e^{i\mathbf{p}\cdot\mathbf{x}},\end{aligned} \tag{III.1}$$

with $w_{\mathbf{p}} := \sqrt{\mathbf{p}^2 + m^2}$. In this manner, the Feynman propagator associated to Δ_F^β may be written, according to (I.61), as

$$\Delta_F^\beta(x) = \theta(x_0)\Delta_\beta^+(x) + \theta(-x_0)\Delta_\beta^-(x_0), \tag{III.2}$$

where θ is the Heaviside step function and $\Delta_\beta^-(x) = \Delta_\beta^+(-x)$.

As discussed in [FR87], Δ_β^+ being the two-point function of a KMS state, it may be extended to a holomorphic function into $\mathcal{S}_- := \{z \in \mathbb{C} : \Im z \in (-\beta, 0)\}$. Due to the form of the kernel

$$x_0 \mapsto e^{-iw_{\mathbf{p}}x_0} + e^{iw_{\mathbf{p}}(x_0 + i\beta)},$$

it may be continued to complex values $z = x_0 + iu$ for $u \in (-\beta, 0)$, which results in an exponential decay for the extended kernel of Δ_β^+. We shall denote this analytic continuation by the same symbol Δ_β^+. Similarly, Δ_β^- may be seen to be extendable over the strip $\mathcal{S}_+ := \{z \in \mathbb{C} : \Im z \in (0, \beta)\}$ in the same manner. In addition, we may conclude that

$$\Delta_\beta^+(z + i\beta, \mathbf{x}) = \Delta_\beta^-(z, \mathbf{x}), \quad z \in S_-.$$

We hence conclude that the function Δ_β^+ defined over the lower strip $\mathcal{S}_-$ equals Δ_β^- defined over $\mathcal{S}_+$, and therefore we may extend the thermal propagator Δ^β to almost the whole of the complex plane by means of this "copy and paste" process in both directions. These observations may be justified considering the following.

The KMS state two-point function (III.1) defines an holomorphic function over the strip $\mathcal{S}_+$ above, and for complex arguments $x_0 + iu$ we have

$$\Delta_\beta^+(x_0 + iu, \mathbf{x}) = \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{p}}{2\omega_\mathbf{p}} \frac{1}{1 - e^{-\beta w_\mathbf{p}}} \left(e^{uw_\mathbf{p}} e^{-iw_\mathbf{p} x_0} + e^{-\beta w_\mathbf{p} - uw_\mathbf{p}} e^{iw_\mathbf{p} x_0} \right) e^{i\mathbf{p}\cdot\mathbf{x}},$$

for $u \in (0, \beta)$. Therefore, we may consider the Fourier series representation of Δ_β^+ within this strip. Along the imaginary axis, omitting the dependence on $\mathbf{x} \in \mathbb{R}^3$ this corresponds to

$$\Delta(\tau) = \sum_{n\in\mathbb{Z}} \hat{\Delta}\left(\frac{2\pi n}{\beta}\right) e^{i\frac{2\pi n}{\beta}\tau}, \quad \hat{\Delta}\left(\frac{2\pi n}{\beta}\right) = \frac{1}{2\beta} \int_{-\beta}^{+\beta} d\tau\, \hat{\Delta}(\tau) e^{-i\frac{2\pi n}{\beta}\tau}.$$

The above expression is what one obtains in the context of the Matsubara formalism of TFT, cf. [LW87]. Considering also the dependences on the real part of the time component and on the spacial component $\mathbf{x} \in \mathbb{R}^3$, this representation becomes instead

$$\begin{aligned} \Delta(x_0 + iu, \mathbf{x}) &= \\ &= \frac{1}{(2\pi)^3} \int dp\, e^{ipx} \sum_{n\in\mathbb{Z}} \frac{e^{i\frac{2\pi n}{\beta}u}}{w_\mathbf{p}^2 + (2\pi n)^2\beta^{-2}} \Big[\delta(p_0 - w_\mathbf{p}) + \delta(p_0 + w_\mathbf{p})\Big] \frac{1}{2}\left(1 + \frac{i2\pi n}{p_0\beta}\right). \end{aligned} \tag{III.3}$$

Furthermore, considering the Fourier transform of the above expression with respect to $x_0, \mathbf{x}$ produces the thermal propagator in momentum space

$$\hat{\Delta}(u, p) = \frac{1}{(2\pi)^3} \sum_{n\in\mathbb{Z}} \frac{e^{i\frac{2\pi n}{\beta}u}}{w_\mathbf{p}^2 + (2\pi n)^2\beta^{-2}} \Big[\delta(p_0 - w_\mathbf{p}) + \delta(p_0 + w_\mathbf{p})\Big] \frac{1}{2}\left(1 + \frac{i2\pi n}{p_0\beta}\right).$$

As the above expressions for the propagators in configuration and in momentum space reveal, these are symmetric under parity transformations $u \to -u$. Furthermore, introducing the **Matsubara frequencies** $w_n := 2\pi n\beta^{-1}$, $n \in \mathbb{Z}$, the Matsubara propagator (as in (II.42)) is then obtained as

$$\widehat{\Delta}_M^\beta = \int dp_0\, \hat{\Delta}(u, p) = \frac{1}{(2\pi)^3} \sum_{n\in\mathbb{Z}} \frac{1}{w_\mathbf{p}^2 + w_n^2} e^{iw_n u}$$

By extending the Fourier series representation of an holomorphic function defined on the strip $0 < \Im z < \beta$ to a periodic function over $\mathbb{C}$, considering the symmetry property of the thermal propagator, we end up with the holomorphic function

$$\Delta^\beta : \{(z, \mathbf{x}) \in \mathbb{C} \times \mathbb{R}^3 : \Im z \neq n\beta,\ n \in \mathbb{Z},\ \text{or } |\Re z| \leq |\mathbf{x}|\} \to \mathbb{C} \tag{III.4}$$

such that

$$\Delta^\beta(z, \mathbf{x}) = \begin{cases} \Delta^+_\beta(z, \mathbf{x}), & \Im z \in \mathcal{S}_-; \\ \Delta^-_\beta(z, \mathbf{x}), & \Im z \in \mathcal{S}_+; \end{cases} \qquad \Delta^\beta(z + in\beta, \mathbf{x}) = \Delta^\beta(z, \mathbf{x}),\ n \in \mathbb{Z},\ z \neq 0, \tag{III.5}$$

and

$$\Delta^\beta(z, \mathbf{x}) = \Delta^\beta(-z, \mathbf{x}). \tag{III.6}$$

In the graphic expansion of thermal expectation values, the thermal propagator above will provide a direct relation between the FL-state and the Matsubara formalism.

In the present section we are interested in the graphic representation of the perturbation series associated to expectation values such as $\omega^{\beta,V} \circ \mathcal{R}_V(A)$, and we consider first the contributions from the Bogoliubov map $\mathcal{R}_V$ to the perturbative expansion of $\omega^{\beta,V} \circ \mathcal{R}_V(A)$. Our analysis will follow a graphic oriented line, as may be seen below. We recollect the form of $\mathcal{R}_V$ as, according to equation (I.47),

$$\mathcal{R}_V(A) = S^{-1}(V) \star \big[S(V) \cdot_T A\big],$$

where A is a finite time-ordered product of local functionals. We may notice within $\mathcal{R}_V$ the presence of three different propagators: besides Δ^+_β employed in the $\star$-product construction, there is the Feynman propagator associated to Δ^+_β cf. (III.2), and the anti Feynman (i.e. anti-time-ordered) propagator $\overline{\Delta^\beta_F}$, which appears in the inverse S-matrix $S^{-1}(V) = \overline{S}(-V)$.

We emphasize that now and henceforth we shall always denote $\star \equiv \star_{\Delta^+_\beta}$ and consider the algebraic product as given in terms of the two-point function of the free β-KMS state Δ^+_β. Hence, as in (I.28) and (I.29), we consider

$$F \star G = M \circ \exp\Big(\hbar \Gamma^{12}_{\Delta^+_\beta}\Big)\big(F \otimes G\big), \quad \Gamma^{12}_{\Delta^+_\beta} = \int dxdy\, \Delta^+_\beta(x - y)\, \frac{\delta}{\delta\phi_1(x)} \otimes \frac{\delta}{\delta\phi_2(y)}$$

for $F, G \in \mathscr{F}_{\mu C}(\mathbb{M})$, with M the multiplication operator $A \otimes B \mapsto AB$ as in 21. Arbitrary products of microcausal observables may be written by means of the extension of Γ over tensor products $A_1 \otimes \cdots \otimes A_n$ as

$$\Gamma^{ij}_{\Delta^+_\beta} = \int dxdy\, \Delta^+_\beta(x - y)\, \frac{\delta}{\delta\phi_i(x)} \otimes \frac{\delta}{\delta\phi_j(y)}$$

where $\delta/\delta\phi_i$ denotes the first functional derivative of the ith element on the tensor product of n functionals, with respect to the field ϕ. Therefore, we may write arbitrary $\star$-products as

$$\begin{aligned} A_1 \star \cdots \star A_n &= M\left[\left(\prod_{i<j} e^{\Gamma_{ij}}\right) A_1 \otimes \cdots \otimes A_n\right] = M\left((e^{\sum_{i<j}\Gamma_{ij}}) A_1 \otimes \cdots \otimes A_n\right) \\ &= M \circ P_n\left(A_1 \otimes \cdots \otimes A_n\right) \end{aligned}$$

with the introduction of the operator

$$P_n : \mathcal{F}^{\otimes n}_{\mu\mathbb{C}}(\mathbb{M}) \to \mathcal{F}^{\otimes n}_{\mu\mathbb{C}}(\mathbb{M}), \quad P_n := e^{\sum_{i<j}\Gamma_{ij}} = \prod_{i<j}\sum_{k=0}^{\infty}\frac{1}{k!}\left(\Gamma^{ij}_{\Delta^+_\beta}\right)^k.$$

For a graphic interpretation of the Bogoliubov map, we consider, as in section I.5, for arbitrary $n \in \mathbb{N}$ the set $\mathcal{G}_n$ of all graphs G with n vertices indexed as $V(G) = \{1, \ldots, n\}$ and an arbitrary but finite number of edges, the number of edges fixed by the number of functionals in the tensor product. The labeling of G is then in one-to-one correspondence with $A_1 \otimes \cdots \otimes A_n$, and for each pair $i, j \in V(G)$, the edges e connecting $i = \mathtt{s}(e)$ to $j = \mathtt{t}(e)$ must consider the non-symmetry of Δ^+_β under change of orientation. In this way, the summation in the definition of P_n above becomes a summation over the number of edges connecting vertices i, j, for all $i, j = 1, \ldots, n$, $i < j$. We may then write this same operator in the rather graphic-oriented form. Denoting $\mathtt{s}(e) \equiv x_e$, $\mathtt{t}(e) \equiv y_e$,

$$P_n = \sum_{G\in\mathcal{G}_n}\frac{1}{sym(G)}\int dxdy \prod_{e\in E(G)}\Delta^+_\beta(x_e - y_e),\ \delta_G.$$

The symbol $sym(G)$, called symmetry factor of the graph G, corresponds to

$$sym(G) = \prod_{\substack{i,j\in V(G)\\ i<j}}\Big(\#\{e \in E(G) : \mathtt{s}(e) = i,\ \mathtt{t}(e) = j\}\Big)!,$$

whereas δ_G correspond to the differential operator over the graph G,

$$\delta_G = \delta^{2|E(G)|}\Bigg/\left[\prod_{i\in V(G)}\left(\prod_{e\in E(G):\mathtt{s}(e)=i}\delta\phi_i(x_e)\prod_{e'\in E(G):\mathtt{t}(e')=i}\delta\phi_i(y_{e'})\right)\right].$$

In addition, arbitrary time-ordered products of local functionals may be treated in the analogous way, via the replacement of Δ^+_β by Δ^β_F in the above equations. The only particular difference concerning time-ordered products of local functionals is the fact that renormalization freedom has to be taken in consideration at each order.

The representation of both $\star$ and $\cdot_T$ presented in the lines above allow for a diagrammatic representation of the Bogoliubov map closely related to the Keldysh-Schwinger formalism. One notice the presence of the anti-S-matrix introducing the same anti-time ordered fields as in the second branch of Keldysh-Schwinger's contours, and thus introducing the equivalent doubling in the degrees of freedom of the field. In effect, the four propagators within $\mathcal{R}_V$ may be all combined in the matrix of propagators

$$D(x) := \begin{pmatrix} \Delta_F^{\beta}(x) & \Delta_{\beta}^{+}(x) \\ \Delta_{\beta}^{+}(x) & \overline{\Delta_F^{\beta}}(x) \end{pmatrix}, \tag{III.7}$$

which is analogous to the Keldysh matrix in the real-time formalism of TFT – see [LW87; Bel00]. In addition, $D(x)$ also contains this doubling of the degrees of freedom. The previous, graphic-oriented description of both $\star$ and $\cdot_T$, along with the introduction of the matrix $D(x)$ in (III.7) implies the establishment of a relation between the real-time formalism and the expansion of $\mathcal{R}_V$, in the form of the following proposition.

Theorem 2. *Let $\phi = (\phi^1, \phi^2) \in \mathcal{E}(\mathbb{M}) \times \mathcal{E}(\mathbb{M})$ and let $A, V_i \in \mathscr{F}_{loc(\mathbb{M})}$ with V_i depending only on ϕ^i, $i = 1, 2$ and $V = V_1 + V_2$. The Bogoliubov map may then be written in terms if the matrix of propagators $D(x)$ in* (III.7) *in a completely analogous way to the Keldysh-Schwinger formalism.*

Proof. Writing the Bogoliubov map with respect to D requires using this propagator in a unique product; this is achieved first by extending $\Gamma^{12}_{\Delta^+_\beta}$ as

$$F \cdot_D G = \widetilde{M} e^{\widetilde{\Gamma}^{12}_D}(F \otimes G), \quad \widetilde{\Gamma}^{12}_D := \sum_{a,b=1,2} \hbar \left\langle D_{ab}, \frac{\delta}{\delta \phi_1^a} \otimes \frac{\delta}{\delta \phi_2^b} \right\rangle$$

with F, G regular functionals over the doubled space of field configurations $\mathcal{E}(\mathbb{M}) \times \mathcal{E}(\mathbb{M})$. We shall denote the space of such functionals as $\widetilde{\mathscr{F}}_{\mathrm{reg}}(\mathbb{M})$, and by $\widetilde{M}$ the extension of M, the multiplication operator $A \otimes B \mapsto AB$ as in definition 21, onto $\widetilde{\mathscr{F}}_{\mathrm{reg}}(\mathbb{M})$. In adittion, D_{ab} are the matrix elements of (III.7) and $\delta/\delta\phi_i^a$ denotes the ath component of the first functional derivative acting upon the i-th element of the tensor product $F \otimes G$. The components a and b correspond to the two real brunches of the Keldysh-Schwinger contour. The operator $\widetilde{\Gamma}^{12}_D$ generalizes then to

$$\widetilde{\Gamma}^{ij}_D := \sum_{a,b=1,2} \hbar \left\langle D_{ab}, \frac{\delta}{\delta \phi_i^a} \otimes \frac{\delta}{\delta \phi_j^b} \right\rangle,$$

where $\delta/\delta\phi_i^a$ denotes the ath component first functional derivative acting upon the i-th element of the tensor product $A_1 \otimes \cdots \otimes A_n \in \widetilde{\mathscr{F}}^{\otimes n}_{reg}(\mathbb{M})$. We then obtain the graphic extension of the above product as

$$\begin{aligned} A_1 \cdot_D \cdots \cdot_D A_n =& \widetilde{M} \left[\left(e^{\sum_{i<j} \widetilde{\Gamma}^{ij}_D} \right) A_1 \otimes \cdots \otimes A_n \right] \\ =& \widetilde{M} \circ \widetilde{P}_n (A_1 \otimes \cdots \otimes A_n), \quad A_i \in \widetilde{\mathscr{F}}_{reg}(\mathbb{M}), \end{aligned}$$

with

$$\widetilde{P}_n := \sum_{G\in\mathcal{G}_n} \frac{1}{sym(G)} \left\langle \prod_{e\in E(G)} D\Big(x_e - y_e\Big), \widetilde{\delta}_G \right\rangle$$

and

$$\widetilde{\delta}_G := \frac{\delta^{2|E(G)|}}{\prod_{i\in V(G)} \Big(\prod_{e\in E(G):\mathtt{s}(e)=i} \delta\phi_i(x_e) \prod_{e'\in E(G):\mathtt{t}(e')=i} \delta\phi_i(y_{e'})\Big)}.$$

The product $\cdot_D$ may be extended to local functionals which separate components of the doubled field $\phi = (\phi^1, \phi^2)$, in the sense of tensor products $A\otimes B \in \mathscr{F}_{loc}^{\otimes k}(\mathbb{M})_1 \otimes \mathscr{F}_{loc}^{\otimes l}(\mathbb{M})_2$, where $\mathscr{F}_{loc}^{\otimes k}(\mathbb{M})_i$ denotes the set of k tensor products of local functional over the space of field configurations with respect to the field $\phi^i \in \mathcal{E}(\mathbb{M})$. In other words, the extension of $\cdot_D$ is performed upon tensor products of local functionals which depend exclusively on one of the ϕ^i components. The set of such restrictively local functionals will be denoted $\widetilde{\mathscr{F}_{1,2-loc}}(\mathbb{M})$. In order to justify the strictness of the above extension, notice that the product of local functionals mixing components ϕ^1 and ϕ^2 result in products $\Delta_\beta^+ \Delta_F^\beta$ with non-local singularities, which, according to the discussion in chapter I, is not a well defined distribution. For instance, we may see such a problematic term appearing in $\phi^1\phi^1 \cdot_D \phi^1\phi^2 \cdot_D \phi^1\phi^1$.

After the extension of $\cdot_D$ to the above particular class of local functionals we may define the S-matrix

$$\tilde{\mathcal{S}} := e^{iV}_{\cdot_D}, \quad V \in \widetilde{\mathscr{F}_{1,2-loc}}(\mathbb{M}).$$

Considering then $V \in \mathscr{F}_{1,2-loc}(\mathbb{M})$ with components V_1, V_2 depending only on ϕ^1, ϕ^2 respectively, we finally obtain that the Bogoliubov map may be written as

$$\mathcal{R}_V(A)(\phi) = \widetilde{M}\Big(\tilde{\mathcal{S}}(V_2) \cdot_D \tilde{\mathcal{S}}(V_1) \cdot_D A_1\Big)(\phi_1, \phi_2)\big|_{\phi_1=\phi_2\equiv\phi}\,, \tag{III.8}$$

where A_1 means the observable $A \in \mathscr{F}_{loc}(\mathbb{M})$ depends only on the 1-component of the doubled field, such as in the real-time formalism. This expression corresponds to the claim of the proposition above. In addition, since the expectation values of products of observables correspond to the evaluation of the product at $\phi = 0$, we obtain

$$\begin{aligned}
\omega^\beta \circ \mathcal{R}_V(A) &= \sum_{n_1,n_2} \frac{i^{n_1}(-i)^{n_2}}{n_1!n_2!} \underbrace{V_2 \cdot_D \cdots \cdot_D V_2}_{n_2} \cdot_D \underbrace{V_1 \cdot_D \cdots \cdot_D V_1}_{n_1} \cdot_D A_1\Bigg|_{(\phi^1,\phi_2)=(0,0)} \\
&= \sum_{n_1,n_2} \frac{i^{n_1}(-i)^{n_2}}{n_1!n_2!} \tilde{M} \sum_{G\in\mathcal{G}_n} \frac{1}{\mathrm{Sym}(G)} \times \\
&\quad\times \left\langle \prod_{e\in E(G)} D\Big(x_e - y_e\Big), \tilde{\delta}_G \right\rangle \underbrace{V_2 \otimes \cdots \otimes V_2}_{n_2} \otimes \underbrace{V_1 \otimes \cdots \otimes V_1}_{n_1} \otimes A_1\Bigg|_{\phi_1,\phi_2=0}\,,
\end{aligned} \tag{III.9}$$

with $n_1 + n_2 + 1 = n$. □

Expressions (III.8) and (III.9) represent the Bogoliubov map contribution to expectation values $\omega^\beta \circ \mathcal{R}_V(A)$, as in the above the cocycle contibution $U(i\beta)$ has been intentionally left aside. As previously mentioned (cf. chapter II), due to [DFP18] we know that in some particular cases the state $\omega^\beta \circ \mathcal{R}_V$ is enough to describe thermal equilibrium for the interacting theory in the large time limit, as the authors show that the clustering property (II.29) implies the return to equilibrium (II.28) holds if the interaction term is space-compactly supported. Therefore, in the particular case of V such as in (II.2) with $h \in \mathcal{C}_0^\infty(\mathbb{R}^3)$, we see that in the large time limit $t \to \infty$, which is also considered in the real-time formalism of TFT, $\omega^\beta \circ \mathcal{R}_V$ completely characterizes thermal equilibrium. Moreover, comparing expressions (III.8) with (II.28) and (II.23), in light of the discussion present in section II.3, it is possible to notice that, in this particular situation, the imaginary branch in the Keldysh-Schwinger contour indeed factorizes, and one is left with the real contributions depicted above only. The same, however, does not hold in the limit $h \to 1$, and there the cocycle contribution has to be considered also. In the following, we shall consider the role of U in the graphic representation of expectation values and establish its relation with the Matsubara formalism. The analysis of the state contribution to the expectation value $\omega^{\beta,V} \circ \mathcal{R}_V(A)$ will be first presented in the context of a compactly supported interaction term as before, and we shall later consider the adiabatic limit. In addition, in considering the role of U to thermal equilibrium characterization, one of our main result corresponds to theorem 3 below, which characterizes the state $\omega^{\beta,V}$ as in integration of connected components depending on imaginary time variables with values within $\mathcal{S}_+^n$.

We shall start by recollecting expression (II.24) describing the state $\omega^{\beta,V}$ in terms of connected components of ω^β, and noticing we may write such connected components in the graphic oriented form

$$\omega^{\beta,c}(A_0 \otimes \cdots \otimes A_n) = \sum_{G \in \mathcal{G}_{n+1}^c} \mathcal{P}_n(A_0 \otimes \cdots \otimes A_n)\big|_{\phi_k = 0\, \forall k=1,\dots,n} \tag{III.10}$$

with

$$\mathcal{P}_n := \prod_{i<j} \frac{1}{n_{ij}!} \int dxdy\, \Delta_\beta^+(x-y) \frac{\delta}{\delta\phi_i(x)} \otimes \frac{\delta}{\delta\phi_j(y)} = \frac{1}{sym(G)} \prod_{e \in E(G)} \mathcal{P}^{\mathtt{s}(e)\mathtt{t}(e)}. \tag{III.11}$$

From this point we obtain the following result. We first explicitly introduce the **n-dimensional symplex**

$$\beta S_n := \{(u_1, \dots, u_n) \in \mathbb{R}^n : 0 < u_1 < \cdots < u_n < \beta < +\infty\},$$

which had already been implicitly employed in the representation of $\omega^{\beta,V}$ in terms of connected components $\omega^{\beta,c}$ in equation (II.24).

Theorem 3. *Let $\Sigma_{2\varepsilon}$ as in section II.2 and let $h \in \mathcal{C}_0^\infty(\Sigma_\varepsilon)$. Then, for any $A \in \mathscr{A}^I(\Sigma_\varepsilon)$ and with V such that $K = \mathcal{R}_V \dot{V}$, the function*

$$\beta S_n \ni (u_1, \dots, u_n) \mapsto F(u_1, \dots, u_n) := \omega^{\beta,c}\left(A \otimes \bigotimes_{k=1}^n \alpha_{iu_k} K\right)$$

has a symmetric extension onto the set

$$\mathcal{C}_n = \{(z_1, \ldots, z_n) \in \mathbb{C}^n : \Re z_j = 0,\ \Im z_j \in (0, \beta),\ z_j \neq z_k \forall j, k = 1, \ldots, n\},$$

where $\mathcal{C}_n = \beta B_n \backslash diag(\mathbb{R}^n)$ *and* $\beta B_n := \{(z_1, \ldots, z_n) \in \mathbb{C}^n : \Re z_j = 0,\ \Im z_j \in (0, \beta)\}$ *and* $diag(\mathbb{R}^n) := \{(z_1, \ldots, z_n) \in \mathbb{R}^n : z_j = z_k \text{ for some } j, k = 1, \ldots, n,\ j \neq k\}$ *is the thick diagonal of* B_n*. In addition, representing* $\mathbf{u} \equiv (u_1, \ldots, u_n)$ *in either* $\beta B_n \backslash diag(\mathbb{R}^n)$ *or* βS_n*, the integration of the* n*th term in perturbation theory* F *may be written as*

$$\int_{\beta S_n} d\mathbf{u} F(\mathbf{u}) = \sum_{G \in \mathcal{G}^c_{n+1}} \frac{1}{sym(G) n!} \int_{\beta B_n} d\mathbf{u} F_G(\mathbf{u}). \tag{III.12}$$

Proof. Let $F : \mathbb{R}^n \to \mathbb{C}$, $F(t_1, \ldots, t_n) := \omega^{\beta,c}(A \otimes \alpha_{t_1} K \otimes \cdots \otimes \alpha_{t_n} K)$, then since F has an analytic extension

$$F(u_1, \ldots, u_n) := \omega^{\beta,c}\big(A \otimes \bigotimes_{k=1}^{n} \alpha_{iu_k} K\big), \tag{III.13}$$

into the symplex βS_n, this theorem refers to enlarging the analytic domain to the above set $\mathcal{C}_n$. The map F may be written in terms of separate contributions to each connected graph with $n+1$ vertices as

$$F(u_1, \ldots, u_n) = \sum_{G \in \mathcal{G}^c_{n+1}} \frac{1}{sym(G)} F_G(u_1, \ldots, u_n)$$

with a finite summation at each fixed perturbation order, since in the present we do not consider the individual expansions of each K. Hence, according to equations (III.10) and (III.11), due to the translation invariance of Δ^+_β we have, by moving the effect of each α_{iu} into the propagators (edges),

$$\begin{aligned} F_G(u_1, \ldots, u_n) = \int dX dY \left[\prod_{e \in E(G)} \Delta^+_\beta (x_e - y_e + i(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)}) \mathbf{e}_0) \right] \times \\ \times \left[\prod_{e \in E(G)} \frac{\delta^2}{\delta \phi_{\mathtt{s}(e)}(x_e) \delta \phi_{\mathtt{t}(e)}(y_e)} \right] \left(A \otimes \bigotimes_{k=1}^{n} K \right) \Big|_{\phi \equiv 0} \end{aligned} \tag{III.14}$$

where $dXdY \equiv dx_1 \ldots dx_{\#E(G)} dy_1 \ldots dy_{\#E(G)}$. We simplify the above equation by writing it as

$$F_G(\mathbf{u}) = \int dX dY \left[\prod_{e \in E(G)} \Delta^+_\beta \big(x_e - y_e + i(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)}) \mathbf{e}_0\big) \right] \Psi_G(X, Y)$$

with $\mathbf{u} \in \beta S_n$ and $\Psi_G(X, Y)$ the differential operator applied to the tensor product as above. The above expression allows for two important observations. First, due to the form of V, and hence of K, $\Psi_G(X,Y)$ defines a compactly supported distribution for each considered A. In addition, due to the form of $\beta\mathcal{S}_n$ we see that $u_j - u_k \in \mathcal{S}_-$ for each pair of arguments of $\mathbf{u}$. Therefore, $F_G(\mathbf{u})$ equals

$$F_G(\mathbf{u}) = \int dXdY \left[\prod_{e\in E(G)} \Delta^\beta\big(x_e - y_e + i(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)})\mathbf{e}_0\big)\right]\Psi_G(X,Y),$$

which differs from the former equation by the substitution of Δ^+_β by the thermal propagator obtained from (III.4). In conclusion, comparing the above expression with the analytic domain of the thermal propagator, we obtain the analytic extension of F. It still remain to prove F is symmetric, and this in effect is a consequence of symmetry of Δ^β.

Let $\sigma : \mathbf{u} \mapsto \sigma(\mathbf{u}) \in \beta\mathcal{S}_n$ a permutation of the arguments of $\mathbf{u} \in B_n$. This is well defined as the thick n-diagonal $diag_n(B_n)$ is excluded from the extended domain of F. Let the same symbol σ denote also the induced permutation over the graph $G \in \mathcal{G}^c_{n+1}$ acting over $V(G) = \{0,\dots,n\}$. Over $E(G)$ the permutation σ has the effect of possibly interchanging targets and sources. I.e., if G is ordered in such a way that $s(e) < t(e)$ then

$$\sigma(e) = \Big(\sigma(\mathtt{s}(\mathtt{e})), \sigma(\mathtt{t}(e))\Big)$$

if $\sigma(\mathtt{s}(\mathtt{e})) < \sigma(\mathtt{t}(e))$, and the converse if otherwise. In fact, for the action of σ over the graph G there are only two possibilities: either $\sigma(\mathtt{s}(e)) = \mathtt{s}(\sigma(e))$, or $\sigma(\mathtt{s}(e)) = \mathtt{t}(\sigma(e))$, the analogous holding also for the target of e. With $\sigma(G)$ the (unique) connected graph with vertices $V(\sigma(G)) = \sigma(V(G))$ and edges $E(\sigma(G)) = \sigma(E(G))$ (maybe equal to G), then $F_{\sigma(G)}(\sigma(\mathbf{u}))$ is such that the propagators there within may be either

$$\begin{aligned}\Delta^\beta\big(x_{\sigma(\mathtt{e})} - y_{\sigma(\mathtt{e})} + i(\sigma(u)_{\mathtt{s}(\sigma(e))} - \sigma(u)_{\mathtt{t}(\sigma(e))})\mathbf{e}_0\big) &= \\ &= \begin{cases}\text{either} & \Delta^\beta\big(x_e - y_e + i(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)})\mathbf{e}_0\big)\\ \text{or} & \Delta^\beta\big(y_e - x_e - i(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)})\mathbf{e}_0\big).\end{cases}\end{aligned}$$

However, due to the parity symmetry of the thermal propagator depicted in equations (III.5) and (III.6), within the symplex $\beta\mathcal{S}_n$ the two latter result are actually the same. This proofs that the invariance of F_G under the action of σ for each edge of G, and thus we conclude $F_G(U) = F_{\sigma(G)}(\sigma(\mathbf{u}))$, and finally the invariance of F under any arbitrary permutation of its arguments.

Additionally, this theorem says that each integration of F_G may be extended from $\beta\mathcal{S}_n$ to $\beta B_n\backslash diag(\mathbb{R}^n)$, which differs from βB_n by a set with null measure. So far we have seen that each function F originally defined on the symplex, may be extended to the box βB_n up to the set of diagonals. The result is then a symmetric function defined over the set $\beta B_n\backslash diag(\mathbb{R}^n)$, which is formed by $n!$ disjoint connected components. Therefore, the integrations over the box βB_n and over the symplex βS_n coincide up to a permutation term $n!$ contained within (III.12). This concludes the proof. □

The above result allows for a change in the expression of $\omega^{\beta,V}$ in terms of connected components of the free β-KMS state. We shall use the latter result to rewrite $\omega^{\beta,V}$ in a Dyson series-like form which takes in consideration the Matsubara formalism.

Theorem 4. *The integration of* (III.12) *over the box is such that*

$$\begin{aligned}\int_{\beta B_n} d\mathbf{u}\, F_G(\mathbf{u}) =& \frac{1}{\beta^{\#E(G)}} \int dP \sum_{N\in\mathbb{Z}^{\#E(G)}} \prod_{e\in E(G)} \Xi_G(P)\times \\ & \times \prod_{1\leq j\leq n} \delta^K \left(\sum_{e\in E(G),\mathbf{t}(e)=j} w_{n_e} - \sum_{e'\in E(G),\mathbf{s}(e')=j} w_{n_{e'}} \right)\end{aligned}$$

where the symbol Ξ_G represents an integral kernel depending on momentum P and δ^K is the Kronecker delta function.

Proof. We start by writing the function F_G relative to $G \in \mathcal{G}^{\rfloor}_{\backslash+\infty}$ in Fourier space. Due to the thermal propagator translation invariance, each integral $F_G(\mathbf{u})$ in equation (III.14) may be also written as

$$F_G(\mathbf{u}) = \int dP \left[\prod_{e\in E(G)} \widehat{\Delta}^\beta\big(u_{\mathbf{s}(e)} - u_{\mathbf{s}(e)}, p_e\big)\right] \hat{\Psi}_G(-P, P),$$

since

$$\begin{aligned}&\int \prod_{i=1}^{n} dx_{0i} dy_{0i} d\mathbf{x}_i d\mathbf{y}_i\, \Psi(x_1, \ldots, x_n, y_1, \ldots, y_n) e^{ip_{0i}x_{0i}} e^{-i\mathbf{p}_i\mathbf{x}_i} e^{-ip_{0i}y_{0i}} e^{i\mathbf{p}_i\mathbf{y}_i} \\ &= \hat{\Psi}(-p_{01}, \mathbf{p}_1, \ldots, -p_{0n}, \mathbf{p}_n, p_{01}, -\mathbf{p}_1, \ldots, \ldots, p_{0n}, -\mathbf{p}_n) \equiv \hat{\Psi}_G(-P, P),\end{aligned}$$

with $\hat{\Delta}^\beta(u, p)$ as in equation (III.4). Assume for a moment that we may change the order of integrations, so that integration in $d\mathbf{u}$ may be performed prior to the integral with respect to dP. Then we consider

$$I_G \equiv \int_{\beta B_n} d\mathbf{u}\, F_G(\mathbf{u}) = \int dP \int_{\beta B_n} d\mathbf{u} \left[\prod_{e\in E(G)} \widehat{\Delta}^\beta\big(u_{\mathbf{s}(e)} - u_{\mathbf{s}(e)}, p_e\big)\right] \hat{\Psi}_G(-P, P), \tag{III.15}$$

and use the Fourier series expression for the thermal propagator, which produces

$$I_G = \int dP \int_{\beta B_n} d\mathbf{u} \left[\prod_{e\in E(G)} \sum_{n_e\in\mathbb{Z}} \tilde{\Delta}^\beta\big(n_e, p_e\big) e^{i\omega_{n_e}[u_{\mathbf{s}(e)} - u_{\mathbf{s}(e)}]}\right] \hat{\Psi}_G(-P, P).$$

We notice we may reorder the product and the summation above as follows. For each edge $e \in E(G)$ the above kernel contains a Fourier series labeled by some n_e; considering the product of one particular term of the series for some edge e with another term belonging to the series relative to some other edge e' we obtain

$$\exp\left(i\frac{2\pi}{\beta}\left[n_e(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)}) - n'_{e'}(u_{\mathtt{s}(e')} - u_{\mathtt{t}(e,)})\right]\right),$$

and hence in the integration I_G we obtain a summation of the exponents over the edges. Namely, when considering all vertices we obtain

$$\exp\left(i\frac{2\pi}{\beta}\sum_{j=1}^{n}\left(\sum_{\substack{e'\in E(G)\\ \mathtt{s}(e)=j}} n_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=j}} n_{e'}\right) u_j\right),$$

i.e. one such a term for each value of the label in the Fourer series. In conclusion, the integration I_G becomes

$$I_G = \int dP \int_{\beta B_n} d\mathbf{u} \sum_{N\in\mathbb{Z}^{\#E(G)}} \exp\left(i\frac{2\pi}{\beta}\sum_{j=1}^{n}\left(\sum_{\substack{e'\in E(G)\\ \mathtt{s}(e)=j}} n_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=j}} n_{e'}\right) u_j\right)\times$$
$$\times\left(\prod_{l\in E(G)} \tilde{\Delta}^{\beta}(n_l, p_l)\right)\hat{\Psi}_G(-P,P),$$

where the summation in $N = (n_1, \ldots, n_{\#E(G)})$ corresponds to the $\#E(G)$ summations over $\mathbb{Z}$. Changing the order of the summation over N with the integration with respect to $d\mathbf{u}$ and using the decomposition of the Kronecker delta as a finite sum of exponentials (see [GR07], for instance) we hence obtain

$$I_G = \frac{1}{\beta^{\#E(G)}}\int dP \sum_{N\in\mathbb{Z}^{\#E(G)}} \prod_{e\in E(G)} \frac{1}{w^2_{\mathbf{p}_e} + w^2_{n_e}}\left[\delta(p_0 - w_{\mathbf{p}_e}) + \delta(p_0 + w_{\mathbf{p}_e})\right]\left(\frac{1}{2} + i\frac{w_{n_e}}{2p_0}\right)\times$$
$$\times \prod_{1\le j\le n} \delta^K\left(\sum_{e\in E(G),\mathtt{t}(e)=j} w_{n_e} - \sum_{e'\in E(G),\mathtt{s}(e')=j} w_{n_{e'}}\right)\hat{\Psi}_G(-P,P), \tag{III.16}$$

where we take advantage of the invariance of the Kronecker delta δ^K under multiplication by a constant in order to obtain an expression in terms of the Matsubara frequencies, $w_n = 2\pi n\beta^{-1}$. The above expression proves the claim up to equation (III.15). In addition, the summation of Matsubara frequencies in the Kronecker delta corresponds to a conservation of such frequencies.

In order to prove equation (III.15), we first of all have to consider the δ distributions within the thermal propagator. In order to use the Lebesgue's dominated convergence theorem, we replace each δ in the propagators by a smooth approximation δ_ϑ and consider the limit $\delta_\vartheta \to \delta$ in the end. The presence of smooth functions in the integral kernel will not affect the decaying properties of certain integrations to be explicitly discussed below.

The integration domain $B_n \backslash diag(B_n)$ corresponds to the disjoint union of $n!$ subsets, each one describing the subtraction of one line of the thick diagonal $diag(B_n)$. In addition, as discussed in the proof of theorem 3 we see that each one of these connected components may be interpreted as a symplex $\beta\mathcal{S}_n$, via some permutation σ. Therefore, for any connected component of $B_n \backslash diag(B_n)$, let $\vartheta \in (0, \beta/(n+1))$ and consider the splitting of this component of $B_n \backslash diag(B_n)$ in two components: one whose nth argument's distance to β is less than ϑ, i.e.

$$\beta\mathcal{S}_n = \beta\mathcal{S}_n^{\downarrow} \sqcup \beta\mathcal{S}_n^{\vartheta}, \quad \beta\mathcal{S}_n^{\vartheta} := \{\mathbf{u} \in \beta\mathcal{S}_n : \beta - u_n < \vartheta\},$$

and $\beta\mathcal{S}_n^{\downarrow}$, the complementary of $\mathcal{S}_n^{\vartheta}$ with respect to $\beta\mathcal{S}_n$. The heuristic idea is that the last condition implies a reduction in the distance between elements u_k, u_{k+1} of $\beta\mathcal{S}_n^{\downarrow}$ in order to accommodate a distance ϑ from u_n to β. Consider then

$$g_G(\mathbf{u}, P) := \prod_{e \in E(G)} \hat{\Delta}^{\beta}(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)})$$

depending on P via the frequencies $w_{\mathbf{p}_e}$, and let

$$I_G^{\downarrow} := \int_{\beta\mathcal{S}_n^{\downarrow}} d\mathbf{u} \int dP\, g_G(\mathbf{u}, P) \hat{\Psi}_G(-P, P).$$

As $\hat{\Psi}_G$ is the Fourier transform of a compactly supported distribution, it is an analytic function, which grows at most polynomially on $|P|$. In addition, due to the presence of the mollifi

ed δ-functions in the propagators, the only directions along which the integral kernel $g_G \hat{\Psi}_G$ may present a non-fast decrease would be $P \equiv 0$ – which means $p_j = 0\ \forall j$. As for the directions on the lightcone, in [FL14], proposition 9 the authors show that, along directions on the future lightcone, $\hat{\Psi}_G(-P, P)$ is also fast decresing. Finally, for $\mathbf{u} \in \beta S^{\downarrow}$ the absolute value

$$|g_G(\mathbf{u}, P)| \leq C \exp\bigg(- \Big(\beta - \sup|u_i - u_j|\Big) w_{\mathbf{p}_k} \bigg),$$

with $\sup|u_i - u_j| < \beta - \vartheta$, is exponentially bounded for some past directed p_k.

The βS_n^{ϑ}-contribution may be treated similarly. Due to the KMS property, the thermal propagator is such that, given the permutation $\pi\ \{1, \ldots, n\} \to \{n, 1, \ldots, n-1\}$ over G, with $\pi(\mathbf{u}) \equiv (u_n, u_1, \ldots, u_{n-1})$, then

$$g_G(u_1, \ldots, u_n, P) = g_{\pi(G)}(u_n - \beta, u_1, \ldots, u_{n-1}, \pi(P)),$$

where $\pi(P) := (\pi(p_1), \ldots \pi(p_{\#E(G)}))$, $\pi(p_k) = -p_k$ if $k = n$ and equal p_k otherwise. Using the translation invariance of the thermal propagator – and thus of g_G, we set

$$(v_1, \ldots, v_n) := (0, u_1 + \beta - u_n, \ldots, u_{n-1} + \beta - u_n)$$

and notice that $\mathbf{u} \in \beta\mathcal{S}_n^{\vartheta} \Leftrightarrow \mathbf{v} \in \beta\mathcal{S}_n^{(1)}$, where $\beta\mathcal{S}_n^{(1)} := \{(v_1, \ldots, v_n) \in \beta\mathcal{S}_n : v_1 < \vartheta\}$.This therefore means that the integration I_G^{ϑ} may be written as

$$I_G^{\vartheta} = \int_{\beta\mathcal{S}_n^{(1)}} d\mathbf{v} \int d\pi(P)\, g_{\pi(G)}(\mathbf{v}, \pi(P))\hat{\Psi}_G(-\pi(P), \pi(P)).$$

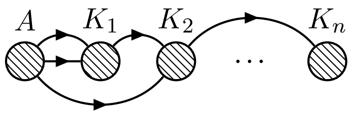
We then iterate the above process and split the latter integration domain as $\beta\mathcal{S}_n^{(1)} = \beta\mathcal{S}_n^{(1)\downarrow} \sqcup \beta\mathcal{S}_n^{(1)\vartheta}$ as before. Focusing on the second connected component, we repeat the previous procedure and now end up with the new region $\beta\mathcal{S}_n^{(2)} := \{\mathbf{v} \in \beta\mathcal{S}_n^{(1)} : v_2 - v_1 < 2\vartheta\}$. Therefore, by repeating this procedure n times, we will end up with an integration region such that the largest distance between v_i, v_j does not exceeds $n \times \vartheta$. Since ϑ is arbitrary, we may now consider the limit $\vartheta \to 0$, and so we conclude that only the $\beta S_n^{\downarrow}$-contribution is relevant. We then explicitly obtain

$$\begin{aligned} I_G^{\downarrow} &:= \int_{\beta\mathcal{S}_n^{\downarrow}} d\mathbf{u} \int dP \left[\prod_{e\in E(G)} \widehat{\Delta}^{\beta}\big(u_{\mathbf{s}(e)} - u_{\mathbf{s}(e)}, p_e\big)\right] \hat{\Psi}_G(-P, P) \\ &= \int_{\mathcal{S}_n^{\downarrow}} d\mathbf{u} \int dP \prod_{e\in E(G)} \left[\frac{1}{(2\pi)^3} \sum_{n\in\mathbb{Z}} \frac{1}{w_{\mathbf{p}_e}^2 + \omega_n^2} \frac{1}{2} \left(1 + \frac{i\omega_n}{p_0}\right) \sum_{\sigma=\pm 1} \delta(p_0 + \sigma w) \times \right. \\ &\quad \left. \times\, e^{i\omega_n (u_{\mathbf{s}(e)} - u_{\mathbf{s}(e)})}\right] \hat{\Psi}_G(-P, P). \end{aligned}$$

We may highlight some important parts of this proof as follows. For $P \not\equiv 0$, which means for not every p_j null, the above kernel is rapidly decreasing as a function of P for all $\mathbf{u} \in \beta\mathcal{S}_{\beta}^{\downarrow}$. Notice this would not true for $\mathbf{u} \in \beta\mathcal{S}_{\beta}^{\vartheta}$. We know already from chapter I and the construction of Δ^{β} that this is truth for non zero momenta, and, in addition, proposition 8 of [FL14] assures that these are directions of rapid decrease of $\hat{\Psi}$. This implies the change of integration order within $\beta\mathcal{S}_n^{\downarrow}$ once we have mollified the Dirac delta functions, as by considering an approximation of δ by a sequence of smooth functions, we may apply Fubini's theorem (the presence of smooth functional also does not affect the directions of rapid decrease of the kernel). □

From the proof of theorem 4 above, we have hence obtained the conservation of Matsubara frequencies, as previously stated. This will become an important elemnet in the set of Feynman rules for thermal perturbative computations, to be discussed in the next section.

Looking back at theorems 2 and 4, in light of the discussion presented in the previous chapter, we see that the expansion of the interacting observable $\mathcal{R}_V(A)$ due to the Bogoliubov map involves a doubling in the degrees of freedom with the introduction of a two-component field and leads to a description equivalent to the real part of Keldysh-Schwinger contour. This however is not enough to describe thermal equilibrium for interacting theories unless the clustering condition (II.29) holds, which leads to return to equilibrium (II.28). This is not the case when considering the adiabatic limit, yet to be further discussed. When we consider the rigorous approach to thermal equilibrium by Fredenhagen and Lindner in [FL14], considering the KMS state $\omega^{\beta,V}$, the effect of $U(i\beta)$ corresponding to the imaginary part integration is equivalent to conservation of Matsubara frequencies, as shown in the latter theorem. We hence conclude that a full description of the thermal equilibrium requires both real-time and Matsubara formalism at each term in the perturbation series, which corresponds to a sum of connected graphs. A graphic representation for the perturbation series, such as



(III.17)

then consists of connected diagrams (bubbles), with inner structure equivalent to the real-time formalism, all of them connected to each other via the thermal propagator and producing itself a connected diagram. In the particular case the bubble-diagrams have their inner structure neglected, we return to the Matsubara formalism, except for the fact that at each vertex we consider a imaginary time extension with a non null real part. This may be seen in the arguments of the thermal propagators in the previous results. On the other hand, if the total diagram is just the union of the connected bubbles, we obtain only Keldysh-Schwinger formalism with the factorization of imaginary contributions. The next step, therefore, is to analyze the adiabatic limit and then conclude with the set of Feynman rules for the graphic expansion obtained.

III.2 The adiabatic limit and Feynman rules for interacting thermal systems

We consider the limit $h \to 1$ in the sense of definition 30 over each term $F(\mathbf{u})$. In order to highlight the dependence of F on h via K we shall now denote it as F^h. The adiabatic limit, however, is considered in a two-steps procedure. First we consider the limit $h \to 1$ of each K, and later on we take the adiabatic limit over F^h. The next proposition will render clear this procedure.

Proposition 25. *With $K = \mathcal{R}_V \dot{V}$, consider*

$$K = \int_{\mathbb{R}^3} d\mathbf{x}\, h(\mathbf{x}) \mathcal{H}^I_h(\mathbf{x}) := \int_{\mathbb{R}^3} d\mathbf{x}\, h(\mathbf{x}) \int dt\, \dot{\chi}(t) \mathcal{R}_V\big(V(t,\mathbf{x})\big).$$

The von Hove limit $\mathcal{H}^I(\mathbf{x}) := \lim_{h\to 1} \mathcal{H}^I_h(\mathbf{x})$ is a well-defined compactly supported kernel.

Proof. As $h \to 1$ we obtain

$$\begin{aligned}\lim_{h\to 1} \mathcal{H}^I_h(\mathbf{x}) &= \lim_{h\to 1} \int dt\, \dot{\chi}(t) \mathcal{R}_V\big(V(t,\mathbf{x})\big) = \int dt\, \dot{\chi}(t) \alpha^V_{(t,\mathbf{x})} \mathcal{R}_V\big(V(0,0)\big) \\ &= \int dt\, \dot{\chi}(t) \mathcal{R}_V \circ \alpha_{(t,\mathbf{x})}\big(V(0,0)\big)\end{aligned}$$

The causal factorization property as per proposition 15 implies the Bogoliubov map does not affect the support of its argument. Therefore, due to the support of $\dot{\chi}$ we conclude the claim. □

Let then

$$F^h(\mathbf{u}) = \int d\mathbf{x} \int d\mathbf{u} \prod_{j=1}^{n} h(\mathbf{x}_j)\omega^{\beta,c}\big(A \otimes \bigotimes_{j=1}^{n} \alpha_{iu_j} \circ \alpha^V_{(0,\mathbf{x}_j)} \mathcal{H}^I(0)\big), \quad d\mathbf{x} \equiv d\mathbf{x}_1 \dots d\mathbf{x}_n. \tag{III.18}$$

We see the adiabatic limit procedure we are considering has been performed up to the interaction term V in $\mathcal{R}_V$. This is covered in the theorem above.

Theorem 5. *The adiabatic limit at each order in perturbation series*

$$F(\mathbf{u}) := \lim_{h\to 1} F^h(\mathbf{u}) = \lim_{h\to 1} \sum_{G\in\mathcal{G}^c_{n+1}} \frac{1}{sym(G)n!} F^h_G(\mathbf{u})$$

is well defined. In addition, it implies momentum conservation at each vertex of each graph $G \in \mathcal{G}^c_{n+1}$.

Proof. The proof of this theorem follows to a large degree the proof of theorem 4. Writing the component of F^h to each graph as in (III.15) with the translations terms in (III.18) results in

$$F^h_G = \int d\mathbf{X} \prod_{j=1}^{n} h(\mathbf{x}_j) \int_{\beta B_n} \int dP \prod_{k=1}^{n} \exp\left(i\mathbf{x}_k \left(\sum_{\substack{e\in E(G)\\ \mathtt{s}(e)=k}} \mathbf{p}_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=k}} \mathbf{p}_{e'} \right)\right) \times$$
$$\times \left(\prod_{e\in E(G)} \hat{\Delta}^\beta\big(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)}, p_l\big) \right) \hat{\Phi}_G(-P, P)$$

with

$$\Phi_G(X,Y) := \prod_{e\in E(G)} \frac{\delta^2}{\delta\phi_{\mathtt{s}(e)}(x_e)\delta\phi_{\mathtt{t}(e)}(y_e)} \Big(A \otimes \bigotimes_{l=1}^{n} \mathcal{H}(0) \Big)\Big|_{\phi\equiv 0}$$

and $\hat{\Phi}_G$ its Fourier transform. Now we may interchange the order of integrations in $d\mathbf{u}$ and dP provided both A and $\mathcal{H}(0)$ are compactly supported – the latter condition following from proposition 25 above. We hence consider the integration with respect to dP of

$$\prod_{k=1}^{n} \exp\left(i\mathbf{x}_k\left(\sum_{\substack{e\in E(G)\\ \mathtt{s}(e)=k}} \mathbf{p}_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=k}} \mathbf{p}_{e'}\right)\right) \times$$
$$\times \underbrace{\int_{\beta B_n} d\mathbf{u} \left(\prod_{e\in E(G)} \hat{\Delta}^{\beta}\big(u_{\mathtt{s}(e)} - u_{\mathtt{t}(e)}, p_l\big)\right) \hat{\Phi}_G(-P,P)}_{=:L(P)}.$$

The function $L(P)$, cf. the argumentation employed in the proof of theorem 4, is rapidly decreasing and thus we can also consider the adiabatic limit $h \to 1$ in the sense of functions, i.e. we may interchange the limit and the integral with respect to each $d\mathbf{x}_j$. This produces

$$\begin{aligned}
\lim_{h\to 1} F_G^h = &\int_{\mathbb{R}^{3n}} d\mathbf{x} \int dP\, L(P) \times \prod_{k=1}^{n} \exp\left(i\mathbf{x}_k\left(\sum_{\substack{e\in E(G)\\ \mathtt{s}(e)=k}} \mathbf{p}_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=k}} \mathbf{p}_{e'}\right)\right)\\
=&(2\pi)^{3n} \int dP\, L(P) \prod_{k=1}^{n} \delta\left(\sum_{\substack{e\in E(G)\\ \mathtt{s}(e)=k}} \mathbf{p}_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=k}} \mathbf{p}_{e'}\right)\\
=&(2\pi)^{3n} \frac{1}{\beta^{\#E(G)}} \int dP \sum_{N\in\mathbb{Z}^{\#E(G)}} \prod_{k=1}^{n} \delta\left(\sum_{\substack{e\in E(G)\\ \mathtt{s}(e)=k}} \mathbf{p}_e - \sum_{\substack{e'\in E(G)\\ \mathtt{t}(e')=k}} \mathbf{p}_{e'}\right) \times\\
&\times \prod_{1\le j\le n} \delta^K\left(\sum_{e\in E(G),\mathtt{t}(e)=j} \omega_{n_e} - \sum_{e'\in E(G),\mathtt{s}(e')=j} \omega_{n_{e'}}\right) \hat{\Phi}_G(-P,P)
\end{aligned}$$

as the rapid decrase of L allows for the interchange between integrations in $d\mathbf{X}$ and dP from the first to the second line, and third line corresponds to writing $L(P)$ as in equation (III.16). The last term establishes the momentum conservation. $\square$

In conclusion, we see that, in the adiabatic limit, there is not only Matsubara frequencies conservation at each bubble vertex of (III.17), but also momentum conservation at each bubble. We may now recollect the previous results in the following. By $\phi(x)$, we denote the kernel of the linear functional Φ_f and consider the graphic representation of

$$G(x_1,\ldots,x_N) := \omega^{\beta,V} \circ \mathcal{R}_V\big(T(\phi(x_1),\ldots,\phi(x_N)\big). \tag{III.19}$$

Due to the results presented in this section, such diagramatic representation is guided by the set of Feynman rules below.

Feynman rules for thermal interacting systems:

1. The nth order contribution to the perturbative expansion of (III.19) corresponds to a finite sum of connected graphs only.
2. In $3n$-dimensional momentum space, to $\mathcal{R}_V\big(T(\hat{\phi}(t_1,\mathbf{p}_1),\ldots,\hat{\phi}(t_N,\mathbf{p}_N))\big) \equiv A$ and to each $\mathcal{H}(0) = \mathcal{R}_V \int dt' \dot{\chi}(t')V(t\,0)$ corresponds a connected diagram; each one of these diagrams is regarded as a bubble, or vertex to the larger diagram; the number of factors $\mathcal{H}(0)$ plus the number of internal vertices for A must sum up to the order in perturbation theory n.
3. Edges in the internal vertices are connected via the propagator $\hat{D}$ in (III.7); bubbles are connected with thermal propagators (III.4).
4. Impose momentum and Matsubara frequency conservation over each bubble.
5. Multiply each graph by the appropriate numeric factor as in (III.12)
6. Perform anti-Fourier transform and integration over the time variables, considering cutoffs $\dot{\chi}$ and χ; if $x_1,\ldots x_n \in \Sigma_\varepsilon$, then $\chi = 1$ and its may be neglected.

Up to now we have presented arguments justifying the use of the real-time formalism in some cases, and pointed the failure of this formalism to describe thermal equilibrium for perturbative systems in general. This analysis drove us to the above set of Feynman rules. We now would like to present some examples of expectation values computation in which the effect of $U(i\beta)$ is not neglectable. This will be the topic of next section.

III.3 Practical computations in perturbative systems

In the following we shall consider the corrections to the self-energy due to $U(i\beta)$ in the presence of two different interaction terms.

III.3.1 $\lambda\phi^2$-theory.

We estimate the expectation value $\omega^{\beta,V} \circ \mathcal{R}_V(\phi^2)$ with the quadratic interaction

$$V(\phi) = \frac{\lambda}{2}\int_{\mathbb{M}} dz\,\chi(z_0)h(\mathbf{z})\phi^2(z), \tag{III.20}$$

where both $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ and $h \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ are as before. This computation will be performed up to first order in perturbation theory, as already at this order we shall notice differences between $\omega^\beta \circ \mathcal{R}_V$ and $\omega^{\beta,V}$. Considering expansion (I.48), it starts as

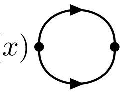
$$\omega^{\beta,V} \circ \mathcal{R}_V(\phi^2) = \frac{\omega^\beta\left(\mathcal{R}_V(\phi^2) \star U(i\beta)\right)}{\omega^\beta\left(U(i\beta)\right)}$$
$$= \omega^\beta\left(\phi^2\right) + \omega^\beta\left(iV \cdot_T \phi^2 - iV \star \phi^2\right) - \int_0^\beta du\, \omega^\beta\left(\phi^2 \otimes \alpha_{iu}\dot{V}\right) + O(\lambda^2),$$

We are therefore mainly interested in the first order difference

$$\Sigma^1_U(\phi^2) := \omega^{\beta,V} \circ \mathcal{R}_V(\phi^2) - \omega^\beta \circ \mathcal{R}_V(\phi^2).$$

According to the notation established in section I.5 this may be represented as

$$\Sigma^1_U(\phi^2) = -\int_0^\beta du \left(\phi^2(x) \quad\quad \alpha_{iu'}\dot{V}(z) \right) = -\int_0^\beta du\, \omega^{\beta,c}\left(\phi^2 \otimes \alpha_{iu}\dot{V}\right)$$



$$= -\int_0^\beta du \int dz\, \dot{\chi}(z_0) h(\mathbf{z}) \alpha_{iu} (\Delta^+_\beta)^2(x-z)$$
$$= \int_0^\beta du \int dz\, \dot{\chi}(z_0) h(\mathbf{z}) \int dp\, (\widehat{\Delta}^+_\beta)^2(p) e^{ip(x-z)} e^{-pu}$$

The square of the KMS state two-point function in momentum space $\widehat{\Delta}^+_\beta$ becomes

$$\mathcal{F}(\widehat{\Delta}^+_\beta)^2(p) = \widehat{\Delta}^+_\beta * \widehat{\Delta}^+_\beta(p) = \int dq\, \widehat{\Delta}^+_\beta(q) \widehat{\Delta}^+_\beta(p-q)$$
$$= \frac{1}{(2\pi)^6} \int dq \left\{ \frac{1}{2w_q} \frac{\delta(q_0 - w_q)}{1 - e^{-\beta w_q}} + \frac{1}{2w_q} \frac{e^{-\beta w_q} \delta(q_0 + w_q)}{1 - e^{-\beta w_q}} \right\} \times$$
$$\times \left\{ \frac{1}{2w_{p-q}} \frac{\delta(p_0 - q_0 - w_{p-q})}{1 - e^{-\beta w_{p-q}}} + \frac{1}{2w_{p-q}} \frac{e^{-\beta w_{p-q}} \delta(p_0 - q_0 + w_{p-q})}{1 - e^{-\beta w_{p-q}}} \right\}.$$

In addition, in the adiabatic limit we obtain

$$h \to 1 \Rightarrow \int d\mathbf{z}\, h(\mathbf{z}) e^{i\mathbf{p}(\mathbf{z})} \to (2\pi)^3 \delta(\mathbf{p}).$$

As each frequency term $w_\mathbf{k}$ depends only on $|\mathbf{k}|$, the integration with respect to $d\mathbf{p}$ in the adiabatic limit then result in equal frequencies $w_\mathbf{p}$ and $w_{\mathbf{p}-\mathbf{q}}$, and thus

$$(\widehat{\Delta}^+_\beta)^2(p) = \frac{1}{(2\pi)^3} \int dq \left\{ \frac{1}{2w} \frac{\delta(q_0 - w)}{1 - e^{-\beta w}} + \frac{1}{2w} \frac{e^{-\beta w} \delta(q_0 + w)}{1 - e^{-\beta w}} \right\} \times$$
$$\times \left\{ \frac{1}{2w} \frac{\delta(p_0 - q_0 - w)}{1 - e^{-\beta w}} + \frac{1}{2w} \frac{e^{-\beta w} \delta(p_0 - q_0 + w)}{1 - e^{-\beta w}} \right\}$$
$$= \frac{1}{(2\pi)^3} \int \frac{dq}{4w^2 (1 - e^{-\beta w})^2} \left\{ \delta(q_0 - w) \left[\delta(p_0 - q_0 - w) + e^{-\beta w} \delta(p_0 - q_0 + w) \right] \right.$$
$$\left. + e^{-\beta w} \delta(q_0 + w) \left[\delta(p_0 - q_0 - w) + e^{-\beta w} \delta(p_0 - q_0 + w) \right] \right\}$$
$$= \frac{1}{(2\pi)^3} \int \frac{d\mathbf{q}}{4w^2 (1 - e^{-\beta w})^2} \left\{ \delta(p_0 - 2w) + 2e^{-\beta w} \delta(p_0) + e^{-2\beta w} \delta(p_0 + 2w) \right\}$$

Hence

$$
\begin{aligned}
-\Sigma^1_U(\phi^2) =&\frac{2}{(2\pi)^3}\int_0^\beta du\int dz_0 d\mathbf{q}dp_0\,\frac{1}{4w^2_{\mathbf{q}}(1-e^{-\beta w_{\mathbf{q}}})^2}\chi(z_0)\Big\{\delta(p_0-2w_{\mathbf{q}})+\\
&+2e^{-\beta w_{\mathbf{q}}}\delta(p_0)+e^{-2\beta w_{\mathbf{q}}}\delta(p_0+2w_{\mathbf{q}})\Big\}e^{ip_0(x_0-z_0)}e^{-p_0u}\\
=&\frac{2}{(2\pi)^3}\int_0^\beta du\int dz_0 d\mathbf{q}dp_0\,\frac{1}{4w^2_{\mathbf{q}}(1-e^{-\beta w_{\mathbf{q}}})^2}\chi(z_0)\Big\{\delta(p_0-2w_{\mathbf{q}})+\\
&+2e^{-\beta w_{\mathbf{q}}}\delta(p_0)+e^{-2\beta w_{\mathbf{q}}}\delta(p_0+2w_{\mathbf{q}})\Big\}e^{ip_0(x_0-z_0)}e^{-p_0u}\\
=&\frac{2}{(2\pi)^3}\int_0^\beta du\int dz_0\int\frac{d\mathbf{q}}{4w^2_{\mathbf{q}}(1-e^{-\beta w_{\mathbf{q}}})^2}\chi(z_0)\Big\{e^{-2w_{\mathbf{q}}u}e^{i2w_{\mathbf{q}}(x_0-z_0)}+\\
&+\beta e^{-\beta w_{\mathbf{q}}}+e^{-2\beta w_{\mathbf{q}}}e^{2w_{\mathbf{q}}u}e^{-i2w_{\mathbf{q}}(x_0-z_0)}\Big\}
\end{aligned}
$$

The integration with respect to dz_0 then produces the Fourier transform of the cutoff functions $\dot{\chi}$,

$$
\begin{aligned}
\Sigma^1_U(\phi^2) =&-\frac{2}{(2\pi)^3}\int_0^\beta du\int\frac{d\mathbf{q}}{4w^2(1-e^{-\beta w})^2}\Big\{e^{2wu}e^{i2wx_0}\widehat{\chi}(-2w)+\beta e^{-\beta w}+\\
&+e^{-2\beta w}e^{-2wu}e^{-i2wx_0}\widehat{\chi}(2w)\Big\}
\end{aligned}
$$

The integrations throughout the symplex becomes

$$
\int_0^\beta due^{\pm 2\omega u}=\frac{e^{\pm 2\beta\omega}-1}{\pm 2\omega},
$$

and hence

$$
\begin{aligned}
&\Sigma^1_U(\phi^2) =\\
&=-\frac{2}{(2\pi)^3}\int\frac{d\mathbf{q}}{4w^2(1-e^{-\beta w})^2}\Big\{\frac{e^{2\beta\omega}-1}{2\omega}e^{i2wx_0}\hat{\chi}(-2w)+\beta e^{-\beta w}+\\
&\quad+\frac{e^{-2\beta\omega}-1}{-2\omega}e^{-2\beta w}e^{-i2wx_0}\hat{\chi}(2w)\Big\}\\
&=\frac{2}{(2\pi)^3}\int\frac{d\mathbf{q}}{4w^2(1-e^{-\beta w})^2}\Big\{\frac{1-e^{2\beta\omega}}{2\omega}\Big[e^{i2wx_0}\hat{\chi}(-2w)+e^{-i2wx_0}\hat{\chi}(2w)\Big]-\beta e^{-\beta w}\Big\}\\
&=\frac{2}{(2\pi)^3}\int d\mathbf{q}\frac{1}{4w^2_{\mathbf{q}}}\Big\{\frac{b_+(w_{\mathbf{p}})+b_-(w_{\mathbf{p}})}{2\omega}\Big[e^{i2wx_0}\hat{\chi}(-2w)+e^{-i2wx_0}\hat{\chi}(2w)\Big]+\\
&\quad-\beta b_+(w_{\mathbf{p}})b_-(w_{\mathbf{p}})\Big\}
\end{aligned}
\tag{III.21}
$$

The oscilatory part of the integral is such that

$$
\lim_{x_0\to\infty}\int\frac{d\mathbf{q}}{4w^2(1-e^{-\beta w})^2}\frac{1-e^{2\beta\omega}}{2\omega}\Big[e^{i2wx_0}\hat{\chi}(-2w)+e^{-i2wx_0}\hat{\chi}(2w)\Big]=0
$$

due to Riemann-Lebesgue lemma. Therefore, in the large time limit we are interested in, the only contribution due to the cocycle $U(i\beta)$, i.e., due to the effect of perturbation upon the state, becomes

$$\Sigma^1_U(\phi^2) = -\frac{1}{(2\pi)^3}\int d\mathbf{q}\,\frac{\beta e^{-\beta w}}{2w^2(1-e^{-\beta w})^2} = -\frac{1}{(2\pi)^3}\int d\mathbf{q}\frac{\beta}{2w^2_{\mathbf{q}}}b_+(w_{\mathbf{q}})b_-(w_{\mathbf{q}}). \tag{III.22}$$

Consequently, the expectation value $\omega^{\beta,V}\circ\mathcal{R}_V(\phi^2)$ becomes

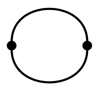
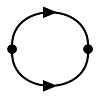
$$\omega^{\beta,V}\circ\mathcal{R}_V(\phi^2) = \omega\circ\mathcal{R}_V(\phi^2) + \Sigma^1_U(\phi^2) + O(\lambda^2),$$

with the contribution from the Bogoliubov map, according to I.48, given by

$$\omega\circ\mathcal{R}_V(\phi^2) = i\omega^\beta\big(V\cdot_T\phi^2 - V\star\phi^2\big) + O(\lambda^2).$$

Up to first order, this term equals

$$\Sigma^1_{\mathcal{R}_V}(\phi^2) := \omega^\beta\left(V\cdot_T\phi^2 - V\star\phi^2\right)$$

$$= \int dz\Bigg(V(z)$$

$$\phi^2(x) \; - \; V(z)$$

$$\phi^2(x)\Bigg)$$

$$= \int dz\chi(z_0)h(\mathbf{z})\Big\{(\Delta^\beta_F)^2(z-x) - (\Delta^+_\beta)^2(z-x)\Big\}.$$

As $\Delta^0_F = \Delta^+_0 + i\Delta_A$ and setting $W_\beta := \Delta^+_\beta - \Delta^+_0$, where Δ^+_0 is the two-point function of the vacuum state, we have, up to renormalization terms,

$$(\Delta^\beta_F)^2 - (\Delta^+_0)^2 = \big(\Delta^0_F + W_\beta\big)^2 - \big(\Delta^+_0 + W_\beta\big)^2 = {\Delta^0_F}^2 - {\Delta^+_0}^2 + i2\Delta_A W_\beta.$$

Therefore,

$$\begin{aligned}\Sigma^1_{\mathcal{R}_V}(\phi^2) &= \int dz h(\mathbf{z})\chi(z_0)\Big((\Delta^0_F)^2 - (\Delta^+_0)^2 + i2\Delta_A W_\beta\Big)(z,x)\\ &= \int dz h(\mathbf{z})\chi(z_0)\int dp_0 d\mathbf{p}\,\mathcal{F}\Big((\Delta^0_F)^2 - (\Delta^+_0)^2 + i2\Delta_A W_\beta\Big)(p)e^{ip_0(z_0-x_0)}e^{-i\mathbf{p}(\mathbf{z}-\mathbf{x})}.\end{aligned}$$

We now consider each integral above separately, the first part being

$$(1) \equiv \int dz h(\mathbf{z})\chi(z_0)\int dp_0 d\mathbf{p}\,\mathcal{F}\Big((\Delta^0_F)^2 - (\Delta^+_0)^2\Big)(p)e^{ip^0(z^0-x^0)}e^{-i\mathbf{p}(\mathbf{z}-\mathbf{x})}.$$

The difference between the square of the Feynman propagator and the two-point function related to the vacuum state of a mass m theory may be obtained by means of the general Kählén-Lehmann formula described in chapter I, cf. equation (I.42). Contribution (1) then becomes

$$\begin{aligned}(1) &= \frac{i}{((2\pi)^3}(-\Box)\int dz_0 dp_0 d\mathbf{p}\,\chi(z_0)\delta(\mathbf{p})\int_{(2m)^2}^{\infty} dM^2\,\rho_m(M^2)\frac{1}{M^2}\hat{\Delta}_A(p,M)e^{ip_0x_0}e^{-i\mathbf{p}(\mathbf{x}-\mathbf{z})}\\ &= \frac{i}{((2\pi)^3}\lim_{\varepsilon\to 0+}\int dz_0 dp_0\,\Box\left[\chi(z^0)e^{ip_0x_0}\right]\int_{(2m)^2}^{\infty} dM^2\,\rho_m(M^2)\frac{1}{(p_0-i\varepsilon)^2-M^2}\\ &= -\frac{1}{(2\pi)^4}\lim_{\varepsilon\to 0+}\int dz_0 dp_0\,\left[ip^0 - i2p^0 + ip^0\right]\dot{\chi}(z^0)e^{ip_0t}\int_{(2m)^2}^{\infty} dM^2\,\frac{\rho_m(M^2)}{2M^3}\times\end{aligned}$$

The remaining contribution to $\Sigma^1_{\mathcal{R}_V}(\phi^2)$ is

$$\begin{aligned}(2) \equiv&\frac{i2}{(2\pi)^3}\int dz', \chi(z_0)h(\mathbf{z})\int dp_0 d\mathbf{p}\,\mathcal{F}\big(\Delta_A W_\beta\big)(p)e^{ip^0(z^0-x_0)}e^{-i\mathbf{p}(\mathbf{z}-\mathbf{x})}\\ =&\frac{i2}{(2\pi)^3}\int dz\,\chi(z_0)h(\mathbf{z})\int dp_0 d\mathbf{p}\,\widehat{\Delta}_A * \widehat{W}_\beta(p)e^{ip_0(z_0-x_0)}e^{-i\mathbf{p}(\mathbf{z}-\mathbf{x})}\end{aligned}$$

The difference between the two-point functions is

$$\begin{aligned}W_\beta(z-x) &= \frac{1}{(2\pi)^3}\int dp\,\frac{1}{1-e^{-\beta p_0}}\varepsilon(p_0)\delta(p_0^2-w_p^2) - \theta(p_0)\delta(p_0^2-w_p^2)\\ &= \frac{1}{(2\pi)^3}\int dp\,\frac{1}{2w_p}\left\{\frac{1}{1-e^{-\beta p_0}}\delta(p_0-w_p) + \frac{e^{-\beta p_0}}{1-e^{-\beta p_0}}\delta(p_0+w_p) - \delta(p_0-w_p)\right\}\\ &= \frac{1}{(2\pi)^3}\int d\mathbf{p}\frac{1}{2w_p}\left\{\frac{e^{-\beta w_p}}{1-e^{-\beta w_p}} + \frac{1}{1-e^{-\beta w_p}}\right\} = \frac{1}{(2\pi)^3}\int d\mathbf{p}\frac{1}{2w_p}\big[1+2b_-(w_\mathbf{p})\big]\end{aligned}$$

Combining this expression with

$$\Delta(z-x) = \frac{-i}{(2\pi)^3}\int d\mathbf{p}\bigg(\frac{e^{-iw_\mathbf{p}(z_0-x_0)}}{2w_\mathbf{p}} - \frac{e^{iw_\mathbf{p}(z_0-x_0)}}{2w_\mathbf{p}}\bigg)e^{-i\mathbf{p}(\mathbf{z}-\mathbf{x})}$$

we obtain, in the adiabatic limit — which again force the frequencies to be equal,

$$(2) = \frac{i2}{(2\pi)^3}\int dz_0\,\theta(z_0-x_0)\chi(z_0)\int d\mathbf{p}\,\left(\frac{e^{-iw_\mathbf{p}(z_0-x_0)}}{2w_\mathbf{p}} - \frac{e^{iw_\mathbf{p}(z_0-x_0)}}{2w_\mathbf{p}}\right)\frac{1}{2w_p}\big[1+2b_-(w_\mathbf{p})\big]$$

The integration in dz^0 now produces

$$\int dz^0\theta(x^0-z^0)\chi(z^0)e^{\pm i2\omega z^0} = \chi(z^0)\frac{e^{\pm i2w_\mathbf{p}z^0}}{\pm i2w_\mathbf{p}}\bigg|_{x^0}^{+\infty} - \int_{x^0}^{+\infty} dz^0\dot{\chi}(z^0)\frac{e^{\pm i2w_\mathbf{p}z^0}}{\pm i2w_\mathbf{p}}.$$

and the above expression becomes

$$\begin{aligned}(2) = \frac{1}{(2\pi)^3}\int d\mathbf{p}\,\bigg\{&\chi(x_0)\frac{e^{i2w_\mathbf{p}x_0} - e^{-i2w_\mathbf{p}x_0}}{i2w_\mathbf{p}} - \int_{x^0}^{+\infty} dz^0\dot{\chi}(z^0)\frac{1}{i2w_\mathbf{p}}\times\\ &\times\left(\frac{e^{-iw_\mathbf{p}(z_0-x_0)}}{2w_\mathbf{p}} - \frac{e^{iw_\mathbf{p}(z_0-x_0)}}{2w_\mathbf{p}}\right)\bigg\}\frac{1}{2w_\mathbf{p}}\big[1+2b_-(w_\mathbf{p})\big]\end{aligned}$$

In the large time limit $x_0 \to 0$, the right hand side in the above expression reduces to

$$(2) = -\frac{1}{(2\pi)^3}\int d\mathbf{q}\,\frac{1}{4\omega^3}\big[1+2b_-(w_\mathbf{p})\big]\Big[\widehat{\chi}(2w)e^{-i2wx_0} - \widehat{\chi}(-2w)e^{i2\omega x^0}\Big]$$

In conclusion, the first order contribution involving solely the correction produced by the Bogoliubov map on the observable is, in the limit $x^0 \to -\infty$,

$$\begin{aligned}\Sigma^1_{\mathcal{R}_V}(\phi^2) &= (1)+(2)\\ &= -\frac{1}{(2\pi)^4}\int d\mathbf{q}\,\frac{1}{4w^3_\mathbf{p}}\big[1+2b_-(w_\mathbf{p})\big]\Big[\widehat{\chi}(2w_\mathbf{p})e^{-i2w_\mathbf{p}x_0} - \widehat{\chi}(-2w_\mathbf{p})e^{i2w_\mathbf{p}x^0}\Big].\end{aligned} \tag{III.23}$$

Up to first order in perturbation theory we obtain, according to equations (III.21) and (III.23), even prior to the large time limit

$$\begin{aligned}&\omega^{\beta,V}\circ\mathcal{R}_V(\phi^2) = \omega^\beta(\phi^2)+\Sigma^1_{\mathcal{R}_V}(\phi^2)+\Sigma^1_U(\phi^2)\\ &= \omega^\beta(\phi^2) + -\frac{1}{(2\pi)^3}\int d\mathbf{q}\,\frac{1}{4\omega^3}\big[1+2b_-(w_\mathbf{p})\big]\Big[\widehat{\chi}(2w)e^{-i2wx_0}-\widehat{\chi}(-2w)e^{i2\omega x^0}\Big]+\\ &-\frac{2}{(2\pi)^3}\int\frac{d\mathbf{q}}{4w^2_\mathbf{q}}\beta b_+(w_\mathbf{p})b_-(w_\mathbf{p}) - \frac{b_+(w_\mathbf{p})+b_-(w_\mathbf{p})}{2w_\mathbf{p}}\Big[e^{i2wx_0}\hat{\chi}(-2w_\mathbf{p})+e^{-i2wx_0}\hat{\chi}(2w_\mathbf{p})\Big]\\ &= -\frac{1}{(2\pi)^3}\int d\mathbf{p}\,\frac{1}{4w_\mathbf{p}}\left[b_+(w_\mathbf{p})b_-(w_\mathbf{p})+\frac{b_+(w_\mathbf{p})+b_-(w_\mathbf{p})}{2w_\mathbf{p}}\right].\end{aligned} \tag{III.24}$$

Looking at the above results, we notice the expectation value computation of ϕ^2 at the state $\omega^{\beta,V}\circ\mathcal{R}_V$ contains a contribution from the cocycle U, corresponding to $\Sigma^1_U(\phi^2)$, and another contribution, $\Sigma^1_{\mathcal{R}_V}(\phi^2)$, exclusively from the Bogoliubov map and which is the result one would obtain by employing the real-time formalism in her/his computations. We shall return to this discussion in this chapter's last section.

III.3.2 $\lambda\phi^3$ theory.

We now consider the same expectation value computation as above except that now we are interested in the interaction term

$$V(\phi) = \frac{\lambda}{3}\int_\mathbb{M} dz\,\chi(z_0)h(\mathbf{z})\phi^3(z). \tag{III.25}$$

Up to second order in perturbation theory, we obtain the expansion

$$\begin{aligned}\omega^{\beta,V}\circ\mathcal{R}_V\Big(\phi\phi\Big) &= \omega^\beta(\phi\phi)+i\omega^\beta\Big(\big[V\cdot_T\phi\phi - V\star\phi\phi\big]\Big)+\omega^\beta\Big(\big[\mathcal{R}_V\phi\phi\big]_2\Big)+\\ &-\int_0^\beta du\,\omega^{\beta,c}\Big(\big[\phi\phi\big]\otimes\alpha_{iu}\dot{V}\Big) - i\int_0^\beta du\,\omega^{\beta,c}\Big(\Big\{\big[V\cdot_T\phi\phi - V\star\phi\phi\big]\Big\}\otimes\alpha_{iu}\dot{V}\Big)+\\ &-i\int_0^\beta du\,\omega^{\beta,c}\Big(\big[\phi\phi\big]\otimes\alpha_{iu}\big[V\cdot_T\dot{V}-V\star\dot{V}\big]\Big)+\\ &+\int_0^\beta du_2\int_0^{u_2}du_1\,\omega^{\beta,c}\Big(\big[\phi\phi\big]\otimes\alpha_{iu}\dot{V}\otimes\alpha_{iu'}\dot{V}\Big)+O(\lambda^3).\end{aligned}$$

We denoted by $[\mathcal{R}_V A]_2$ the second order terms within $\mathcal{R}_V A$, for simplicity. For the particular case of interaction term $V = \lambda\phi^3$, the above expression simplifies, as

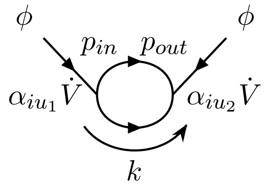
$$V = \lambda\phi^n,\, n > 2 \Rightarrow \omega^\beta\Big(\big[V \star \phi\phi - V \cdot_T \phi\phi\big]\Big) = \omega^{\beta,\,c}\Big(\big[\phi\phi\big] \otimes \alpha_{iu}\dot{V}\Big) = 0.$$

Therefore, in this case the cocycle contribution at second order in perturbation theory to the self-energy Σ^2_U becomes

$$\Sigma^2_U = -i\int_0^\beta du\, \omega^{\beta,\,c}\Big(\Big\{\big[V \cdot_T \phi\phi - V \star \phi\phi\big]\Big\} \otimes \alpha_{iu}\dot{V}\Big) +$$
$$-\, i\int_0^\beta du\, \omega^{\beta,\,c}\Big(\big[\phi\phi\big] \otimes \alpha_{iu}\big[V \cdot_T \dot{V} - V \star \dot{V}\big]\Big) + \int_0^\beta du_2 \int_0^{u_2} du_1\, \omega^{\beta,\,c}\Big(\big[\phi\phi\big] \otimes \alpha_{iu_1}\dot{V} \otimes \alpha_{iu_2}\dot{V}\Big)$$

We shall first consider contribution

$$(3) \equiv \int_0^\beta du_2 \int_0^{u_1} du_1\; \omega^{\beta,\,c}\Big(\big[\phi(x)\phi(y)\big] \otimes \alpha_{iu_1}\dot{V} \otimes \alpha_{iu_2}\dot{V}\Big) = \int_0^\beta du_2 \int_0^{u_1} du_1$$



$$= \int_0^\beta du_2 \int_0^{u_1} du_1 \int dz_1 dz_2\, \Delta^+_\beta(x, z_1)(\Delta^+_\beta)^2(z_1, z_2)\Delta^+_\beta(y, z_2)\alpha_{iu_1}\dot{\chi}(z^0_1)\alpha_{iu_2}\dot{\chi}(z^0_2)h(\mathbf{z}_1)h(\mathbf{z}_2),$$

where we represented as $p_{in/out}$ the momenta of the incoming/outcoming field in the diagramatic expression. In Fourier space the above contribution becomes

$$(3) = \int_0^\beta du_2 \int_0^{u_2} du_1 \int dz_1 dz_2 dp_{in} dk dp_{out}\, \alpha_{iu_1}\widehat{\Delta}^+_\beta(p_{in})(\widehat{\Delta}^+_\beta)^2(k)\alpha_{iu_2}\widehat{\Delta}^+_\beta(p_{out})\times$$
$$\times\, \dot{\chi}(z^0_1)\dot{\chi}(z^0_2)h(\mathbf{z}_1)h(\mathbf{z}_2)e^{ip^0_{in}x^0}e^{iz^0_1(k^0 - p^0_{in})}e^{-iz^0_2(k^0 + p^0_{out})}e^{ip^0_{out}y^0}e^{-i\mathbf{p}_{in}\mathbf{x}}e^{-i\mathbf{p}_{out}\mathbf{y})}.$$

Both the symplex and the time components of the external legs integrations may be performed independently. Having passed to Fourier space, the cocycle contribution becomes

$$\int_0^\beta du_2 \int_0^{u_2} du_1\, \dot{\chi}(z^0_1)\dot{\chi}(z^0_2)\alpha_{iu_2}\big(e^{-iz^0_2(k^0 + p^0_{out})}\big)\alpha_{iu_1}\big(e^{iz^0_1(k^0 - p^0_{in})}\big)$$
$$= \int_0^\beta du_2 \int_0^{u_2} du_1\, \dot{\chi}(z^0_1)\dot{\chi}(z^0_2)e^{i(z^0_1 - iu_1)(k^0 - p^0_{in})}e^{-i(z^0_2 - iu_2)(k^0 + p^0_{out})}$$
$$= \int_0^\beta du_2 \int_0^{u_2} du_1\, \dot{\chi}(z^0_1)\dot{\chi}(z^0_2)e^{u_1(k^0 - p^0_{in})}e^{-u_2(k^0 + p^0_{out})}e^{iz^0_1(k^0 - p^0_{in})}e^{-iz^0_2(k^0 + p^0_{out})},$$

and therefore the integrations in du_1 and du_2 result in

$$S^{(3)}_2(\beta) \equiv \int_0^\beta du_2 \int_0^{u_2} du_1 e^{u_1(k^0 - p^0_{in})}e^{-u_2(p^0_{out} + k^0)}$$
$$= \frac{1}{(k^0 - p^0_{in})}\left\{\frac{1 - e^{-\beta(p^0_{in} + p^0_{out})}}{(p^0_{in} + p^0_{out})} - \frac{1 - e^{-\beta(p^0_{out} + k^0)}}{(p^0_{out} + k^0)}\right\}.$$

As for the integrations with respect to dz^0, we obtain

$$\int dz_1^0 dz_2^0\, \dot\chi(z_1^0)\dot\chi(z_2^0)e^{iz_1^0(k^0-p_{in}^0)}e^{-iz_2^0(k^0+p_{out}^0)} = \widehat{\dot\chi}(p_{in}^0-k^0)\widehat{\dot\chi}(p_{out}^0+k^0).$$

In addition, in the adiabatic limit we obtain, for the space integrations $d\mathbf{z}$,

$$\int d\mathbf{z}_1 \int d\mathbf{z}_2\, h(\mathbf{z}_1)h(\mathbf{z}_2)e^{-i\mathbf{z}_1(\mathbf{k}-\mathbf{p}_{in})}e^{i\mathbf{z}_2(\mathbf{k}+\mathbf{p}_{out})} \to (2\pi)^6\delta(\mathbf{k}-\mathbf{p}_{in})\delta(\mathbf{k}+\mathbf{p}_{out}).$$

Contribution (3) may now be written as

$$(3) = \frac{Z}{(2\pi)^6}\int dp_{in}dkdp_{out}\,\widehat{G}(p_{in},p_{out},k)\widehat{\chi}(p_{in}^0-k^0)\widehat{\chi}(p_{out}^0+k^0)e^{ip_{in}^0x^0}e^{ip_{out}^0y^0}e^{-i\mathbf{p}_{in}\mathbf{x}}e^{-i\mathbf{p}_{out}\mathbf{y}},$$

where Z is a symmetrization factor and

$$\widehat{G}(p_{in},p_{out},k) := \widehat{\Delta}_\beta^+(p_{in})(\widehat{\Delta}_\beta^+)^2(k)\widehat{\Delta}_\beta^+(p_{out})S_2^{(3)}(\beta)\delta(\mathbf{k}-\mathbf{p}_{in})\delta(\mathbf{k}+\mathbf{p}_{out}).$$

The *in* and *out* contributions in $\widehat{G}$ are given, according to (II.8), by

$$\widehat{\Delta}_\beta^+(p) = \frac{1}{2\omega_p}\Big\{b_+(\omega_p)\delta\big(p_0-\omega_p\big) + b_-\big(\omega_p\big)\delta\big(p_0+\omega_p\big)\Big\},$$

and thus $\widehat{\Delta}_\beta^+(p_{in})\widehat{\Delta}_\beta^+(p_{out})$ contains a combination of terms with equal modes $b_+(w)^2$, $b_-(w)^2$, plus terms with different modes $b_+(w)b_-(w)$, with with $w_\mathbf{p} \equiv w_\mathbf{p}(p_{in}) = w_\mathbf{p}(p_{out})$ in the adiabatic limit. The contribution with b_+^2, for instance, results in

$$\int dp_{in}^0 dp_{out}^0\,(\widehat{\Delta}_\beta^+)^2(k)S_2^{(3)}(\beta)\delta(p_{in}^0-w_\mathbf{p})\delta(p_{out}^0-w_\mathbf{p})\widehat{\chi}(p_{in}^0-k^0)\widehat{\chi}(p_{out}^0+k^0)e^{ip_{in}^0x^0}e^{ip_{out}^0y^0}$$

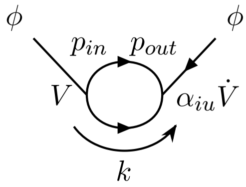
Considering then the large time limit $t \equiv x^0+y^0 \to +\infty$, the Riemann-Lebesque lemma then implies that the above contribution vanishes. Since the term with b_-^2 differs from the former one by a change $w \to -w$, also this contribution vanishes, and we are left only with terms with opposite modes $b_+(w)b_-(w)$ from $\widehat{G}$. Heuristically, this corresponds to considering only on-shell momenta in the adiabatic limit, but selecting incoming and outgoing momentum with opposite orientations. Therefore, we obtain

$$\begin{aligned}(3) =& \frac{1}{(2\pi)^6}\int dk\,(\widehat{\Delta}_\beta^+)^2(k)\Bigg\{\big|\widehat{\chi}(w_\mathbf{k}-k^0)\big|^2 e^{-iw_\mathbf{p}(x^0+y^0)}\left[\frac{\beta}{k^0-w_\mathbf{p}} - \frac{1-e^{-\beta k^0+w_\mathbf{p}}}{(k^0-w_\mathbf{p})^2}\right] + \\ &+ \big|\widehat{\chi}(w_\mathbf{k}+k^0)\big|^2 e^{iw_\mathbf{p}(x^0+y^0)}\left[\frac{\beta}{k^0+w_\mathbf{p}} - \frac{1-e^{-\beta k^0+w_\mathbf{p}}}{(k^0+w_\mathbf{p})^2}\right]\Bigg\}\frac{b_+(w_\mathbf{p})b_-(w_\mathbf{p})}{4w_\mathbf{p}^2}. \quad \text{(III.26)}\end{aligned}$$

Now addressing contribution (1), we have

$$(1) = -i\int_0^\beta du\,\omega^{\beta,c}\Big(\Big\{\big[V\cdot_T\phi\phi - V\star\phi\phi\big]\Big\}\otimes\alpha_{iu}\dot V\Big)$$

$$= -i\int_0^\beta du$$



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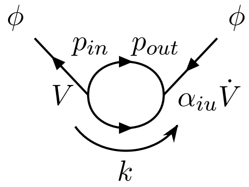


$$\begin{aligned}
&= -i\int_0^\beta du\int dz_1dz_2\Big[\Delta_F^\beta(x,z_1) - \Delta_\beta^+(z_1,x)\Big](\Delta_\beta^+)^2(z_1,z_2)\alpha_{iu}\Delta_\beta^+(y,z_2)\chi(z_1^0)\dot\chi(z_2^0)\\
&\quad\times h(\mathbf{z}_1)h(\mathbf{z}_2)\\
&= \frac{i^2}{(2\pi)^6}\int_0^\beta du\int dz_1dz_2dp_{in}dkdp_{out}\,\hat\Delta_A(p_{in})\hat\Delta_\beta^2(k)\hat\Delta_\beta(p_{out})\theta(z_1^0-x^0)\chi(z_1^0)\dot\chi(z_2^0)\times\\
&\quad\times h(\mathbf{z}_1)h(\mathbf{z}_2)e^{ip_{in}(z_1-x)}e^{ik(z_1-z_2)}e^{ip_{out}(y-z_2)}e^{-p^0_{out}u}
\end{aligned}$$

Considering the decompositions $\Delta = \Delta_R - \Delta_R$ and $\Delta_F = \Delta_+ + i\Delta_A$, the propagator in the incoming momenta may be written as above. For this contribution also the symplex integral may be computed directly and results

$$S_2^{(i)}(\beta) \equiv \int_0^\beta du\,e^{-u(k^0+p^0_{out})} = \frac{1-e^{-\beta(k^0+p^0_{out})}}{(k^0+p^0_{out})}.$$

Furthermore, the integration in dz_2^0 results in its Fourier transform evaluated at $k^0+p^0_{out}$, while for dz_1^0 we integrate by parts and obtain

$$\begin{aligned}
\int dz_1^0\,\theta(z_1^0-x^0)\chi(z_1^0)e^{iz_1^0(k^0-p^0_{in})} &= \int_{x^0}^{+\infty} dz_1^0\,\chi(z_1^0)e^{iz_1^0(p^0_{in}+k^0)}\\
&= \chi(z_1^0)\frac{e^{iz_1^0(k^0-p^0_{in})}}{i(k^0-p^0_{in})}\Bigg|_{x^0}^{+\infty} - \int_{x^0}^{+\infty} dz_1^0\,\dot\chi(z_1^0)\frac{e^{iz_1^0(k^0-p^0_{in})}}{i(k^0-p^0_{in})}\\
&= \cancelto{0}{\chi(z_1^0)\frac{e^{iz_1^0(k^0-p^0_{in})}}{i(k^0-p^0_{in})}\Bigg|_{x^0}^{+\infty}} - \int_{-\infty}^{+\infty} dz_1^0\,\dot\chi(z_1^0)\frac{e^{iz_1^0(k^0-p^0_{in})}}{i(k^0-p^0_{in})}.
\end{aligned}$$

The first term in the right hand side above becomes zero in the large time limit to be considered at the end. The causal propagator related to the external leg with momentum p_{in} is transformed into the Wightman function of the β-KMS state by means of the relation

$$\hat\Delta_\beta(p) = \frac{i\hat\Delta(p)}{1-e^{-\beta p^0}}.$$

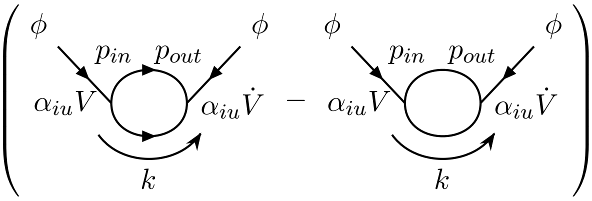
Analogously to the case of contribution (3), considering the inner form of $\widehat{\Delta}^+_\beta$ the terms with b_+^2 or b_-^2 depending on $t^0 = 2(x^0 + y^0)$ vanish in the large time limit $t^0 \to 0$. We hence obtain

$$
\begin{aligned}
(1) =& \frac{1}{(2\pi)^6} Z \int dk\, (\widehat{\Delta}^+_\beta)^2(k) \Bigg\{ \left|\widehat{\chi}(k^0 - w_{\mathbf{p}})\right|^2 e^{i2w_{\mathbf{k}}t} \left[\frac{1 - e^{\beta(k^0 - w_{\mathbf{k}})}}{(k^0 - w_{\mathbf{p}})^2}\right] \frac{b_-(w_{\mathbf{k}})}{4w_{\mathbf{k}}^2} + \\
&- \left|\widehat{\chi}(k^0 + w_{\mathbf{p}})\right|^2 e^{-i2w_{\mathbf{k}}t} \left[\frac{1 - e^{-\beta(k^0 + w_{\mathbf{k}})}}{(k^0 + w_{\mathbf{p}})^2}\right] \frac{b_+(w_{\mathbf{k}})}{4w_{\mathbf{k}}^2} \Bigg\}.
\end{aligned}
$$

Finally, contribution (2) corresponds to

$$
(2) = -i \int_0^\beta du\, \omega^{\beta,c}\Big([\phi\phi] \otimes \alpha_{iu}\big[V \cdot_T \dot{V} - V \star \dot{V}\big] \Big)
$$

$$
- i \int_0^\beta du
$$



$$
\begin{aligned}
&= -i \int_0^\beta du \int dz_1 dz_2 \alpha_{iu} \Delta_\beta(x, z_1) \Big(\Delta_\beta^2 - \Delta_\beta^{F\,2}\Big)(z_1, z_2) \alpha_{iu} \Delta_\beta(y, z_2) \chi(z_1^0) \dot{\chi}(z_2^0) h(\mathbf{z}_1) h(\mathbf{z}_2) \\
&= -i \int_0^\beta du \int dz_1 dz_2 \alpha_{iu} \widehat{\Delta}^+_\beta(p_{in}) \Big[(\widehat{\Delta}^+_\beta)^2 - (\widehat{\Delta}^\beta_F)^2\Big](k) \widehat{\Delta}^+_\beta(p_{out}) \chi(z_1^0) \dot{\chi}(z_2^0) \\
&\times h(\mathbf{z}_1) h(\mathbf{z}_2) e^{ip_{in}(x - z_1)} e^{ik(z_1 - z_2)} e^{ip_3(y - z_2)}
\end{aligned}
$$

The difference between squared propagators may be treated by means of the Kählén-Lehmann regularization procedure discussed in chapter I, as employed before. We hence obtain for the *in* leg, for a suitable choice of renormalization term,

$$
\begin{aligned}
Q(x, z_1) :=& \big[(\Delta_F^\beta)^2 - (\Delta_\beta^+)^2\big](x - z_1) \\
=& - i\theta(-x^0) \left\{ \int_{4m^2}^{+\infty} dM^2\, \rho_2(M) \Delta(x - z_1; M) + 2\Delta(x - z_1) W_\beta(x - z_1) \right\}
\end{aligned}
$$

The symplex integration for (2) is

$$
S_2^{(2)}(\beta) \equiv \int_0^\beta du\, e^{-u(p^0_{out} + p^0_{in})} = \frac{1 - e^{-\beta(p^0_{in} + p^0_{out})}}{(p^0_{in} + p^0_{out})},
$$

and, besides for the internal lines which have already been treated, the computation of this contribution follows the same lines as the previous ones: the integrations in z_1^0 and z_2^0 may be computed directly, and considering the adiabatic and the large time limit we obtain

$$(2)_{c=0} = \frac{1}{(2\pi)^3}\beta Z \int dk\,\widehat{Q}(k)\Bigg\{e^{-i2w_{\mathbf{p}}t}\left[\frac{1}{(p_0^2 - w_{\mathbf{p}})} - \frac{|\hat{\chi}(p_0^2 - w_{\mathbf{p}})|^2}{(p_0^2 - w_{\mathbf{p}})}\right] + \tag{III.27}$$

$$+ e^{i2w_{\mathbf{p}}t}\left[\frac{1}{(p_0^2 + w_{\mathbf{p}})} - \frac{|\hat{\chi}(p_0^2 + w_{\mathbf{p}})|^2}{(p_0^2 + w_{\mathbf{p}})}\right]\Bigg\}\frac{b_+(w_{\mathbf{p}})b_-(w_{\mathbf{p}})}{4w_{\mathbf{p}}^2}. \tag{III.28}$$

To this expression we add the contribution coming from the renormalization term,

$$\frac{1}{(2\pi)^3}cZ\int_0^\beta du \int dz^0 dp_{in}^0 dp_{out}^0 dk\, \dot{\chi}(z^0)\chi(z^0)\widehat{\Delta}_\beta^+(p_{in}^0, \mathbf{k})\widehat{\Delta}_\beta^+(p_{out}^0, \mathbf{k})e^{-u(p_{out}^0 + p_{in}^0)} \times$$
$$\times\, e^{ip_{in}^0(z^0 - t_1)}e^{ip_{out}^0(z^0 - t_2)},$$

In the large time limit we have

$$(2)_c = \frac{1}{(2\pi)^3}c\beta\frac{b_+(w_{\mathbf{p}})b_-(w_{\mathbf{p}})}{4w_{\mathbf{p}}^2} \tag{III.29}$$

We should perhaps emphasize that c cannot depend on β, as the renormalization term in state independent.

Before concluding this chapter, we estimate the total second order contribution to $\omega^{\beta,V} \circ \mathcal{R}_V(\phi\phi)$ for $\tau = 0 = \mathbf{p}$ in the large time limit $t \to +\infty$. Term $\widehat{Q}$ in (2) is composed of

$$\mathcal{F}(\Delta_\beta^+ W_\beta)(k) = \frac{1}{(2\pi)^6}\int d\mathbf{q}_1 d\mathbf{q}_2\,\frac{b_+(w_2)}{4w_1w_2}\delta(\mathbf{k} - \mathbf{q}_1 - \mathbf{q}_2)e^{-\beta w_2}\Big[\delta(k^0 - w_1 - w_2) +$$
$$- \delta(k^0 + w_1 - w_2) + \delta(k^0 - w_1 + w_2) - \delta(k^0 + w_1 + w_2)\Big]$$

and

$$\mathcal{F}\bigg(\int_{4m^2}^{+\infty} dM^2\,\rho_2(M)i\Delta(x;M)\bigg)(k) = \int_{4m^2}^{+\infty} dM^2\,\rho_2(M)\varepsilon(k^0)\delta\big((k^0)^2 - w_{\mathbf{k}}^M\big)$$
$$= -\,\varepsilon(k^0)\theta\big((k^0)^2 - w_{\mathbf{k}}^{4m^2}\big)\rho_2\big(\sqrt{(k^0)^2 - |\mathbf{k}|^2}\big),$$

where $w_i \equiv w_{\mathbf{q}_i}$ and $w_{\mathbf{k}}^\mu$ corresponds to the frequency $w_{\mathbf{k}}$, with mass term μ. We notice that both the above expressions are odd functions of k^0, the first due to the signs in front of each δ and the second due to $\varepsilon(k^0)$. Considering then the contribution $(2)_{c=0}$ in (III.27) in light of this fact, we see that the whole integrand in (III.27) is an odd function, since its part which is not described in the two expressions above is an even function. Consequently, the integration with respect to dk^0 returns zero, and the contribution of (2) reduces to the renormalization term (III.29).

As for contributions (1) and (3), the square of $\widehat{\Delta}_\beta^+$ may computed as before by means of the convolution theorem, which results.

$$(\widehat{\Delta}_\beta^+)^2(k) = \frac{1}{(2\pi)^6}\int d\mathbf{q}_1 d\mathbf{q}_2\,\frac{b_+(w_1)b_+(w_2)}{4w_1w_2}\delta(\mathbf{k} - \mathbf{q}_1 - \mathbf{q}_2)\Big[\delta(k^0 - w_1 - w_2) +$$
$$+ \delta(k^0 + w_1 - w_2)e^{-\beta w_1} + \delta(k^0 - w_1 + w_2)e^{-\beta w_2} + \delta(k^0 + w_1 + w_2)e^{-\beta(w_1 + w_2)}\Big]$$

By selecting the case $\mathbf{k} = 0$, the above integration is restricted to $\mathbf{q}_1 = -\mathbf{q}_2$, which forces the frequencies to be equal as $w_1 = w_2 \equiv w$. Since the integrand then depends only on $|\mathbf{q}|^2$, the integration may be performed in spherical coordinates. We end up with the total result

$$\begin{aligned}\Sigma_U^2 =& \frac{1}{(2\pi)^6} c\beta \frac{b_+(m)^2}{4m^2} e^{-\beta m} + \frac{1}{(2\pi)^6} \frac{\pi}{8} \frac{e^{-\beta m}}{m^2} b_+(m) \int_{2m}^{\infty} dM \sqrt{1 - \frac{4m^2}{M^2}} b_+ \left(\frac{M}{2}\right)^2 \times \\ & \times \left[\beta b_+(m)(1 - e^{-\beta M}) \left(\frac{|\hat{\dot\chi}(M-m)|^2}{M-m} + \frac{|\hat{\dot\chi}(M+m)|^2}{M+m} \right) + \right. \\ & + (e^{-\beta m} - e^{-\beta M}) \left(\frac{|\hat{\dot\chi}(M-m)|^2}{(M-m)^2} \right) (e^{-\beta(M+m)} - 1) \left(\frac{|\hat{\dot\chi}(M+m)|^2}{(M+m)^2} \right) + \\ & \left. - 2e^{-\beta \frac{M}{2}} |\hat{\dot\chi}(m)|^2 \frac{1}{m^2 b_+(m)} \right]. \end{aligned} \tag{III.30}$$

III.4 Conclusions and remarks.

We based our analysis on a system composed of a real, massive scalar field propagating over Minkowski space. We supposed the system to be initially both free and prepared at thermal equilibrium at inverse temperature $\beta > 0$. In particular, the condition of initial thermal equilibrium for the free theory translated into considering a unique KMS state ω^β. At an arbitrary instant $t = -2\varepsilon$, $\varepsilon > 0$, we then introduced a local, polynomial interaction term of the general form (II.2), with time cutoff as in (I.37). The form of the cutoff χ represented also the interaction term smoothly turned on and stable as of a subsequent instant $t = -\varepsilon$. At a later time, supposing the system had reached again thermal equilibrium, we considered the expectation value of certain observables, with the initail KMS state modified into $\omega^{\beta,V}$. Following [FL14], we see that thermal equilibrium property for the perturbatiove theory is then characterized by the state $\omega^{\beta,V}$. For the particular case of compactly supported interaction, the thermalization hypothesis has been legitimated by the return to equilibrium property, described in [DFP18], which holds provided the interaction term has compact spacial support, as discussed in proposition 24. However, we again emphasize that the construction of a thermal equilibrium state $\omega^{\beta,V}$ in [FL14; Lin13] discussed in the previous chapters does not require the restriction to compactly supported interaction terms. In order to concretely illustrate our arguments and conclusions, we particularly considered quadratic and cubic interactions and the self-energy estimations above. The discussion in the previous section allows for the present conclusions.

Equation (III.30) corresponds to the difference Σ_U^2 between the FL-analysis and the real-time formalism, estimated at second order in perturbation theory for the case of a $\lambda\phi^3$-interacting theory, and which tends to zero as $\beta \to +\infty$. In the Σ_U^2 contribution to the self-energy, there is a dependence on the cutoff function χ, via the Fourier transform of $\dot\chi$. While in [FL14] the authors proved that $\omega^{\beta,V}$ does not depend on χ, the fact that Σ_U^2 is χ-dependent indicates that the real-time formalism, reobtained by ignoring the cocycle $U(i\beta)$ contribution, presents a sensibility to how the interaction is turned on. In addition, we observe that, in the limit $\chi \to \theta$, the integration with respect to dM in (III.30) diverges, as in this case $\mathcal{F}\dot{\chi} = cte$. Therefore, the steeper is the curve χ in the interval $(-2\varepsilon, -\varepsilon)$, (and, consequently, the more $\dot{\chi}$ tends to a δ-function) the larger is the factor Σ_U^2. This discussion is in agreement with the so-called Bogoliubov prescription, described for instance in [LW87], which states the requirement that the interaction term considered ought to be smoothly turned on. In Thermal Field Theory, the Bogoliubov prescription is considered within the so-called *Thermal Wick theorem*. Rather than a theorem, this is an assumption over the system, which should allow for neglecting initial correlation functions (thus prior to the introduction of the interaction term) in perturbative computations. In [LS50; Bog62; LW87] this prescription is shown to hold if the interaction is *adiabatically*, i.e smoothly turned on. Our aim here is not to discuss this prescription itself, but merely to stress a connection between the real-time formalism and the Fredenhagen-Lindner analysis.

In order to consider the adiabatic limit $\chi \to 1$, we consider a smooth cutoff χ as in (I.49), but now with $\chi|_{t\geq 1} \equiv 0$ and $\chi|_{t<1} \equiv 0$. Let now $(\chi_n)_{n\in\mathbb{N}}$ be a sequence defined as $\chi_n(t) := \chi(t/n)$. In this way, in the limit $n \to \infty$ we obtain $\chi_n \to 1$, and, as a result, an interaction term supported in the whole space $\mathbb{M}$. The adiabatic limit is then equivalent to the time limit often considered in the physics literature $t_{in} \to -\infty$, mentioned in the previous chapter, which corresponds to the interaction being turned on at an arbitrarily distant instant t_{in}. In addition, performing the limit $\chi \to 1$ in this way produces also $\dot{\chi}_n \to 0$, which does not follow if we had considered $\chi \to 1$ via $\alpha_t\chi$ for $t \to +\infty$. The suppression of $\dot{\chi}$ as the limit $\dot{\chi}$ implies an always-defined interaction term, with no contribution from its turning on on expectation values. Moreover, for $n \to \infty$, $\mathcal{F}\dot{\chi}(p_0) = \mathcal{F}\dot{\chi}(np_0)$ vanishes for $p_0 \neq 0$, since the Fourier transform of $\dot{\chi}$ is a rapidly decreasing function. Consequently, in the adiabatic limit $\chi \to 1$, the difference Σ_U^2 reduces to the first term in the right hand side of (III.30), which does not depend on χ.

As for this contribution to the total difference Σ_U^2, the renormalization constant $c \in \mathbb{C}$ may be picked in such a way that it is null. Since the renormalization constant is state independent, due to the principle of general covariance described in [HW01; BFV03], it may not depend on β. It is possible to consider $c = 0$ in particular, and then, in the adiabatic limit $\chi \to 1$, we have that the real-time and the Fredenhagen and Lindner formalism coincide for the case of a $\lambda\phi^3$-theory in the analysis of Σ_U, provided care is taken in the order in which the limits $\chi \to 1$ and $h \to 1$ are taken, as discussed in chapter II (cf. discussed after equation (II.29), in particular).

The situation is substantially different for the case of a $\lambda\phi^2$-theory, as we may see from subsection III.3.1. In this context, the difference between the FL-analysis and the results obtained from the real-time formalism is represented in equations (III.21) and (III.22), the latter referring to the large time limit situation. Considering equation (III.22), which does not depend on χ, $\dot{\chi}$ or its Fourier transform, we notice that, in the presence of quadractic interaction terms, the real-time formalism is not equivalent to the FL-state. In addition, in the case of a $\lambda\phi^4$-theory, the interaction term contains a $\lambda\phi^2$ contribution proportional to the thermal mass in the algebra $(\mathscr{F}_{\mu C}[\![\hbar]\!], \star_{\Delta_\beta^+})$ due to the action of the algebra $*$-isomorphism described in chapter I, and as discussed in chapter

II. Again, we refer to [DHP17] for details. Therefore, we conclude the above results represent contributions to be found also in the $\lambda\phi^4$-theory.

In conclusion, a general description of thermal equilibrium for interacting, perturbative theories is only provided via the FL-state, while the real-time formalism lacks an intrinsic and independent analytic property for the physical interpretation of a thermal equilibrium state, as discussed after theorem 1 in chapter II. Moreover, although in particular situations the two descriptions may agree, as has been anticipated already from chapter II when we discussed the return to equilibrium property, this is not the case in general. In particular, we have seen one case of a computation in which the cocycle contribution does factorizes, as suggested in the context of TFT, and another in which this contribution may not be ignored. We hence conclude that the perturbation series representation of expectation values for interesting interacting theories, such as ϕ^2 and ϕ^4, may produce accurate results for thermal equilibrium systems only by considering the cocycle $U(i\beta)$ contribution. In addition, when considering estimates for the self-energy for the $\lambda\phi^2$-theory, we obtained, in equation (III.24), a final result given by the sum of two contributions, $\Sigma^1_U + \Sigma^1_{\mathcal{R}_V}$, respectively detailed in equations (III.22) and (III.23). While term $\Sigma^1_{\mathcal{R}_V}$ corresponds to the non-vanishing contribution coming from the cocycle $U(i\beta)$, and hence it is the result we would have obtained considering only the Matsubara formalism, $\Sigma^1_{\mathcal{R}_V}$ considers only the effect of the Bogoliubov map over the observable ϕ^2. Therefore, this latter contribution to the total estimation for the self-energy in thermal equilibrium results from considering the real-time formalism instead, and we finally see that a complete, perturbative description of this expectation value requires the combination of both formalisms of TFT, in the sense that the cocycle $U(i\beta)$ in the Fredenhagen and Lindner's state $\omega^{\beta,V}$ cannot be neglected. This illustrates our previous statement that a complete, perturbative characterization of thermal equilibrium demands considering both formalisms of TFT together.

IV. Secular Effects in perturbative Algebraic Quantum Field Theory

The appearance of a polynomial dependence on time in the perturbative expansion of expectation values in QFT, with polynomial degree proportional to the order of perturbation, is called a **secular effect**. That is, this effect is characterized by dependence on time of the nth-order term in the perturbative expansion of some expectation value, via a polynomial of degree proportional to n. The nth-order term refers to the contribution proportional to λ^n, being λ the perturbation parameter. Therefore, secular effects are proper of perturbation theory.

Although it is well known that the perturbation series for interacting theories hardly ever converges, its truncation at a certain order in the perturbation parameter provides accurate results in many cases (see e.g. [PS95] for examples and discussions). The situation is, however, substantially different in the presence of a secular growth in time. In order to illustrate this statement, consider the perturbative expansion of the abstract expectation value $\omega(A)$ of an interacting theory, for some observable A and some state ω. In this heuristic discussion, we shall not explicitly address how interaction manifests over the state or the observable. Rather, suppose $\omega(A)$ may be written as a formal power series in terms of a perturbation parameter λ as

$$\omega(A) = \omega(A)_0 + \lambda\omega(A)_1 + \lambda^2\omega(A)_2 + \dots,$$

where each $\omega(A)_j \in \mathbb{C}$ may depend on time. As a truncation of the perturbation series, we consider an approximation of $\omega(A)$ by the first, finitely many terms of the above series. Consider then a truncation at arbitrary order N. It may be a suitable approximation to $\omega(A)$, provided the parameter $\lambda \ll 1$ implies that the first N contributions numerically prevail over the $(N+1)$th. However, if each individual term in this approximation presents a polynomial dependence on time with degree proportional to the power of the fix parameter λ, i.e. $\omega(A)_n \propto \lambda^n t^{an}$ for some $a > 0$, then, after a long enough time has passed, the factor t^{an} should prevail over the dependence on λ. This has two consequence. First, for any truncation at arbitrary order of the perturbation series, after a long interval the higher order terms in λ should become numerically larger in absolute value than terms of lower order, thus contradicting the basic assumption for truncation of the perturbation series. Moreover, the perturbative representation of $\omega(A)$ is evidently divergent in time, which may be in apparent contradiction with properties of the state ω, in some particular situations.

The second point mentioned above has to be understood noticing that secular effects are an artifact of perturbation theory. Therefore, whenever the expectation value $\omega(A)$ may be also exactly calculated, such divergence should not be present in this result, an apparent contradiction of results and contrary to the Principle of Perturbative Agreement discussed in subsection I.4.5. In the last few chapters, we have mentioned an example of interacting theory which allows for both a perturbative and an exact analysis, namely a real scalar theory with interaction term proportional to ϕ^2. This case will be further treated in the present chapter.

It has been pointed out in the physics literature how such divergences should appear in different interacting theories. For instance, in [AAP14] the authors analyze the coupling of a charged scalar field with an external electrical field. In addittion, in [AGP16] it is shown how in the collapse of a star and formation of a Schwarzschild black hole such effect reveals, with an analysis on the relation between such divergences and Hawking radiation. In the just mentioned papers, but also in other publications (see also [AP15] and references there mentioned), it is argued that the secular growth corresponds to the failure of perturbation theory in providing meaningful results for expectation values. In [AAP14; AGP16] the authors use the Keldysh-Schwinger formalism to show how such polynomial divergences appear in the Keldysh propagator. These divergences, however, would not depend on the particular form of the propagators employed, and may also be noticed in the computation of two-point functions of free states.

However, we shall see in this chapter that secular divergences are not an intrinsic effect of the perturbative expansion of expectation values. It fact, it is a consequence of a choice of state, and it should disappear when we consider certain states. In the context of this thesis, we shall be particularly interested in the analysis of thermal equilibrium states. Therefore, considering for instance the perturbative expansion of an expectation value with respect to $\omega^{\beta,V}$ should present no such divergence, since the state is translation invariant.

In this chapter we show how secular growth appears in the perturbative computation of two-point functions for the case of a real scalar field in the presence of a simple self-interaction term of the form of a mass correction. This is similar to the analysis presented in [AAP14] for the coupling between the quantum scalar field and an external electric potential. Furthermore, as in this case it is possible to obtain exact results for the interacting theory, since, in this particular situation, the perturbation series converges, we use this example to illustrate the fact that secular divergences are a result of how the perturbative approach to expectation values estimation is performed. In other words, we show that the appearance of secular divergences does not mean the break of perturbation theory for interacting theories, instead it comes from treating a stationary state with respect to the free dynamics as a stationary state for the interacting dynamics. Secular effects are, hence, shown to come from bad choice of state. Indeed, we show that if the interacting system is in thermal equilibrium or vacuum, for instance, secular divergences cannot be present in the expectation values results.

The present chapter is structured as follows. In the first section, we shall treat a particular interacting system in both a perturbative and in an exact manner. Whereas the perturbative treatment will result in secular divergent terms, the result from the exact analysis shall not. This illustrates the fact that secullar effects are characteristic of perturbation theory, and may be found only in this context and in certain cases. This will be presented in a different language of AQFT, and at the end of section 1 we discuss how secular effects may be observed in this context. In section 2 we then present an illustrative example of a system in a steady-state, which presents no secular divergence.

This chapter is based on a research project which, by the time this thesis was written, had not been concluded yet. Therefore, in the following we present the first results obtained and indicate a dynamical stability result for certain states. Unfortunately, we shall not be able to present the proof for this latter conclusion.

IV.1 Secular effects in scalar field theories with mass-like interaction terms

As before, we consider a real, massive scalar field with mass $m > 0$ propagating over $\mathbb{M}$. We are interested in systems which are initially free, interacting nor with itself nor with any external field or thermal reservoir at finite temperature, but which presents a self-interaction term at later times. For the absence of interaction with an external thermal reservoir at finite temperature, we understand a system which is initially either in the vacuum state, or in a KMS state at finite temperature $\beta > 0$. In particular, the kind of interaction term we shall be interested in at first is a mass-like correction term. I.e., we restrict to systems which, at the algebraic level, are described by a Lagrangian as (II.1) in the particular form

$$\mathcal{L} = \mathcal{L}_0 + Q = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 + Q, \quad Q := -\frac{1}{2}\delta m^2 \int dtd\mathbf{x}\,\chi(t)h(\mathbf{x})\phi^2(t,\mathbf{x}), \tag{IV.1}$$

which implies the Klein-Gordon equation of motion of the form

$$(\Box + m^2)\phi = Q' = -\chi h \delta m^2 \phi, \tag{IV.2}$$

with the presence of a self-interaction term Q, whose functional derivative w.r.t. the field ϕ we denote as Q'. The term $\delta m^2 > 0$ has the form of a mass correction, and the cutoff function $\chi \in C^\infty(\mathbb{R})$, $0 \leq \chi \leq 1$, is in particular set as

$$\chi(t) = \begin{cases} 0 & t \leq -2\varepsilon \\ 1 & t \geq -\varepsilon. \end{cases} \tag{IV.3}$$

for some arbitrary $\varepsilon > 0$.

The interacting theory may be treated via a perturbative approach to quantum field theory. In particular, we shall be interested in perturbative methods within algebraic quantum field theory. However, due to this specific mass-like interaction, considering the adiabatic limit $h \to 1$, one might attempt to address the interacting theory as a free one, but with a mass term $\mu^2(t) := m^2 + \delta m^2 \chi(t)$ where χ is as in above. At the level of states this means to consider states ω^Q whose two-point function Δ_+^Q solve the equation of motion

$$\left[\Box + \mu^2(t)\right] \Delta_+^Q(x, y) = 0, \quad \mu^2(t) := m^2 + \delta m^2 \chi(t). \tag{IV.4}$$

Therefore, due to the Principle of Perturbative Agreement, briefly discussed in chapter I, the above theory may be approached in two different, though equivalent ways. In this section we intend to analyze the consequences of these two approaches in different circumstances. First, we consider the well-posedness of the Cauchy problem for equation (IV.4) prior to the adiabatic limit, and later extend it to the limit case $h \to 1$. Similarly to the discussion concerning the Fredenagen and Lindner analysis in chapter II, we shall also consider a compactly supported cutoff χ at the first place, and later adapt our analysis to contain a cutoff such as in (IV.3). In the present context, the Cauchy problem 3 assumes the following particular form. Since the Cauchy problem for smooth function is well posed as discussed in proposition 3, the dynamical equation (IV.4) will be considered later via modes decomposition. Throughout this chapter, we shall always be working in the adiabatic limit $h \to 1$.

Proposition 26. *Consider the differential operator $P := \Box + \mu^2$ acting on smooth functions in $\mathcal{E}(\mathbb{M})$, with $\mu^2 \in C^\infty(\mathbb{M})$ given by $\mu^2(t, \mathbf{x}) := m^2 + \delta m^2 \chi(t) > 0$, with $\chi \in \mathcal{C}^\infty(\mathbb{R})$ as above. In addition, for arbitrary but fixed $\varepsilon > 0$, let $\Sigma := \{-2\varepsilon\} \times \mathbb{R}^3$ a Cauchy surface of $\mathbb{M}$. Then, for given $f_0, f_1 \in \mathcal{C}_0^\infty(\Sigma)$, there exists $f \in \mathcal{C}^\infty(\mathbb{M})$ solution to the Cauchy problem $Pf = 0$ with initial condition*

$$\begin{cases} f|_\Sigma = f_0, \\ \partial_0 f|_\Sigma = f_1. \end{cases} \tag{IV.5}$$

We notice that, as the differential operator P differs from the Klein-Gordon operator $\Box + m^2$ by a smooth term, their principal symbols coincide and so, according to definition I.2, P is also normally hyperbolic.

A generic solution f to the Cauchy problem may be written via mode decomposition as

$$f(x) = \frac{1}{(2\pi)^3} \int d^3\mathbf{p} \Big\{ T_\mathbf{p}(x_0) \hat{\psi}_1(\mathbf{p}) + \overline{T_\mathbf{p}}(x_0) \hat{\psi}_2(\mathbf{p}) \Big\} e^{i\mathbf{p}(\mathbf{x}-\mathbf{y})}$$

for suitable smooth functions $\hat{\psi}_1, \hat{\psi}_2$, and modes $T_\mathbf{p}$ such that

$$\left[\partial_t^2 + w_\mathbf{p}^2(t)\right] T_\mathbf{p} = 0. \tag{IV.6}$$

Solutions to the Cauchy problem for the two-point function Δ_+^Q in equation (IV.4) may then be obtained from solutions to the dynamical problem for smooth functions, and we shall be particularly interested in the decomposition of vacuum and KMS states. In general, however, the modes $T_{\mathbf{p}}$ must also satisfy

$$\dot{\overline{T}}_p(t_x)T_p(t_y) - \overline{T}_p(t_x)\dot{T}_p(t_y) = i. \tag{IV.7}$$

Equation (IV.4) corresponds to the dynamical equation in Fourier space, whereas (IV.7) is the Wronskian from Klein-Gordon equation in configuration space, which implements over the modes the requirement that the antysymmetric part of states correspond to the causal propagator. Although exact expressions for the modes T may be obtained only in certain conditions (see comments in [AAP14] for instance), these will not necessary for our analysis.

The two-point function of vacuum and KMS states then respectively reduce to

$$\Delta_0^{+,Q}(x,y) = \frac{1}{(2\pi)^3}\int d^3\mathbf{p}\, \overline{T_{\mathbf{p}}}(t_x)T_{\mathbf{p}}(t_y)e^{-i\mathbf{p}(\mathbf{x}-\mathbf{y})}, \tag{IV.8}$$

$$\Delta_+^{\beta,Q}(x,y) = \frac{1}{(2\pi)^3}\int d^3\mathbf{p}\left\{b_+(\mathbf{p})\overline{T_{\mathbf{p}}}(t_x)T_{\mathbf{p}}(t_y) + b_-(\mathbf{p})T_{\mathbf{p}}(t_x)\overline{T_{\mathbf{p}}}(t_y)\right\}e^{-i\mathbf{p}(\mathbf{x}-\mathbf{y})}, \tag{IV.9}$$

where, for $v \in \mathbb{M}$, we denote $t_v \equiv v^0$. From equation (II.8), we also recall that

$$b_+(\mathbf{p}) := \frac{1}{1-e^{-\beta w_{\mathbf{p}}}}, \quad b_-(\mathbf{p}) := \frac{1}{e^{\beta w_{\mathbf{p}}}-1} = e^{-\beta w_{\mathbf{p}}}b_+(\mathbf{p}).$$

The above two-point functions are interpreted as respectively describing vacuum or KMS states, in the sense that each of the functions $T_{\mathbf{p}}$ correspond to free state modes with mass m for $t < -2\varepsilon$. In equation (IV.9), terms $w_{\mathbf{p}}$ in the factors $b_\pm(\mathbf{p})$ could be replaced with $(\mathbf{p}^2 + m^2 + \delta m^2)^{1/2}$, in order to describe the two-point function of a KMS state in the future of Σ. Hence, we consider the Cauchy problem discussed in the latter two propositions in Fourier space, by writing the two-point functions in the above forms. As for $t < -2\varepsilon$ the modes reduce to

$$T^0_{\mathbf{p}}(t) = \frac{e^{-iw_{\mathbf{p}}t}}{\sqrt{2w_{\mathbf{p}}}}, \tag{IV.10}$$

with $w^2(t) = \mathbf{p}^2 + m^2$, which correspond to the free modes in Minkowski space, the initial conditions discussed previously are then implemented in Fourier space via $T_{\mathbf{p}}|_{t\leq -2\varepsilon} = T^0_{\mathbf{p}}$. This is nothing but the condition that each state ω^Q should reduce to the corresponding free state with mass m at earlier times than -2ε. I.e., prior to $t = -2\varepsilon$, $\Delta_0^{+,Q}$ corresponds to the Minkowski vacuum two-point function with mass m, whereas $\Delta_+^{\beta,Q}$ coincides with the free β-KMS state two-point function with mass m in the same region.

Before further addressing the interacting theory as a free theory with a time-dependent mass term, we consider the perturbative description of the same theory, considering $\delta m^2\chi(t)$ as a perturbation parameter over the free theory. From the modes decomposition and the general equation of motion in Fourier space, (IV.6) may be written as

$$(\partial_t^2 + w_{\mathbf{p}}^2)T_{\mathbf{p}}(t) = -\delta m^2\chi(t)T_{\mathbf{p}}(t).$$

This treatment consists, in addition, of supposing $T_{\mathbf{p}}(t)$ a power series with parameter $\delta m^2\chi(t)$, as

$$T_{\mathbf{p}}(t) = \sum_{n\geq 0} \tau_{\mathbf{p}}^{(n)}(t), \tag{IV.11}$$

This produces the following result, which precludes the described secular effects.

Proposition 27. *Let $T_{\mathbf{p}}(t)$ be a solution to $(\partial_t^2 + w_{\mathbf{p}}^2)T_{\mathbf{p}}(t) = -\delta m^2\chi(t)T_{\mathbf{p}}(t)$, with $T_{\mathbf{p}} = T_{\mathbf{p}}^0$ cf. equation* (IV.10) *for $t < -2\varepsilon$. Then,*

(i). there exist a sequence of $C^2(\mathbb{R})$ functions $(\tau_{\mathbf{p}}^{(n)})_{n\in\mathbb{N}_0}$, such that $T_{\mathbf{p}}$ may be written as a (convergent) power series in the parameter δm^2 as in equation (IV.11)*;*

(ii). the n-th term of the above power series of $T_{\mathbf{p}}(t)$ is such that

$$\tau_{\mathbf{p}}^{(n)}(t) = e^{iw_{\mathbf{p}}t}c_n(\mathbf{p})t^n + \mathcal{O}(t^{n-1}), \quad \forall n \in \mathbb{N},$$

with constants $c_n(\mathbf{p}) \in \mathbb{C}$ given by

$$c_n(\mathbf{p}) := -\frac{i}{(2w_{\mathbf{p}})^{n+1/2}}\delta m^2, \quad \forall n \in \mathbb{N}. \tag{IV.12}$$

Proof. We first consider item *(i)*. Set $\Lambda(t) := \delta m^2\chi(t)$. Solving the inhomogeneous equation at each order in the perturbation parameter $\Lambda(t)$ results in

$$\begin{aligned}
(\partial_t^2 + w_{\mathbf{p}}^2)\tau_{\mathbf{p}}^{(0)}(t) &= 0,\\
(\partial_t^2 + w_{\mathbf{p}}^2)\tau_{\mathbf{p}}^{(1)}(t) &= -\Lambda(t)\tau_{\mathbf{p}}^{(0)}(t),\\
&\dots\\
(\partial_t^2 + w_{\mathbf{p}}^2)\tau_{\mathbf{p}}^{(n)}(t) &= -\Lambda(t)\tau_{\mathbf{p}}^{(n-1)}(t).
\end{aligned}$$

The first equation above is the free Klein-Gordon equation in momentum space. Considering the mode which solves this equation $T_{\mathbf{p}}^0(t)$, we obtain

$$\begin{aligned}
\tau_{\mathbf{p}}^{(0)}(t) &= T_{\mathbf{p}}^0(t);\\
\tau_{\mathbf{p}}^{(1)}(t) &= -\Delta_R\left(\Lambda T_{\mathbf{p}}^0\right)(t);\\
&\dots\\
\tau_{\mathbf{p}}^{(n)}(t) &= \Delta_R^n\left(\Lambda T_{\mathbf{p}}^0\right)(t).
\end{aligned}$$

with Δ_R the retarded propagator of the mass m free scalar theory in 3-momentum space, cf. (I.10), and with $T_{\mathbf{p}}^0(t)$ the free mode in equation (IV.10). Explicitly, the next few terms of $T_{\mathbf{p}}(t)$ are

$$\begin{aligned}
\tau_{\mathbf{p}}^{(1)}(t) &= -\int_{\mathbb{R}} dt'\, \frac{\theta(t-t')\sin(w_{\mathbf{p}}(t-t'))}{w_0}\Lambda(t')\frac{e^{iw_0t'}}{\sqrt{2w_{\mathbf{p}}}},\\
\tau_{\mathbf{p}}^{(2)}(t) &= \int_{\mathbb{R}^2} dt'dt''\, \theta(t-t')\theta(t'-t'')\frac{\sin(w_{\mathbf{p}}(t-t'))}{w_{\mathbf{p}}}\frac{\sin(w_{\mathbf{p}}(t'-t''))}{w_{\mathbf{p}}}\Lambda(t)\Lambda(t'')\frac{e^{iw_{\mathbf{p}}t''}}{\sqrt{2w_{\mathbf{p}}}},
\end{aligned}$$

or, in general,

$$\tau_{\mathbf{p}}^{(n)}(t) = (-1)^n \int_{\mathbb{R}^n} dt_1 \dots dt_n \, \frac{e^{iw_{\mathbf{p}}t_n}}{\sqrt{2w_{\mathbf{p}}}} \prod_{j=0}^{n-1} \left[\theta(t_j - t_{j+1}) \frac{\sin\left(w_{\mathbf{p}}(t_j - t_{j+1})\right)}{w_{\mathbf{p}}} \Lambda(t_{j+1})\right],$$

with $t_0 \equiv t$. The above expression consists of n integrations of bounded functions, which, due to the presence of the θ-functions, may be performed within the region

$$S_n := \{(t_1, \dots, t_n) \in \mathbb{R}^n : -\infty < -2\varepsilon < t_n < \dots < t_1 < t\}.$$

Given the support of χ in each $\Lambda(t_j)$, it hence corresponds to n integrations over the finite interval $(-2\varepsilon, t_{j+1})$, $j = 0, \dots, n-1$. In addition, the integrand in each term is a bounded, smooth function. Therefore, for arbitrary but fixed t each integral exists and each $\tau_{\mathbf{p}}^{(n)}$ is a well-defined function of t.

Considering the general term for the series, we may estimate

$$\begin{aligned}
\left|\sum_n \tau_{\mathbf{p}}^{(n)}(t)\right| &\leq \sum_n \left|\tau_{\mathbf{p}}^{(n)}(t)\right| \\
&\leq \sum_n \int \frac{dt_1 \dots dt_n}{\sqrt{2w_{\mathbf{p}}}} \prod_{j=0}^{n-1} \left|\frac{\theta(t_j - t_{j+1})\Lambda(t_{j+1})}{w_{\mathbf{p}}}\right| \\
&\leq \sum_n \frac{1}{\sqrt{2w_{\mathbf{p}}}} \frac{(\delta m^2)^n}{n! w_{\mathbf{p}}^n} (2\varepsilon + t)^n = \frac{1}{\sqrt{2w_{\mathbf{p}}}} \exp\left(\frac{\delta m^2}{w_{\mathbf{p}}}(2\varepsilon + t)\right).
\end{aligned}$$

Hence, for each fixed t the series converge. This concludes the proof of item *(i)*.

Consider the first term $\tau_{\mathbf{p}}^{(1)}$ which differs from the free one. It equals

$$\begin{aligned}
\tau_{\mathbf{p}}^{(1)}(t) &= \frac{1}{\sqrt{2}w_{\mathbf{p}}^{3/2}} \int_{-\infty}^{t} dt' \, \Lambda(t') \left(\frac{e^{iw_0(t-t')} - e^{-iw_0(t-t')}}{i2}\right) e^{iw_0 t'} \\
&= \frac{-i}{(2w_{\mathbf{p}})^{3/2}} \delta m^2 e^{iw_0 t} \int_{-2\varepsilon}^{t} dt' \, \chi(t') + \frac{-i}{(2w_{\mathbf{p}})^{3/2}} \delta m^2 \int_{-2\varepsilon}^{t} dt' \, \chi(t') e^{-iw_0(t-2t')} \\
&= \frac{-i}{(2w_{\mathbf{p}})^{3/2}} \delta m^2 \left\{ e^{iw_0 t} \left[\int_{-2\varepsilon}^{-\varepsilon} dt' \, \chi(t') + \int_{-\varepsilon}^{t} dt'\right] + \int_{-\infty}^{t} dt' \, \chi(t') e^{-iw_0(t-2t')} \right\}
\end{aligned}$$

where, for all $\varepsilon > 0$,

$$\delta m^2 \int_{-2\varepsilon}^{-\varepsilon} dt' \, \chi(t') = -\delta m^2 \int_{-2\varepsilon}^{-\varepsilon} dt' \, t' \dot{\chi}(t') \in \mathbb{R}.$$

The second term in the last line for $\tau_{\mathbf{p}}^{(1)}$ then is proportional to t and diverges as we consider the limit $t \to \infty$. The third integration, on the other hand, after an integration by parts may be written as

$$\int_{-\infty}^{t} dt' \, \chi(t') e^{-iw_0(t-2t')} = -i\chi(t') \frac{e^{-iw_0(t-2t')}}{2w_0}\bigg|_{-\infty}^{t} + i \int_{-\infty}^{t} dt' \, \dot{\chi}(t') \frac{e^{-iw_0(t-2t')}}{2w_0}.$$

Both terms in the right hand side above are bounded in absolute value. In addition, in the limit $t \to +\infty$ the second integral becomes proportional to the Fourier transform of a compactly supported smooth function, $\mathrm{supp}\,\dot{\chi} \subset [-2\varepsilon, 0]$, and hence remains finite. We then see that the first order polynomial term t in $\tau_{\mathbf{p}}^{(1)}$ is not canceled by any other, and it is the only non bounded contribution.

Having shown the first order term in perturbation series may be written as in the statement of this present proposition and has a divergent term proportional to t, we proceed by induction. Suppose the n-th term of the power series $\tau_p^{(n)}(t)$ may be written in terms of constants $c_n(\mathbf{p})$ in (IV.12) t^n, then the $(n+1)$-th term is, for some smooth function f such that $|f(t)| \leq \alpha t^{n-1}$ with $\alpha \in \mathbb{R}$,

$$
\begin{aligned}
\Delta_R\Big((\Delta_R^n)^n\, (T_{\mathbf{p}}^0)\Big)(t) &= \Delta_R\Big(c_n(\mathbf{p})\; t'^{\,n} + f\Big)(t) \\
&= \int dt'\, \frac{\theta(t-t')\sin(w_0(t-t'))}{w_0}\delta m^2 \chi(t') \frac{e^{iw_0 t'}}{\sqrt{2w_0}} \Big(c_n(\mathbf{p})\; t'^{\,n} + f\Big)(t') \\
&= \frac{c\delta m^2}{i2w_0}\int_{-2\varepsilon}^{t} \Big[e^{iw_0 t} - e^{-iw_0(t-2t')}\Big][t'^n + f(t')]\chi(t') \\
&= c_{n+1}(\mathbf{p}) \int_{-\varepsilon}^{t} dt'\, \Big[e^{iw_0 t} - e^{-iw_0(t-2t')}\Big][t'^n + f(t')]. \\
&= c_{n+1}(\mathbf{p}) \int_{-\varepsilon}^{t} dt'\, t'^n + \mathcal{O}(t^{n-1}).
\end{aligned}
$$

The second integration in the latter line above may be performed by parts to produce a term proportional to t'^n, plus another integration involving t'^{n-1}, and so on. The remaining terms in the integration produce contributions of order at most n. $\square$

The latter proposition asserts the existence of secular divergences in the modes from equations (IV.8) and (IV.9). Considering the above result within the vacuum state two-point fucntion (IV.8) , we consider the truncated series at order n for the modes within the two-point function. This produces

$$
\Delta_0^{+,Q}(x,y)\Big|_n = \frac{1}{(2\pi)^3}\sum_{k=0}^{n}\int d^3\mathbf{p}\, \sum_{l=0}^{k} \tau_{\mathbf{p}}^{(l)}(t_x)\overline{\tau_{\mathbf{p}}^{(n-l)}}(t_y),
$$

where $B(t_x, t_y, \mathbf{p})$ is some function of t_x, t_y and $\mathbf{p}$ bounded with respect to its first two arguments. Considering only the term of order n, we set $k = n$ and neglect the first summation, thus considering

$$
\sum_{l=0}^{n} \tau_{\mathbf{p}}^{(l)}(t_x)\overline{\tau_{\mathbf{p}}^{(n-l)}}(t_y) = \sum_{l=0}^{n} c_l(\mathbf{p}) t_x^l c_{n-l}(\mathbf{p}) t_y^{n-l}.
$$

Introducing the result of the previous proposition into the integral kernel then implies that the perturbation series representation of $\Delta_0^{+,Q}(x,y)$ described above has a polynomial dependence on time, with polynomial degree equals to the perturbation degree.

The same result may be obtained for $\Delta_+^{\beta,Q}$ in an analogous way. This proofs the presence of secular effect for the states in (IV.8), (IV.9) when the modes decomposition is treated via perturbation theory as in proposition 27.

In proposition 27 and the above discussion we see that, treating the interaction term $\Lambda(t) = \delta m^2 \chi(t)$ perturbatively, expectation values with respect to a β-KMS state of the free theory are divergent in the limit $t_x + t_y \to \infty$. The fact that the perturbative computations consider only states of the free theory is indeed of fundamental importance to obtain the secular divergences. Indeed, in the proof of proposition 27 we see that secular divergences arise from writing the solution of the interacting dynamical equation with the retarded propagator of the free theory; the positive frequency terms cancel an oscillating dependence in time which provokes the polynomial dependence in t. If, however, we had not based our analysis upon an expansion with respect to a free state, already the dynamical equation for each mode $T_{\mathbf{p}}$ would have been of a different form. As a matter of fact, had we considered the interacting system at thermal equilibrium as per the Fredenhagen and Lindner description, we would not have obtained secular divergences. We shall return to this point in the next subsection below.

Instead of addressing equations (IV.8) or (IV.9) from the perspective of a free theory with time-dependent squared mass $m^2 + \delta m^2 \chi(t)$, we may perform an alternative perturbation treatment which reveals the absence of secular divergence in expectation values. Again, from the PPA we know that the perturbative description of this system must not show such effect. The idea in comparing these two treatments for the same dynamical equation is to show that secular effects are characteristic of perturbation theory. I.e., although certain perturbative expansions of expactation values may not produce secular divergences, these can only be obtained when we consider the perturbation series of expectation values. Therefore, if we are able to exactly compute the given expectation value, the result must not contain such divergences.

In the paragraphs above we shall consider the exact treatment for equations (IV.8) and (IV.9), and show that no secular effect emerges from the exact analysis. As a conclusion, we shall see that secular divergences are an artifact of perturbation theory indeed. In order to show that the modes $T_{\mathbf{p}}$ have no polynomial dependence on time, we shall consider the so-called adiabatic modes

$$T_p^a(t) := \frac{1}{\sqrt{2w(t)}} \exp\left(-i \int_{-\infty}^t dt'\, w(t')\right),$$

where $w^2(t) = \mathbf{p}^2 + \mu^2(t)$, as in above. As we shall see explicitly in the next theorem, these are not a solution to equation (IV.6). For $t < -2\varepsilon$, these modes correspond to the free modes with square mass m^2, whereas in the (adiabatic) limit $\chi \to 1$ they equal the free modes with square mass $m^2 + \delta m^2$. We shall then prove that the difference between modes $T_{\mathbf{p}}$ and $T_{\mathbf{p}}^a$ is bounded in time, and as so is $T_{\mathbf{p}}^a$, we shall conclude there may be no secular divergences in modes $T_{\mathbf{p}}$, such as we encountered in proposition 27.

With the adiabatic modes we construct the function

$$\omega^a(x, y) := \frac{1}{(2\pi)^3} \int d^3\mathbf{p}\, \overline{T_{\mathbf{p}}^a}(t_x) T_{\mathbf{p}}^a(t_y) e^{i\mathbf{p}(\mathbf{x}-\mathbf{y})}, \tag{IV.13}$$

and consider the differences $\omega_0^Q - \omega^a$, $\omega_\beta^Q - \omega^a$ in order to prove the theorem below, which is contrary to the appearance of secular divergences. The function ω^a is not a solution to the dynamical equation, and also should not be seen as the two-point function of some state.

Theorem 6. *The two-point functions of ω_{vac}^Q and ω_β^Q are both bounded in time.*

Proof. The adiabatic modes

$$T^a_{\mathbf{p}}(t) = \frac{1}{\sqrt{2w(t)}} \exp\left(-i\int^t dt'\, w(t')\right),$$

with $w(t)$ as above, coincide with the free modes in the past and solve the differential equation

$$\left(\partial_t^2 + w^2(t)\right) T^a_{\mathbf{p}}(t) = -\lambda(t) T^a_{\mathbf{p}}(t), \quad \text{with } \lambda(t) := \frac{1}{2w(t)}\left(\ddot{w}(t) - \frac{3}{2}\frac{\dot{w}^2(t)}{w(t)}\right).$$

I.e. they fail to solve equation (IV.4) for $T^a_{\mathbf{p}}$ by an error given by $\lambda(t)$. We treat this error as a perturbation parameter in the equation for the modes T_p, associated to ω^Q. Hence, consider

$$\left[\partial_t^2 + w^2(t) + \lambda(t)\right] T_p(t) = \lambda(t) T_p(t)$$

and, similarly to the previous analysis, we construct modes $T_p(t)$ as a power series,

$$T_p(t) = \sum_{n\geq 0} \tau_p^{(n)}(t) \quad \Rightarrow \quad \left[\partial_t^2 + w^2(t) + \lambda(t)\right] \sum_{n\geq 0} \tau_p^{(n)}(t) = \lambda(t) \sum_{n\geq 0} \tau_p^{(n)}(t),$$

now with $\tau_{\mathbf{p}}^{(0)} = T^a_{\mathbf{p}}$. Order by order in the perturbation parameter λ, the last equation becomes

$$\begin{cases} \left[\partial_t^2 + w^2(t) + \lambda(t)\right] \tau_p^{(0)}(t) = & 0 \\ \left[\partial_t^2 + w^2(t) + \lambda(t)\right] \tau_p^{(1)}(t) = & -\lambda(t)\tau_p^{(0)}(t) \\ \dots & \\ \left[\partial_t^2 + w^2(t) + \lambda(t)\right] \tau_p^{(n)}(t) = & -\lambda(t)\tau_p^{(n-1)}(t) \end{cases}$$

Solving each differential equation we obtain

$$\tau_p^{(0)}(t) = T_p^a(t),\ \lambda\tau_p^{(1)}(t) = \Delta_R^a(\lambda T_p^a(t)),\ \dots\ \tau_p^{(n)}(t) = \left(\Delta_R^a \circ M_\lambda\right)^n (T_p^a)(t)$$

in the sense of pairing composition. We denote M_λ as the multiplication by $\lambda(t)$ operator, and Δ_R^a is the retarded fundamental solution of the equation for the adiabatic modes, which involves the differential operator $\partial_t^2 + w^2(t) + \lambda(t)$. Therefore, we obtain

$$\Delta_R^a(\lambda T_p^a)(t) = \int dt_1\, \theta(t-t_1)\frac{1}{\sqrt{w(t)w(t_1)}}\lambda(t_1)\sin\left(\int_{t_1}^t d\tau w(\tau)\right) T_p^a(t_1)$$

$$\begin{aligned}\left(\Delta_R^a \circ M_\lambda\right)^2 (T_p^a)(t) = &\int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \frac{\lambda(t_1)}{\sqrt{w(t)w(t_1)}}\frac{\lambda(t_2)}{\sqrt{w(t_1)w(t_2)}}\sin\left(\int_{t_1}^t d\tau_1 w(\tau_1)\right)\times \\ &\times \sin\left(\int_{t_2}^{t_1} d\tau_2 w(\tau_2)\right) T_p^a(t_2),\end{aligned}$$

and the general term is expressed by

$$\begin{aligned}(\Delta_R^a \circ M_\lambda)^n\, (T_p^a)(t) = &\int_{-\infty}^{t} dt_1 \cdots \int_{-\infty}^{t_{n-1}} dt_n\, \frac{\lambda(t_1)}{w(t)} \dots \frac{\lambda(t_n)}{w(t_n)} \sin\left(\int_{t_1}^{t} d\tau_1 w(\tau_1)\right) \times \dots \\ &\cdots \times \sin\left(\int_{t_n}^{t} d\tau_n w(\tau_n)\right) T_p^a(t_n).\end{aligned}$$

The perturbative treatment to the dynamical equation for the modes T_p contrasts significantly with the previous perturbative method, as the power series for $T_p(t)$ is not only convergent, but also bound in time. This might be seen from the estimations

$$\begin{aligned}\left|\sum_{n\geq 0} (\Delta_R^a \circ M_\lambda)^n\, (T_p^a)(t)\right| \leq &\sum_{n\geq 0} \left|(\Delta_R^a \circ M_\lambda)^n\, (T_p^a)(t)\right| \\ \leq &\sum_{n\geq 0} \frac{1}{n!} \int_{-\infty}^{t} dt_1 \cdots \int_{-\infty}^{t} dt_n \left|\frac{1}{\sqrt{2w(t)}} \frac{\lambda(t_1)}{w(t_1)} \cdots \frac{\lambda(t_n)}{w(t_n)}\right| \\ \leq &\frac{1}{\sqrt{2w(t)}} \exp\left(\int_{-\infty}^{\infty} dt' \left|\frac{\lambda(t')}{w(t')}\right|\right)\end{aligned} \tag{IV.14}$$

where the form of $\lambda(t)$ allows extending the integration to $+\infty$. This is seen from

$$\frac{\lambda(t)}{w(t)} = \frac{1}{2w^2(t)}\left[\ddot{w}(t) - \frac{3}{2}\frac{\dot{w}^2(t)}{w(t)}\right] = \frac{\delta m^2}{4w^3}\left\{\ddot{\chi}(t) - \dot{\chi}(t)\left[\frac{\delta m^2 \dot{\chi}(t)}{2w^2} - \frac{3}{2w}\right]\right\} \leq C \in \mathbb{R}. \tag{IV.15}$$

Since χ is a smooth, compactly supported function, and since the integrand λ/w is decreases at least as $\sim 1/w^3$, the integral in the exponent converges. The last inequality in the previous estimation then implies the perturbation series is absolutely convergent, and bounded as a function of t. The same analysis shows also the difference between $T_p(t)$ and the adiabatic modes T_p^a are bounded, as

$$\left|T_p - T_p^a\right| \leq \frac{1}{\sqrt{2w(t)}} \left|\exp\left(\int_{-\infty}^{+\infty} dt' \left|\frac{\lambda(t')}{w(t')}\right|\right) - 1\right|$$

Suppose now ω^Q is built from the vacuum state of the free theory ω_{vac}. Its two point function therefore is

$$\omega_{vac}^Q(x,y) = \frac{1}{(2\pi)^3} \int d\mathbf{p}\, \overline{T}_p(t_x) T_p(t_y) e^{i\mathbf{p}(\mathbf{x}-\mathbf{y})},$$

and regularization is obtained by the subtraction of adiabatic modes. Work in the three-dimensional momentum space for simplicity,

$$\begin{aligned}\hat{\omega}_{vac}^Q(t_x, t_y, \mathbf{p}) = &\overline{T}_p(t_x) T_p(t_y) - \overline{T}_p^a(t_x) T_p^a(t_y) \\ = &\overline{T}_p(t_x)\left[T_p(t_y) - T_p^a(t_y)\right] + \left[\overline{T}_p(t_x) - \overline{T}_p^a(t_x)\right] T_p^a(t_y)\end{aligned}$$

Therefore the absolute value of the expectation value of the two-point function is

$$\begin{aligned}|\hat{\omega}^Q_{vac}(t_x,t_y,\mathbf{p})| \leq & \left|\overline{T}_p(t_x)\right| \left|T_p(t_y) - T^a_p(t_y)\right| + \left|\overline{T}_p(t_x) - \overline{T}^a_p(t_x)\right| \left|T^a_p(t_y)\right| \\ \leq & \frac{C}{\sqrt{w(t_x)w(t_y)}} \left|\exp\left(\int_{-\infty}^{+\infty} dt' \left|\frac{\lambda(t')}{w(t')}\right|\right) - 1\right|\end{aligned}$$

for some $C \in \mathbb{R}$. The integration of the above term in 3-momentum space is well defined, again due to the support of $\dot{\chi}$ and equation (IV.15). We emphasize the importance of term -1 within the module above, in contrast to estimation (IV.14), which implies the integral with respect to dp converges. In particular, this means not only that we may extend the integration of λ/w up to $+\infty$ as stated above; but also that $|\hat{\omega}^Q_{vac}(t_x,t_y,\mathbf{p})|$ behaves at least as $\sim 1/w^4$. Precisely, the term in the exponential may be estimated as

$$\begin{aligned}&\frac{\delta m^2}{4w^3}\left\{\ddot{\chi}(t) - \dot{\chi}(t)\left[\frac{\delta m^2 \dot{\chi}(t)}{2w^2} - \frac{3}{2w}\right]\right\} \leq \\ &\qquad \leq \frac{\delta m^2}{4(|\mathbf{p}^2| + m^2)^{3/2}}\left\{\ddot{\chi}(t) - \dot{\chi}(t)\left[\frac{\delta m^2 \dot{\chi}(t)}{2(|\mathbf{p}|^2 + m^2)} - \frac{3}{2(|\mathbf{p}|^2+m^2)^{1/2}}\right]\right\} \\ &\qquad \leq \frac{C}{(|\mathbf{p}|^2+m^2)^{3/2}}\left(1 - \frac{1}{(|\mathbf{p}|^2+m^2)} - \frac{1}{(|\mathbf{p}|^2+m^2)^{1/2}}\right)\end{aligned}$$

for some constant $C \in \mathbb{R}$. As a consequence we have

$$\begin{aligned}|\hat{\omega}^Q_{vac}(t_x,t_y,\mathbf{p})| \leq & \int d|\mathbf{p}|\, |\mathbf{p}|^2 \frac{2}{\sqrt{w(t_x)w(t_y)}} \times \\ & \times \left|\exp\left(\int_{-\infty}^{+\infty} dt' \frac{\delta m^2}{4w^3(t')}\left\{\ddot{\chi}(t') - \dot{\chi}(t')\left[\frac{\delta m^2\dot{\chi}(t')}{2w^2(t')} - \frac{3}{2w(t')}\right]\right\}\right) - 1\right| \\ \leq & C' \int \frac{d|\mathbf{p}|\, |\mathbf{p}|^2}{\sqrt{w(t_x)w(t_y)}} \left|\exp\left(\frac{C}{(|\mathbf{p}|^2+m^2)^{3/2}}\right) - 1\right| \\ \leq & C' \int \frac{d|\mathbf{p}|\, |\mathbf{p}|^2}{\sqrt{|\mathbf{p}|^2+m^2}} \frac{1}{(|\mathbf{p}|^2+m^2)^{3/2}}.\end{aligned}$$

The discussion is analogous if we consider the KMS state ω^Q_β instead. As presented in proposition **??**, its singular part is subtracted via the same procedure adopted for the vacuum state ω^Q_{vac}, and the integration in $d^3\mathbf{p}$ is well defined. In addition, the boundness of $\hat{\omega}^Q_\beta$ w.r.t. t is then analogous to the case with ω_{vac}. In this case we write

$$\begin{aligned}\hat{\omega}^Q_\beta(t_x,t_y,\mathbf{p}) =& b_+(p)\overline{T}_p(t_x)T_p(t_y) - \overline{T}^a_p(t_x)T^a_p(t_y) + b_-(p)T_p(t_x)\overline{T}_p(t_y) \\ =& b_+\left[\overline{T}_p(t_x) - \overline{T}^a_p(t_x)\right]T^a_p(t_y) + b_+\overline{T}^a_p(t_x)\left[T_p(t_y) - T^a_p(t_y)\right] + \\ & + (1-b_+)\overline{T}^a_p(t_x)T^a_p(t_y) + b_-T_p(t_x)\overline{T}_p(t_y) \\ =& (b_+ + b_-)\left[\overline{T}_p(t_x) - \overline{T}^a_p(t_x)\right]T^a_p(t_y) + b_+\overline{T}^a_p(t_x)\left[T_p(t_y) - T^a_p(t_y)\right] + \\ & + b_-T_p(t_x)\left[\overline{T}^a_p(t_y) - \overline{T}^a_p(t_y)\right].\end{aligned}$$

We then proceed with estimations analogous to the previous case with ω^Q_{vac}, considering that $b_\pm$ is a bounded function of $\mathbf{p}$ for the massive theory – in addition, b_- being also a fast decreasing function. We hence obtain

$$|\hat{\omega}^Q_\beta(t_x, t_y, \mathbf{p})| \leq \frac{C}{\sqrt{2w(t_x)w(t_y)}} \left| \exp\left(\int_{-\infty}^{+\infty} dt' \left| \frac{\lambda(t')}{w(t')} \right| \right) - 1 \right|,$$

and we proceed as before. $\square$

IV.1.1 Secular Effects in perturbative AQFT.

In pAQFT the secular growth presents in a equivalent manner. We present a brief discussion and indicate how the divergences revealed in proposition 27 might be seen in this framework.

In this context we ought to emphasize how perturbation theory is performed when considering expectation values computations, since, as discussed already throughout this thesis, it is necessary to consider the effect of interaction both upon observables and states separately. Therefore, when addressing the perturbative estimation of an abstract expectation value, it is necessary to explicitly consider the effect of interaction upon all the objects involved. In order to illustrate this statement, consider the squared-field observable, whose formal kernel we represent as ϕ^2, and the interacting observable represented by $\mathcal{R}_Q\phi^2$. When considering the expectation value $\omega^{\beta,V}\big(\mathcal{R}_Q\phi^2(x)\big)$, we may conclude in advance that its computation may not present any secular divergent contribution, since $\omega^{\beta,V}$ is a thermal equilibrium state of the interacting theory and, hence, α^Q_t-invariant, where α^Q_t is the dynamical operator defined in equation (II.15). This may be recollected in the form of the following proposition.

Proposition 28. *Expectation values of observables of the interacting theory in thermal equilibrium are time-independent. Hence, they may present no secular divergence.*

Proof. After the interaction $Q(t)$ was turned on and a long enough time has passed, in such a manner that the system returned to thermal equilibrium, it is characterized by a KMS state ω^Q_β which differs from the KMS state of the free theory. The time evolution of the system is, besides, now given by the interacting time evolution α^Q_t rather than the free evolution operator; this might be seen as a "*switch to the interacting picture*", in the spirit of chapter II. Then, as $\omega^Q_\beta \circ \alpha^Q_t = \omega^Q_\beta$, we conclude the absence of secular effects. $\square$

However, if we neglect the effect of the interaction term Q upon one of the elements within $\omega^{\beta,V} \circ \alpha^Q_t\big(\mathcal{R}_V\phi^2(x)\big)$, the time invariance may be replaced by the secular effect. We shall further justify this with the estimations below. Nevertheless, we may see that the difference in results obtained in expectation values computations, provoked by implementing the action of interaction upon different elements in different manners, reveals that secular effect is not an intrinsic failure of perturbation theory. Instead, it is a consequence of neglecting the effect of interaction upon the state and/or the dynamics, and hence, in this present example, of misinterpreting a thermal equilibrium state for the free theory as a thermal equilibrium state for the interacting one. In this subsection we shall illustrate this by considering the expectation value $\omega^{\beta,V} \circ \alpha_t^Q\big(\mathcal{R}_V\phi^2(x)\big)$, but substituting $\omega^{\beta,V}$ by ω^β, and therefore choosing a state which is not invariant under the given dynamics.

Without further introduction, in the presence of the polynomial interaction $Q(t)$, we first consider the up to first order expansion of $\omega^\beta \circ \mathcal{R}_Q(\phi^2(x))$,

$$\omega^\beta \circ \mathcal{R}_Q\left(\phi^2(x)\right) = \omega^\beta(\phi^2(x)) + i\omega^\beta\left(Q \cdot_T \phi^2 - Q \star \phi^2\right) + H.O.,$$

where ω^β is the β-KMS of the free theory with mass m. Whereas the zeroth order term does not present secular divergent growth in time, since it is a free observable evaluated with respect to the KMS state of the free theory, which is translation invariant, the first order contribution equals

$$\begin{aligned}\omega^\beta\big(Q \cdot_T \phi^2 - Q \star \phi^2\big) =&\\ =2\int dz\,\left[\Delta_F^2(z,x) - \Delta_+^2(z,x)\right]\chi(t)\delta m^2 + 4\int dz\,\Delta_A(z,x)W_\beta(z,x)\chi(t)\delta m^2.&\end{aligned}$$

The first integral is treated as in chapter III, subsection III.3.1 as

$$\left[\Delta_F^2(z,x) - \Delta_+^2(z,x)\right] = -\Box\int_{4m^2}^{+\infty} dM^2\rho_2(M^2)\frac{1}{M^2}i\Delta_A(z-x,M) + c\delta(z-x)$$

where c is a renormalization constant. Due to the form of the advanced propagator, this contribution to the first order term of $\omega^\beta \circ \mathcal{R}_V(\phi^2)$ is bounded in time. The remaining contribution to the first order term is proportional to

$$\begin{aligned}&\int dz\,\theta(x_0 - z_0)\Delta(z,x)W_\beta(z,x)\chi(z_0)h(\mathbf{z}) =\\ &\quad= \int dz\theta(x_0 - z_0)\chi(z_0)h(\mathbf{z})\int dp\,\mathcal{F}(\Delta W_\beta)(p)e^{ip(x-z)}\\ &\quad= \int_{-\infty}^{x_0} dz\,\chi(z_0)h(\mathbf{z})\int \frac{dp}{(2\pi)^6}dq\,\frac{b_-(2)}{4w_1w_2}\left[b_+(1)\delta(q_0 - w_1) + b_-(1)\delta(q_0 + w_1)\right]\\ &\qquad\times\left[\delta(p_0 - q_0 - w_2) + \delta(p_0 - q_0 - w_2)\right]e^{ip(x-z)}\end{aligned}$$

In the adiabatic limit $h \to 1$, with $w_1 = w_2 \equiv w$ we obtain the integration with respect to $d\mathbf{q}$

$$\int d\mathbf{q}\,\frac{b_+(w)b_-(w)}{4w^2}\Big\{\delta(p_0 - 2w) + 2\delta(p_0) + e^{-\beta w}\delta(p_0 + 2w)\Big\}.$$

In the $\delta(p_0)$ contribution, the dependence with respect to z_0 lies entirely within $\chi(z_0)$, and therefore the dz_0 integration reduces to

$$\int_{-\varepsilon}^{x_0} dz_0\chi(z_0) = \int_{-\varepsilon}^{0} dz_0\,\chi(z_0) + t'\big|_{-\varepsilon}^{x_0}$$

which presents a secular growth when we consider the large time limit $x_0 \to \infty$, which corresponds to supposing an ever lasting mass perturbation δm^2. By considering the limit of zero temperature $\beta \to +\infty$, we may notice this divergence is also present when the vacuum state of the free theory is considered.

The computation just performed correspond to the first terms appearing in the expansion of $\omega^\beta \circ \alpha_t^Q(\mathcal{R}_Q\phi^2)$ with respect to the Bogolubov map, with the interacting dynamics α_t^Q from equation (II.15) constructed with the local interaction term Q. Therefore, we conclude that expectation values of certain interacting observables, with respect to the free theory KMS state ω^β, may present secular divergences when the observable evolves according to the interacting dynamics. In this situation, we notice an interplay between elements of the interacting and the free theory: the expectation value $\omega^\beta \circ \alpha_t^Q(\mathcal{R}_Q\phi^2)$ consists of an interacting observable $\mathcal{R}_Q\phi^2$, which evolves according to α_t^Q, evaluated with respect to the free state ω^β. If, however, the expectation value had been estimated with respect to the interacting state $\omega^{\beta,V}$, since it is α_t^Q-invariant the secular divergence would not have been present, in the same manner as $\omega^\beta(\phi^2)$ may not contain a secular effect.

In addition to this discussion about the relation between the free state ω^β and the interacting dynamics α_t^Q, the perturbative analysis of $\omega^\beta \circ \alpha_t^Q$ has to be compared with the return to equilibrium property discussed in chapter II, proposition 24. As previously, provided care is taken in considering the limits $h \to 1$ and $t \to +\infty$ in the precise order, $\omega^\beta \circ \alpha_t^Q$ coincides with the KMS state for the interacting theory $\omega^{\beta,V}$, which, as argued above, cannot produce expectation values with secular effect. This again illustrates how such effects are characteristic of perturbative expansions.

Performing instead a perturbative analysis of $\omega^\beta \circ \alpha_t^Q(\mathcal{R}_Q\phi^2)$, focused now exclusively on the time evolution of the interacting theory, up to first order we obtain, cf. equation (II.24),

$$\omega^\beta \circ \alpha_t^Q\left(\mathcal{R}_Q\phi^2\right) = \omega^\beta\left(\mathcal{R}_Q\phi^2\right) + i\int_{-\infty}^t dt_1\, \omega^\beta\left(\left[\alpha_{t_1}\mathcal{R}_Q\,\dot{Q}, \alpha_t\mathcal{R}_Q\phi^2\right]\right) + O(\lambda^2).$$

It is possible to prove that the above integral in the right hand side results in a term proportional to t. The interacting observable $\mathcal{R}_Q\phi^2$, which is not to be expanded in a perturbation series in the present, contains cutoffs $\chi(z_0)$ throughout its terms, while $R_Q\dot{Q}$, on the other hand, has compact support $\dot{\chi}$. Expanding $\mathcal{R}_Q\dot{Q}$ to first order produces

$$\int_{-\infty}^t dt_1 \int dz\, \dot{\chi}(z_0 - t_1 + t)\omega^\beta\big(\phi^2(z) \star \mathcal{R}_Q\phi^2(x) - \mathcal{R}_Q\phi^2(x) \star \phi(z)\big).$$

We observe that the dependence on t_1 is entirely contained within the cutoff $\dot{\chi}$. Changing order of integrations we obtain

$$\int_{-\infty}^t dt_1\, \dot{\chi}(z_0 - t_1 + t) = \chi(z_0 + t - t_1)\big|_{-2\varepsilon}^t = \chi(z_0) - \chi(z_0 + t + 2\varepsilon).$$

Although a complete result from the perturbative series above requires considering also the perturbative expansion of $\mathcal{R}_Q\phi^2$, it is possible to notice that the integration of the latter result, smeared with a smooth, non compactly supported function, produces an infinite divergence of order one. This may thus be generalized to observables $\mathcal{R}_Q A$ with $A \in \mathscr{F}_{loc}(\mathbb{M})$, $\operatorname{supp} A \subset J_+(\operatorname{supp}\chi)$, other than ϕ^2.

In this subsection, we have then seen how, in the context of perturbative AQFT, secular effects may emerge from expectation values computations when the state and the dynamical evolution mix the free and the interacting theory, but that such effects may not occur in certain cases, when the effect of interaction is considered upon both these objects. We shall return to this discussion in the future.

In the next section we intend to deepen the analysis of secular effects in AQFT by treating a simple model of a non equilibrium steady state.

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