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OS TEOREMAS DE SINGULARIDADE VALEM SE CONSIDERARMOS EFEITOS QUÂNTICOS?

Lissa Campos

Orientador: Prof. Dr. João Carlos Alves Barata

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Banca Examinadora:

Prof. Dr. João Carlos Alves Barata - Orientador (IFUSP)
Prof. Dr. Daniel Augusto Turolla Vanzella (IFSC)
Prof. Dr. André Gustavo Scagliusi Landulfo (UFABC)

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DO SINGULARITY THEOREMS HOLD IF WE CONSIDER QUANTUM EFFECTS?

Lissa de Souza Campos

Supervisor: Prof. Dr. João Carlos Alves Barata

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Examining Committee:

Prof. Dr. João Carlos Alves Barata - Supervisor (IFUSP)
Prof. Dr. Daniel Augusto Turolla Vanzella (IFSC)
Prof. Dr. André Gustavo Scagliusi Landulfo (UFABC)

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¹In the end of chapter 10 of “Small Treatise of the Great Virtues”, by André Comte-Sponville

Ignoro si creí alguna vez en la Ciudad de los Inmortales:
pienso que entonces me bastó la tarea de buscarla.
[El inmortal, J. L. Borges]

ABSTRACT

There are two quantum loopholes in the Singularity Theorems of General Relativity: violations of the classical energy conditions and quantum fluctuations of the spacetime geometry. In this dissertation, we study the first loophole and approach Singularity Theorems through the energy condition. We review the algebraic approach of Quantum Field Theory for the Klein-Gordon field and, within it, we review the derivation of a quantum energy inequality for Hadamard states on globally hyperbolic spacetimes. However quantum energy inequalities cannot be directly applied to Singularity Theorems, we show that generalized Hawking and Penrose Theorems are proven considering weakened energy conditions inspired by them. Hence, Singularity Theorems do hold under subtle quantum effects. The question of whether interaction or backreaction effects could break them is still open; there are reasons to expect both answers.

Keywords: Singularity Theorems; General Relativity; Negative energy; Quantum energy inequalities; Algebraic Quantum Field Theory.

RESUMO

Há duas brechas quânticas nos Teoremas da Singularidade em Relatividade Geral: violações das condições clássicas de energia e flutuações quânticas da geometria do espaço-tempo. Nesta dissertação, estudamos a primeira brecha e abordamos os Teoremas da Singularidade através da condição de energia. Revisamos a abordagem algébrica de Teoria Quântica de Campos para o campo de Klein-Gordon e, neste formalismo, revisamos a derivação de uma desigualdade quântica de energia para os estados de Hadamard em espaços-tempos globalmente hiperbólicos. Apesar das desigualdades quânticas de energia não poderem ser aplicadas diretamente nos Teoremas de Singularidade, mostramos que generalizações dos Teoremas de Hawking e Penrose são provadas considerando condições de energia enfraquecidas inspiradas por elas. Assim sendo, os Teoremas de Singularidade continuam valendo se considerarmos efeitos quânticos sutis. A questão de se efeitos de interação ou efeitos de “backreaction” poderiam quebrá-los ainda está em aberto; há razões para se esperar ambas as respostas.

Palavras-chave: **Teoremas de Singularidade; Relatividade Geral; Energia Negativa; Desigualdades quânticas de energia; Teoria Quântica de Campos Algébrica.**

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1

A QUESTION: SINGULARITY THEOREMS UNDER THE LIGHT OF QUANTUM PHYSICS

Where we see what lead us to the problem of finding quantum energy inequalities in the context of Algebraic Quantum Field Theory.

The Standard Cosmological Model gives us the following information: the universe had a beginning some 14 billion years ago. This model lies in the realm of General Relativity and corresponds to the Friedman-Lemaître-Robertson-Walker solution to the Einstein equations. The “beginning” of the universe is leisurely known as “Big Bang”, and academically referred to as “cosmological singularity”. In fact, there are two types of singularities within General Relativity, besides the cosmological one, there are the Black Hole ones—which correspond to the Schwarzschild solution of the Einstein equations. Both these solutions rely on symmetry hypotheses: the cosmological solution assumes an homogeneous and isotropic universe and the Black Hole solution assumes spherical symmetry. For many years, these symmetries were held suspect for causing the singular behaviour of these solutions.

Actually, a solution to the Einstein equations is just a metric—it does not fix the topology of the spacetime. So, let’s call the pair metric *and* spacetime, a spacetime solution; to obtain one of these—which is not necessarily unique—we first need to choose a matter model, solve Einstein equations and then chose a spacetime: for a vacuum model without cosmological constant we get Minkowski spacetime (or, for example, its compactification into a torus), for a vacuum around a spherical mass model we get Schwarzschild spacetime, for a perfect fluid universe we get Friedman-Lemaître-Robertson-Walker spacetime. These solutions are somewhat simplified models. Yet, even if we knew all types of matter, their proportions in the universe and the equations of motion governing it, it would be impossible to know the exact form of $T_{\mu\nu}$ and obtain the geometry of our universe.

Singularity Theorems are two things, at least. First, they constitute a way of obtaining information about the geometry of the spacetime without specifying a matter model or solving Einstein equations. If we impose physically reasonable conditions on the energy-momentum tensor—called energy conditions—by the Einstein equations we can translate this to a condition on the curvature tensors and get something out of it. Second, the Singularity Theorems exonerate the symmetries of the particular solutions as being the cause of their

singular behaviour and clarified, within a general well-defined formalism, sufficient conditions that lead to singular spacetimes.

The strong energy condition is the one of Hawking Singularity Theorem, which corresponds to the Cosmological singularity, and the null energy condition is the one of Penrose Singularity Theorem, which corresponds to the Black Hole singularity; the strong and the null energy conditions are examples of classical energy conditions—classical in the sense that they are non-quantum—and these are all constructed by physically reasonable assumptions; basically, each of them answers in a different way the question: where and for whom is energy positive?

On the other hand, Quantum Field Theory gives us several examples of violations of the classical energy conditions. We can explicitly construct states with negative local energy densities and we can actually measure the Casimir effect. Thus, one way of considering quantum effects on Singularity Theorems is through the energy condition.

We first review Singularity Theorems, in section 1.1, to understand what they are, their connection with particular solutions of Einstein equations and their general role in the study of singularities in General Relativity. Then, we study the existence of negative energy, in section 1.2, to accept that all classical energy conditions are violated within Quantum Field Theory. Yet, Quantum Field Theory also restrict these violations; bounds on the duration and magnitude of negative energy can be directly derived from its formalism—these bounds are called quantum energy inequalities, and are introduced in section 1.2.3.

The study developed here is within a semi-classical analysis, we are considering quantum matter on a classical background, and in order to define a quantized energy density and search for quantum energy inequalities on general curved spacetimes, we go to the algebraic approach of Quantum Field Theory—the transition from Minkowski spacetime to general curved spacetimes is justified in section 1.3. And a review of the algebraic approach of Quantum Field Theory for the Klein-Gordon field, as well as the mathematical preliminaries—regarding Microlocal Analysis—is given in chapter 2.

The goal of this first chapter is to set the problem and this is done in an informal way; moreover, I assume the reader is familiar with both General Relativity and Quantum Physics, for example with the terms: Einstein equations, spacetime, wave-functions, Hilbert spaces. On the other hand, chapter 2 is mathematically rigorous and more self-contained.

In chapter 3, we understand how we can use the quantum energy inequalities to study singularities in General Relativity; first, in section 3.1, we use the formalism of chapter 2 for the derivation of the quantum energy inequality on general curved backgrounds, as done by Fewster [32] in 2000. Then, by reviewing Fewster and Galloway's work [37] of 2011, we see two generalized Singularity Theorems: in the cosmological context and in the black hole context; in the end of this chapter, we can finally answer the question:

—Do Singularity Theorems hold if we consider quantum effects?

There are two ways of interpreting the search for an answer to that. One is (expecting a negative answer): singularities are not a disaster for General Relativity since at Planck scale we must consider also Quantum Physics, hence if all works out fine at this scale with both theories, then they are both fine. The other possible way is: General Relativity does break, we do need a new theory and to settle the ground for this new theory, we can start working with the interaction between General Relativity and Quantum Physics. Either way, it is relevant to study this interaction.

1.1 Singularity Theorems in General Relativity..

Where we understand the nature of Singularity Theorems and the impact of the ones from the 60's on the debate concerning singularities in General Relativity.

The study of singularities in General Relativity emerged concomitantly with General Relativity itself. A few months after Einstein's publication "On the general theory of relativity" in November 1915, Schwarzschild obtained the first exact solution to Einstein equations—which indeed already presented a singularity. It took a long debate, from 1916 to 1973, until singularities gained a mathematical precise definition and Singularity Theorems, a well-defined structure. This debate on singular solutions to the Einstein equations was marked by works of too many scientists to fit in this dissertation, among them were Friedman, Lemaître, Raychaudhuri, Penrose and Hawking.

The Singularity Theorems of Penrose [88] and Hawking [71] from the 60's made it clear that singularities should be accepted as endemic of General Relativity—*singularities are a part of generic solutions*. Their mathematical precise definition of singularity, however, did not solve the debate. There is not a *correct* definition for a singularity in General Relativity; the consensus on that is, seemingly, that we cannot have one¹. In this section, I will use the term *singularity* in a broadly manner—as indicating some mathematical irregularity or some physical quantity blowing up or the vanishing of spacetime itself—until we define it formally.

First, I will give a brief description of the debate on singularities in General Relativity, using as an example the cosmological singularity—the one of the now known as Friedman-Lemaître-Robertson-Walker solution. We will see how, within a different formalism, Hawking obtained a cosmological singularity without a (high)symmetry hypothesis or even solving Einstein equations. Furthermore, we will establish the nature of a Singularity Theorem by constructing a statement of a "Pattern Singularity Theorem".

To illustrate the debate on singularities in General Relativity, we will see the evolution of the debate on the cosmological singularity, by discussing the following results²:

1922 Friedman obtained a dynamical solution that vanished in finite time [58];

1932 Lemaître argued that anisotropy could not prevent it [82];

1955 Raychaudhuri highlighted a geometrical identity [95];

1965 Penrose introduced the concept of closed trapped surface [88];

1966 Hawking's theorem settled the debate on the symmetry hypothesis [71].

Friedman, inspired by Einstein and De Sitter solutions, studied, in 1922, the possible spacetime solutions³ such that for each constant time t , corresponds a three dimensional spherically symmetric space:

¹In appendix A, one can find a discussion on this topic based on Geroch's article "What is a singularity in General Relativity?", published in 1968.

²The history of singularities in General Relativity is an extensive one, for a nice review see [30].

³A curiosity for a not-in-a-hurry reader: General Relativity was suppose to be a Theory of Gravitation—in the sense that the equations were suppose to describe the movement of things, and not to give us weird spacetime solutions. In spite of that, Einstein tried to show that his equations were compatible with the

$$ds^2 = R^2(dx_1^2 + \sin^2 x_1 dx_2^2 + \sin^2 x_1 \sin^2 x_2 dx_2^2 dx_3^2) + M^2 dx_4^2;$$

where R is a function of time $x_4 = t$ and M is an arbitrary function. For each t , space has curvature constant on x_1, x_2, x_3 ; but, since $R = R(x_4)$, space curvature has a time dependence. He showed that this is a non-stationary generalization for Einstein and De Sitter solutions: replacing $R^2 \rightarrow \frac{-R^2}{c^2}$, it reduces to Einstein solution for $M = 1$ and to De Sitter solution for $M = \cos x_1$.

There is another possible solution. Setting $M = 1$ (without loss of generality), the Einstein equations gives a set of two ordinary differential equations for R in terms of T_{00} and Λ . By an analysis of this set, Friedman found that—for certain values of Λ , let's conveniently consider it zero— R goes to zero in a finite time. Thus, *if we allow a dynamical solution, Einstein equations tell us that spacetime itself will vanish*.

Independtly of Friedman, Lemaître also obtained a dynamical solution in 1927 [81] that was a non-stationary generalization of Einstein and De Sitter solutions; furthermore, he used the expanding universe model to explain the observational data that Hubble obtained in 1926 of distances and radial velocities of galaxies⁴. In the 30's, the expansion of the universe was widely accepted, but the singularity of the spacetime solutions was still controversial⁵.

Friedman singular solution was taken as a mathematical artifact due to the symmetry hypothesis. Under Einstein suggestion, Lemaître studied, in 1932, if anisotropy could avoid this “catastrophic” vanishing of a dynamical spacetime; he considered the line segment:

$$ds^2 = -b_1^2 dx_1^2 - b_2^2 dx_2^2 - b_3^2 dx_3^2 + b_4^2 dx_4^2;$$

where b_1, b_2 and b_3 are functions of time $t = x_4$. Defining R by: $\sqrt{-g} = b_1 b_2 b_3 = R^3$, Lemaître found that

$$3\frac{\ddot{R}}{R} = \frac{\kappa}{2}(T_1^1 + T_2^2 + T_3^3 - T_4^4) - \frac{1}{3}I^2;$$

where $\kappa = 8\pi G$ is a constant and I is a function of b_1, b_2, b_3 and its firsts derivatives. Thus, I represents the anisotropy of space.

If $T_1^1 + T_2^2 + T_3^3 - T_4^4$ is negative—which was assumed to hold for all physically reasonable spacetimes⁶—then \ddot{R} is negative. Therefore, if \dot{R} is negative, then R will be zero at some time and the spacetime volume will vanish. Furthermore, the equation above indicates that *anisotropy, beyond not preventing the collapse, could actually enhance it*.

existing conception of the universe (immutable and eternal)—to obtain this static universe compatibility, he introduced the cosmological constant Λ . But then, De Sitter obtained a solution for the adapted equation—with Λ —by setting $T_{\mu\nu} = 0$. Einstein was not fond of that because General Relativity was suppose to establish the relation between matter and gravity, so a curved vacuum solution was not reasonable.

⁴Lemaître also calculated a rate of expansion of $\sim 600 \text{ km/s/Mpc}$, which Hubble calculated to $\sim 500 \text{ km/s/Mpc}$ with some new data two years later and which nowadays is said to be $\sim 70 \text{ km/s/Mpc}$. With this new data, Hubble was able to confirm the linear relation that is now known as “Hubble law”.

⁵The use of the word “widely” in this sentence is justified by the fact that even Einstein proposed, in 1931, a model for an expanding universe—known nowadays as “Einstein-Friedman model”. This also justifies the use of the word “controversial” at the end, because this model corresponds to an universe that does not collapses to a singularity—it restarts expanding. A nice historical reference for Einstein's reactions to the dynamical models is [86].

⁶This holds if we consider the strong energy condition for the perfect fluid universe, for example.

An interesting feature of this argument is that Lemaître did not use a matter model; he assumed a condition on $T_{\mu\nu}$ and for this, the result above could be called a primordial Singularity Theorem.

The basis, however, of all Singularity Theorems was Raychaudhuri's work in 1955. He—like Lemaître—argued that anisotropy could not keep spacetime from collapsing, but Raychaudhuri's proof was highly geometrical and for this, Raychaudhuri's result is often considered the first Singularity Theorem. His major contribution was to notice the importance of a geometrical identity known today as *Raychaudhuri equation*, which is a crucial part of the mathematical formalism of Singularity Theorems.

Consider a congruence of timelike geodesics and let V^μ be the tangent vector field of this congruence with $V^\mu V_\mu = -1$. The gradient of V^μ can be split into three quantities: a symmetric traceless part, an antisymmetric part and the trace part. The symmetric traceless part is called the *shear* $\sigma_{\mu\nu} := \nabla_{(\mu} V_{\nu)} - \frac{1}{3}\theta h_{\mu\nu}$, where $h_{\mu\nu} := g_{\mu\nu} + V_\mu V_\nu$ is the metric of the space orthogonal to V^μ ; the antisymmetric part is the *vorticity* $\omega_{\mu\nu} := \nabla_{[\mu} V_{\nu]}$ and the trace is the *expansion* (also called *divergence*) $\theta := \nabla_\mu V^\mu$. Raychaudhuri equation characterize the flow of this congruence:

$$\dot{\theta} = -\frac{1}{3}\theta^2 - \sigma_{\mu\nu}\sigma^{\mu\nu} + \omega_{\mu\nu}\omega^{\mu\nu} - R_{\mu\nu}V^\mu V^\nu. \quad (1.1.1)$$

If $\dot{\theta} \leq 0$, we have *geodesic focusing*. The equation above tell us that the shear acts in favor of the focusing, while rotation acts against it⁷. Focusing by itself, however, does not generally lead to a singularity.

What Raychaudhuri equation represents is a way of obtaining information about the movement of a certain configuration of free particles without solving the Einstein equations. If we represent the trajectories of these free particles with the geometrical object V^μ , then their movement is always characterized by the geometrical identity (1.1.1)—the term $R_{\mu\nu}V^\mu V^\nu$ is the one that contain particular information of the spacetime on which these particles are. In this picture, “geodesic focusing” is intuitively equivalent to “gravity is attractive”. We can think of a dust model for the universe with this intuitive interpretation and expect to obtain information about a possible spacetime collapse.

Raychaudhuri considered the case of an irrotational dust, so: $\omega_{\mu\nu} = 0$. Moreover, $R_{\mu\nu}V^\mu V^\nu \geq 0$ —known as *convergence condition*—is trivially satisfied for the dust model, since $T_{00} \geq 0$. Then, Raychaudhuri equation implies:

$$\dot{\theta} + \frac{1}{3}\theta^2 \leq 0.$$

For a synchronous coordinate system for the dust flow⁸:

$$\theta = \frac{\partial}{\partial t} \ln \sqrt{-g},$$

thus $\theta \rightarrow -\infty$ implies $g \rightarrow 0$.

⁷This is expected by an analogy with centrifugal forces. Moreover, Gödel showed that rotation could prevent singularity formation in the sense that he found a singularity-free exact solution by considering a rotating universe [65].

⁸This is nicely explained in [66, Pg281]

After Raychaudhuri's publication⁹, physicists undertook clarifying the following question: how does $g \rightarrow 0$ connect with a singularity in spacetime? A flat spacetime (which is naturally non-singular) can have focal points or caustics of geodesic congruences. In the early 60s, the notion of a spacetime singularity was definitely not clear, the definition of singularity came only after Penrose and Hawking Theorems, with a backwards analysis.

Penrose's theorem from 1965 is considered the Singularity Theorem of greatest impact in General Relativity; it was the first singularity result that did not rely on any symmetry hypothesis. Penrose introduced the concept of *closed trapped surfaces*—which was crucial for many of the subsequent results on Singularity Theorems and on other subjects—a nice reference for understanding the impact of this concept and this theorem is [107].

Theorem 1.1. [72, Pg261,Thm1](Penrose Singularity Theorem) *If the spacetime M contains a non-compact Cauchy surface \mathcal{S} and a closed future-trapped surface \mathcal{T} , and if the convergence condition holds for null V^μ , then there are future incomplete null geodesics.*

The idea of the proof is: if M is null geodesically complete, then the boundary of the future of \mathcal{T} is compact and this is inconsistent with \mathcal{S} being non-compact. Implicitly, Penrose introduced the notion of geodesic incompleteness as defining a singularity¹⁰:

The existence of a singularity can never be inferred (...) without an assumption such as completeness of the manifold under consideration[88, Pg58,Col2].

Since the 60's, geodesic incompleteness of the spacetime has been taken as signaling a singularity—the definition follows.

Definition. A spacetime is singular if it is not geodesically complete, *i.e.* if the geodesics cannot be extended to arbitrarily large parameter values.

By using Penrose Theorem, Hawking finally settled the symmetry hypothesis question on the cosmological singularity. A few months after Penrose's publication, Hawking proved that any expanding universe close to the homogeneous and isotropic model have a closed trapped surface [71]. The existence of a trapped surface does not rely on coordinate systems or symmetry assumptions; it is defined by an inequality—thus, it is stable under small perturbations. In the subsequent years, Hawking published several results on Singularity Theorems. In 1970, he and Penrose published a general version that compactified all their previous work [72, Pg266,Thm2]. The following theorem is one of Hawking Singularity Theorems, analogous to [72, Pg272,Thm4] in the cosmological context.

Theorem 1.2. [66, Thm8.9](Hawking Singularity Theorem) *Consider a spacetime with a matter model such that*

$$T_{\mu\nu}u^\mu u^\nu - \frac{1}{2}g^{\mu\nu}T_{\mu\nu} \geq 0 \text{ for all timelike unit } u^\mu,$$

⁹and Komar's publication in 1956, who had obtained—apparently independently of Raychaudhuri—similar results.

¹⁰Another curiosity for a not-in-a-hurry reader: physicists first assumed that Penrose's singularity implied divergence of density or something like that, but, in fact, it did not! Then Hawking and Ellis published a theorem analogous to Penrose, for a homogeneous model generalizing Shepley's result for perfect fluid. It continued unclear what was indeed being demonstrated in these singularity theorems. Then Geroch published his dialog and the conclusion was “ok, we will continue in this unclear state.”

and suppose that the expansion satisfies $\theta \leq \theta_0 < 0$ on a Cauchy hypersurface. Then the spacetime is singular. If we consider $\theta \geq \theta_0 > 0$, we get a singularity to the past of S —“The Big Bang”.

The above condition on $T_{\mu\nu}$ is called *strong energy condition*, which is one of the classical energy conditions we will discuss in the establishment of the Pattern Singularity Theorem. For now, let’s just take it as a *convergence condition* that allows us to use Raychaudhuri equation.

Proof. This is a one-paragraph sketch of the proof, to illustrate.

Let spacetime be a 4-dimensional globally hyperbolic Lorentzian manifold denoted by (M, g) and let it be *singular* if it is not geodesically complete. Let S be a Cauchy hypersurface in M and let p be a point in S for which the expansion (divergence of a congruence) is a negative constant θ_0 . If (M, g) satisfies the strong energy condition, geometrically we have for the Ricci tensor: $Ric(V, V) \geq 0$, for any smooth vector field V over M . The condition on the Ricci tensor impose a condition on the expansion of synchronized observers; we can then prove, using Raychaudhuri’s equation, that a timelike geodesic c_p passing through p and orthogonal to S contains a conjugate point to S not far from S , at a distance of at most $-\frac{\theta_0}{3}$ to the future. Therefore, we know that c_p does not maximize length between S and a point q further from the conjugate point. This contradicts the fact that we should have a maximizing timelike geodesic orthogonal to S . Which lead us to conclude that no future-directed timelike geodesic orthogonal to S can be extended further from that conjugate point. $\therefore (M, g)$ is singular. \square

The results shown here are to illustrate the debate on singularities in General Relativity and to show the power of the Singularity Theorems. By 1973, all ingredients of a Singularity Theorem had been clarified; a remarkable review on the status of the art at that time is [72]. Singularity Theorems can be generalized by the following:

Theorem 1.3. [106, Pg796](Pattern Singularity Theorem) *If a spacetime, obeying Einstein equations, satisfies:*

- i) *an Initial/Boundary Condition;*
- ii) *an Energy Condition;*
- iii) *a Global Causal Condition;*

then, it is singular.

Let’s understand the ingredients of this Pattern Singularity Theorem.

i) An Initial/Boundary Condition

An initial/boundary condition is necessary to ensure that geodesics start focusing. In the more physical point of view, it characterizes what kind of situation is being considered. Some examples of possible condition i):

1. The entire universe is strictly expanding at the moment, *i.e.* the expansion of the geodesics orthogonal to a hypersurface is positive—this suits the cosmological model, as we saw in Raychaudhuri’s and Hawking’s results¹¹;
2. There exists a closed trapped surface and a non-compact Cauchy surface—this suits the collapsing of a star, as used by Penrose;
3. The universe is spatially finite—this suits a closed universe.

The idea of an initial/boundary condition is to give a set that is or will become a closed trapped surface; example 1 is actually saying that the universe had a closed trapped surface in the past. If the set does not become trapped, then there is incompleteness. If the set does become trapped and if the future Cauchy development of the initial set is not the entire future, then the boundary of the domain is non-compact and there is incompleteness too. Let’s see the definition of a closed trapped surface, as given by Wald in [99, Pg239].

Definition 1.4. (Closed trapped surface) A closed trapped surface \mathcal{T} is a compact, smooth, spacelike, two-dimensional surface such that the expansion θ of both sets (*i.e.* “ingoing” and “outgoing”) of future directed null geodesics orthogonal to \mathcal{T} is everywhere negative.

Note that an open trapped surface is not an useful concept: any point in Minkowski spacetime lies in an open trapped surface. Also, the compactness in the definition above is crucial, since, intuitively, something trapped at infinity does not make sense.

ii) An Energy Condition

In the first half of the 19th century, energy conditions were used indiscriminately—just as physically reasonable conditions. After Raychaudhuri’s work, energy conditions leveled up to convergence conditions. By 1973, energy conditions were given names and became one of the ingredients of Singularity Theorems.

Some condition on the energy-momentum tensor is needed since every smooth Lorentzian manifold satisfies the Einstein equations for some energy-momentum tensor. The energy conditions are not derived from any physical theory¹², they impose where and for whom “energy is positive”. By the Einstein equations we can consider the energy conditions as geometric conditions and, as we saw before, together with Raychaudhuri’s equation they constrain the geodesics expansion and enforce them to focus.

The *classical energy conditions*—extensively used in the last century—are characterized for being conditions given at points of the spacetime. A singularity theorem that has a classical energy condition as condition **i**) is called a Classical Singularity Theorem. Let’s take a look at these conditions.

The simplest energy condition is the **weak energy condition**(WEC). It is a natural condition within classical physics and states that the local energy density is non-negative in

¹¹One could wonder how reasonable it is to impose an initial or boundary condition on the entire universe; yet, this is a personal question that will not be addressed here. My answer is implicit in this dissertation.

¹²We will see that this is not the nature of quantum inequalities—these are derived within QFT, since within QFT we choose $T_{\mu\nu}$.

every observer's rest frame, *i.e.* "All observers see non-negative energy" $\Rightarrow T_{00} \geq 0$. It holds in any frame if it holds in one frame for any configuration, so:

$$T_{\mu\nu}u^\mu u^\nu \geq 0 \quad \text{for all timelike } u^\mu. \quad (1.1.2)$$

The weakest energy condition is the **null energy condition**(NEC), which, in spite of not having the same intuitive interpretation as the WEC, is obtainable up to a normalization by taking the light-like limit from the above:

$$T_{\mu\nu}k^\mu k^\nu \geq 0 \quad \text{for all null } k^\mu. \quad (1.1.3)$$

A stronger one is the **dominant energy condition**(DEC), which we can interpret as "All observers see a causal flux of energy-momentum":

$$T_{\mu\nu}u^\mu v^\nu \geq 0 \quad \text{for all future-pointing timelike } u^\mu \text{ and } v^\nu. \quad (1.1.4)$$

The **strong energy condition**(SEC) implies that the sum of the local energy density and the local pressures is non-negative. It has a misleading name since it neither implies WEC nor NEC and states that:

$$T_{\mu\nu}u^\mu u^\nu - \frac{1}{2}g^{\mu\nu}T_{\mu\nu} \geq 0 \quad \text{for all timelike unit } u^\mu. \quad (1.1.5)$$

For a perfect fluid universe—as the FLRW spacetime—we have the following diagram:

$$\begin{array}{ccc} DEC & \Rightarrow & WEC \\ & \downarrow & \\ NEC & \Leftarrow & SEC \end{array}$$

A good review on Energy Conditions is [24] and on their Cosmological Implications, [113].

iii) A global causal condition

A causality condition is needed to forbid backwards time travel and to guarantee the existence of maximal geodesics. Gödel's pathological model of a rotating and complete universe with closed timelike curves made the former necessary. If condition iii) is the existence of a Cauchy surface S , then one can prove that between any two points of the the Cauchy development of S , which is globally hyperbolic, there is a geodesic with maximizing proper time. Maximal geodesics cannot have focal points and this guarantees the contradiction between conditions i) and iii).

A spacetime contains a Cauchy surface if and only if it is globally hyperbolic; equivalently¹³, if and only if the causality condition holds and that the intersection of the causal past of a point with the causal future of another point is always compact. Intuitively, we are trying to say that there are no naked singularities in spacetime—the global hyperbolicity hypothesis is also known as the strong cosmic censorship conjecture (or in words not so used anymore "a strong form of the principle of determinism" [84, Pg118]).

¹³These definitions and equivalences are discussed in appendix B, Theorem B.18.

Proof. (symbolic proof for the symbolic Theorem 1.3)

Condition **i**) starts the focusing of geodesics, condition **ii**) ensures the focusing continues to a focal point. Condition **iii**) forbids focal points, then there is geodesic incompleteness. \square

To find a stronger version of a singularity theorem, one must weaken some hypothesis. The initial/boundary condition is essential, but just for the beginning of the focusing of geodesics; the global causal condition is less restrictive than the others, physically intuitive and mathematically convenient. Therefore, to weaken the energy condition sounds a good idea. Furthermore, it is known that, within quantum physics, energy can assume negative values in a sense to be made precise. This is a well-founded way to justify the analysis and the weakening of the energy condition.

Before discussing negative energy in the next section, let's pause for a quote that illustrates the impact of Singularity Theorems:

“The situation has changed since the discovery of Penrose (and later by Hawking and Geroch), of new theorems which reveal a connection between the existence of a singularity (of unknown type) and some very general properties of the equations, which bear no relation to the choice of reference system.”[78, Pg78]

1.2 Negative Energy within Quantum Field Theory

Where we are convinced we need to consider negative energies if we take Quantum Field Theory into account—but not too negative, and not for too long...

General Relativity alone cannot describe nature for lengths smaller than the Planck scale, so what if we try to see Classical Singularity Theorems under the light of Quantum Physics?¹⁴ It is well-known that all classical energy conditions are violated within Quantum Field Theory: Quantum Physics says negative energy exist, at least for some time. First, we convince ourselves that negative energy must be taken into account. In section 1.2.1, we review a clear proof of the existence of negative energy within Local Quantum Field Theory given by Epstein, Glaser and Jaffe [31] in 1965; and in section 1.2.2, we discuss the most notorious example of a classical energy condition violation—the Casimir effect [22]—which has strong experimental support [80]. Then, in section 1.2.3, we understand the transition of abandoning the classical energy conditions and searching for a quantum energy inequality.

1.2.1 A simple formal proof within Local Quantum Field Theory

Where we see a simple and clear proof of the existence of negative energy in the context of Local Quantum Field Theory.

In 1964, Wightman and Streater published the book “PCT, Spin and Statistics and all that” [111] on which they gathered concisely the known results of Local Quantum Field Theory. In the same year, Wightman showed, in [118], that fields cannot be defined at points

¹⁴A nice reference on quantum loopholes in Singularity Theorems is [50].

of spacetime. He proved that in every local quantum field theory with a vacuum there exists a point associated with a trivial algebra of observables. Henceforth, Wightman justified the characterization of fields as *distributions*. What is called *Wightman fields* are operator valued generalized functions over (usually) the Schwartz space \mathcal{S} or the space of smooth compactly supported functions \mathcal{D} . The framework of both [111, 118] is known nowadays as *Wightman Axioms* and has several similar versions.

In this context of Local Quantum Field Theory, in 1965, Epstein, Glaser and Jaffe [31] gave a simple and clear proof of the existence of negative energy density. In this section, we review how this was done. We take a look at the framework, some definitions, a theorem and two lemmas to prove the main result; although this take a few pages to do it carefully, it is important to justify the search of a quantum inequality that is studied in this dissertation.

Framework: Wightman Axioms, as stated in [31]

Axiom 1: $\exists \mathcal{H}$ a Hilbert space with a dense subspace D_0 . Pure states are unitary rays in \mathcal{H} ;

Axiom 2: \exists a continuous unitary representation $U(a, 1)$ of the group of translations in $\mathcal{L}(\mathcal{H})$, with $U(a, 1)D_0 \subset D_0$;

Axiom 3: P^μ is defined by $U(a, 1) = \exp(iP^\mu a_\mu)$ and satisfies a *stability condition*—also called *spectrum condition*: its spectrum must be in the future cone¹⁵ $\overline{V^+}$. In particular, P^0 is positive; yet, we will see that even so, T^{00} is not positive—not even if smeared with a positive function;

Axiom 4: \exists one or several local fields $\varphi_1, \dots, \varphi_N$. The definition of a *local field* follows.

Definition 1.5. (local field) A local field $\varphi(x)$ is an operator-valued distribution such that $\forall f \in \mathcal{D}$

$$\varphi(f) = \int \varphi(x)f(x)dx \quad \text{is defined on } D_0 \text{ and } \varphi(f)D_0 \subset D_0;$$

Axiom 5: For a local field φ : $U(a, 1)\varphi(x)U(a, 1)^{-1} = \varphi(x+a)$ and

$$[\varphi(x), \varphi_j(y)] = [\varphi(x), \varphi(y)] = 0 \text{ for } (x-y)^2 < 0 \text{ and } j \in \{1, \dots, N\};$$

Axiom 6: $\exists!$ (up to a phase) $\Psi_0 \in D_0$, called *vacuum*, such that $U(a, 1)\Psi_0 = \Psi_0$.

Remark 1.6. The condition $\varphi(f)D_0 \subset D_0$ does not have an intuitive physical motivation; is *ad hoc*, but allows us to define and work with the objects we need in a simple manner—in particular, construct polynomials of smeared field operators.

Definition 1.7. (Local quantum field theory) A theory that satisfies the Wightman axioms above will be called here¹⁶ a *local quantum field theory*. Note that this version is for Minkowski spacetime, a framework generalization to curved spacetimes was done in 1978 by Isham [75].

¹⁵i.e. the support of the spectral measure $dE(p)$ of $U(a, 1) = \int e^{ipa}dE(p)$ consists of points p of spacetime such that $p^2 > 0$ and $(p^0)^2 > 0$; a nice reference for irreducible unitarily representations of the Poincaré group is [108, Sec. 9.4]

¹⁶In section 1.3, we comment on the use of the term “Local Quantum Field Theory” in the broad sense

A local quantum field theory gives us a collection of possible measurements; the expectation value of the observable φ smeared with a test function f at the state $\Psi \in \mathcal{H}$ is represented by objects like $\langle \Psi, \varphi(f)\Psi \rangle$. A compactly supported test function assimilates the conception that a measurement is always performed by a finite extension apparatus during a finite time. To each open set \mathcal{O} of spacetime there is an associated local algebra of observables, say $\mathcal{A}(\mathcal{O})$, that is generated by the local fields $\varphi_1, \dots, \varphi_N$ smeared with test functions such that $\text{supp } f \subset \mathcal{O}$.

Going to the von Neumann algebras context, it is well-known that if a vector Ω is cyclic for an algebra, say \mathcal{M} , then Ω is separating for the commutant algebra \mathcal{M}' . For the local algebras associated with spacetime open sets, the ones which we are considering, we have a similar result: a cyclic vector for $\mathcal{A}(\mathcal{O})$ is separating for each local field on \mathcal{O} . Let's see what is a cyclic vector, a separating vector and the statement of the result.

Definition 1.8. (Ω cyclic for $\mathcal{A}(\mathcal{O})$) A vector $\Omega \in \mathcal{H}$ is said to be cyclic for the local algebra $\mathcal{A}(\mathcal{O})$ if

$$\overline{\mathcal{A}(\mathcal{O})\Omega} = \mathcal{H}.$$

Note that the above is the usual definition in the von Neumann algebras context.

Definition 1.9. (Ω separating for $\varphi(x)$) A vector $\Omega \in \mathcal{H}$ is said to be separating for a local field $\varphi(x)$ if for any test function f :

$$\varphi(f)\Omega = 0 \Rightarrow \varphi(f) = 0.$$

The following theorem is the well-known result [111, Thm4-3,Pg139]. Recall that, if \mathcal{O} is a region of spacetime, its causal complement \mathcal{O}' is the set of points of spacetime that are spacelike separated from points in \mathcal{O} .

Theorem 1.10. (Cyclic \Rightarrow separating) *Let Ω be a cyclic vector for $\mathcal{A}(\mathcal{O})$, where \mathcal{O} is an open set of spacetime such that \mathcal{O}' is not empty and $T \in \mathcal{A}(\mathcal{O})$, then*

$$T\Omega = 0 \Rightarrow T = 0.$$

Proof. The proof is really simple. Take $\Psi = P'\Omega$ for some $P' \in \mathcal{A}(\mathcal{O}')$ and $\Phi \in D_0$, since $\langle \Psi, T^*\Phi \rangle = \langle T\Psi, \Phi \rangle = \langle TP'\Omega, \Phi \rangle = 0$ and $\overline{\mathcal{A}(\mathcal{O})\Psi} = \overline{\mathcal{A}(\mathcal{O}')\Psi} = \mathcal{H}$, then $T\Psi = 0$. Since vectors like $P'\Omega$ span \mathcal{H} , we have that $T = 0$. \square

It is important to consider cyclic vectors for two reasons. One is that we would like to do Quantum Physics in terms of vacuum expectation values—which does need a cyclic vacuum. The other reason is that the Reeh-Schlieder Theorem tells us that if a vector is cyclic for the algebra $\mathcal{A}(M)$, for the whole Minkowski spacetime M , then it is cyclic for $\mathcal{A}(\mathcal{O})$, for each open set $\mathcal{O} \subset M$. With this in mind, we can translate the theorem above to our context by the statement:

If the vacuum Ψ_0 is cyclic for the algebra generated by the local fields $\varphi_1, \dots, \varphi_N$, then Ψ_0 is separating for every local field φ .

By now, we have a local quantum field theory, we have states, an algebra of observables and a vacuum. We are ready to define an energy-momentum tensor.

Definition 1.11. (Energy-momentum tensor) $T^{\mu\nu}(x)$ is an energy-momentum tensor for a local quantum field theory if it is a local field such that:

- i) $\frac{\partial}{\partial x^\mu} T^{\mu\nu}(x) = 0$.
- ii) $\int_\sigma T^{\mu\nu}(x) d\sigma_\mu(x) = P^\nu \forall$ spacelike plane σ ;
- ii') $(\Psi_0, T^{\mu\nu}(x) \Psi_0) = 0$.

Property ii) implies ii'), since:

$$\lim_{f \rightarrow 1} \int_{x^0=t} (\Psi_0, T^{0\nu}(x) \Psi_0) f(x) d^3x = (\Psi_0, P^\nu \Psi_0) = 0$$

for $0 \leq f \leq 1$, $f \in \mathcal{D}(\mathbb{R}^3)$ tends to 1 in $\mathcal{C}(\mathbb{R}^3)$. Since it holds in any coordinate system, $(\Psi_0, T^{\mu\nu}(x) \Psi_0) = a^{\mu\nu}$ is independent of x and $a^{\mu\nu} = 0$.

In which sense does this definition of $T^{\mu\nu}(x)$ can be interpreted as an energy-momentum tensor? We do not have an operator associated to the amount of energy and momentum in a volume V of spacetime

$$P(V) = \int_V T^{0\nu}(t, \vec{x}) d\vec{x},$$

so we must focus on the object $T^{\mu\nu}(f)$. Classical physics would say $\int T^{00}(x) f(x) \geq 0$ and a quantum analogue would be $(\Phi, T^{00}(f) \Phi) \geq 0$, but this does not hold, not even for a positive test function f , due to the following result [31, Thm1]:

Theorem 1.12. (Incompatibility) *Let $T(x)$ be a local field and f a positive test function in \mathcal{D} such that $(\Phi, T(f) \Phi) \geq 0 \forall \Phi \in D_0$. Suppose there exists a vector $\Omega \in D_0$ and an integer m such that $(\Omega, T(f)^m \Omega) = 0$. If Ω and Ψ_0 are separating for T , then $T = 0$.*

For the proof, we will need the following two lemmas 1.13 and 1.14, which correspond, respectively, to [31, Lem1] and [31, Lem2].

Lemma 1.13. Let A be an operator with a dense domain D_A such that for all $\Phi \in D_A$: $(\Phi, A\Phi) \geq 0$. Let $\Omega \neq 0$ be a vector such that $A^n \Omega \in D_A, n \in \mathbb{N}$. Assume $(\Omega, A^m \Omega) = 0$ for some natural m . Then $A\Omega = 0$.

Proof. Consider the case of an odd exponent $(\Omega, A^{2r+1} \Omega) = 0$, for some $r \in \mathbb{N}$. $\forall \Phi, \Psi \in D_A$, by the Cauchy-Schwartz inequality:

$$|(\Phi, A\Psi)|^2 = |(A^{1/2}\Phi, A^{1/2}\Psi)|^2 \leq (A^{1/2}\Phi, A^{1/2}\Phi)(A^{1/2}\Psi, A^{1/2}\Psi) = (\Phi, A\Phi)(\Psi, A\Psi);$$

thus $(\Psi, A\Psi) = 0 \Rightarrow (\Phi, A\Psi) = 0 \forall \Phi \in D_A \Rightarrow A\Psi = 0$. For the even case exponent, we have that if $(\Omega, A^{2q} \Omega) = 0$ for some natural q , then $\|A^q \Omega\|^2 = 0$, thus $A^q \Omega = 0$.

If $(\Omega, A^m \Omega) = 0$ for some natural m , we can apply the odd and even cases repeatedly until we obtain $A\Omega = 0$. \square

Lemma 1.14. Let T be a local field and f a positive test function in \mathcal{D} , not identically zero. If $T(f)\Psi_0 = 0$, then $T(x)\Psi_0 = 0$, i.e. $T(g)\Psi_0 = 0 \forall g \in \mathcal{D}$.

Proof. Let $T(f) = 0$ and suppose $T(x)\Psi_0 \not\equiv 0$. Since

$$\begin{aligned} (\Psi_0, T(x+a)T(y+a)\Psi_0) &= (\Psi_0, U(a,1)T(x)U(a,1)^{-1}U(a,1)T(y)U(a,1)^{-1}\Psi_0) \\ &= (U(a,1)^{-1}\Psi_0, T(x)T(y)U(a,1)^{-1}\Psi_0) \\ &= (\Psi_0, T(x)T(y)\Psi_0), \end{aligned}$$

we can define the distribution $F(x-y) \equiv F(x-y, 0) \equiv F(x, y) := (\Psi_0, T(x)T(y)\Psi_0)$. Then

$$T(x)\Psi_0 \not\equiv 0 \Rightarrow F(x) \not\equiv 0.$$

Moreover, since

$$\begin{aligned} F(x) &= (\Psi_0, T(x)T(0)\Psi_0) = (\Psi_0, U(x,1)T(0)U(x,1)^{-1}T(0)\Psi_0) \\ &= (T(0)U(x,1)^{-1}\Psi_0, U(x,1)^{-1}T(0)\Psi_0) \\ &= (T(0)\Psi_0, U(x,1)^{-1}T(0)\Psi_0) \\ &= (\Psi, U(x,1)^{-1}\Psi), \text{ for } \Psi := T(0)\Psi_0 \in D_0 \\ &= \int e^{-ipx}(\Psi, dE(p)\Psi) \geq 0 \text{ by the spectrum condition in Axiom 3,} \end{aligned} \tag{1.2.1}$$

then F is of positive type in Hörmander sense [74, Pg38], *i.e.* $F(g) = \int F(x)g(x)dx \geq 0$, for all positive $g \in \mathcal{D}$.

Consider the convolution between F and f , which is well-defined since $\text{supp } f$ is compact:

$$F * f(x) = \int F(x-y)f(y)dy = \int (\Psi_0, T(x)T(y)\Psi_0)f(y)dy;$$

$T(f) = \int T(y)f(y)dy = 0$ implies $F * f(x) = 0$. Taking the inverse Fourier transform, denoted by a tilde, we get:

$$\tilde{F}(p)\tilde{f}(p) = 0, \text{ where } \tilde{F}(p) = \int e^{ipx}F(x)dx.$$

Let's switch the representation of $\tilde{F}(p)$ from the configuration space to energy-momentum space. Since F is a positive type distribution in Hörmander sense, then F is a positive measure [74, Thm2.1.7]; thus \tilde{F} is also of positive type in the Hörmander sense. Moreover, F and \tilde{F} are also of positive type in the Reed and Simon sense [96, Pg14], *i.e.* let $\hat{f}(x) = f(-x)$, $\forall f \in \mathcal{D}$:

$$\begin{aligned} F(\hat{f} * f)(p) &= \int F(y)(\hat{f} * f)(y)dy = \int F(y)\hat{f}(y-x)f(x)dxdy = \int F(y)f(x-y)f(x)dxdy \\ &= \int F(y)f(x-y)f(x)dxdy = \int F(x-y)f(y)f(x)dxdy \\ &= \int (\Psi_0, T(x)T(y)\Psi_0)f(x)f(y)dxdy \\ &= (\Psi_0, T(f)T(f)\Psi_0) \\ &= \|T(f)\Psi_0\|^2 \\ &\geq 0. \end{aligned}$$

It is clear that the above implies that \tilde{F} is also of positive type in the Reed and Simon sense. This means we can apply Bochner-Schwartz Theorem [96, ThmIX.10], thus \tilde{F} is the Fourier transform of a positive finite measure μ :

$$\tilde{F}(p) = \int e^{-ipx} d\mu(p). \quad (1.2.2)$$

Equation (1.2.1) implies that $\text{supp}\mu \in \overline{V^+}$. As done in [118, Pg416], from equation (1.2.2) with a quick detour through two holomorphic functions and invoking Bogoliubov-Vladimirov Theorem, we get:

$$\tilde{F}(0) = \int d\mu(p) = \int \mathcal{P}(-ip) d\lambda(p);$$

where $\mathcal{P}(-ip)$ is a polynomial in $(-ip)$ and λ is a Lorentz invariant measure with support in $\overline{V^+}$. Therefore, the support of \tilde{F} , which is Lorentz invariant and is in $\overline{V^+}$, is a union of upper sheets of hyperboloids $p^2 = m^2$. Furthermore, $\text{supp}\tilde{F}$ must be in the set of zeros of \tilde{f} , since $\tilde{F}(p)\tilde{f}(p) = 0$. By hypothesis, $f \geq 0$, $f \in \mathcal{D}$ and $f \not\equiv 0$, thus we have for $\tilde{f} \in \mathcal{S}$ that:

\tilde{f} cannot vanish at zero or in the entire future cone,

$$\text{since both would imply } \tilde{f}(0) = \int f(x) d(x) = 0 \Rightarrow f(x) \equiv 0.$$

Since, for *some* $m > 0$, \tilde{F} is not zero on the upper sheet of the hyperboloid $p^2 = m^2$, $\tilde{f}(p)$ must vanish there, *i.e.* for some $m > 0$:

$$\tilde{f}(p)\delta(p^2 - m^2)\Theta(p_0) = 0 \Rightarrow \frac{1}{i} \int \Delta^+(x-y)f(y)dy = \Delta^+ * f(x) = 0,$$

where $\Delta^+(x-y)$ is the well-known retarded green solution. Finally, we can find a contradiction: for spacelike x , $\Delta^+(x)$ is positive; so we can take x large enough such that $f(x)$ is positive and obtain a positive value for $\Delta^+ * f(x)$, $\therefore T(x)\Psi_0 = 0$. \square

Proof. (of Theorem 1.13) Given the hypothesis of Theorem 1.12, Lemma 1.13 tell us that $T(f)\Omega = 0$. Then, if Ω is separating for the local fields, we have $T(f) = 0$. Which, if Ψ_0 is separating also, is equivalent to $T(f)\Psi_0 = 0$. Lemma 1.14 tells us that $T(f)\Psi_0 = 0 \Rightarrow T(x)\Psi_0 = 0$; thus we have $T(g)\Psi_0 = 0$ for all test functions g , therefore $T = 0$. \square

A local quantum field theory with an energy-momentum tensor and a cyclic vacuum trivially satisfies the hypothesis of the theorem. The following is a simplified statement of the main result:

Theorem 1.15. (simplified version of 1.12) *Let $T^{\mu\nu}(x)$ be an energy-momentum tensor for a local quantum field theory and $f \in \mathcal{D}$ a positive function such that $(\Phi, T^{\mu\nu}(f)\Phi) \geq 0$ for all $\Phi \in D$. If Ψ_0 is separating for $T^{\mu\nu}$, then $T^{\mu\nu} \equiv 0$ for all μ and ν .*

That is, a positive energy density is incompatible with a local quantum field theory.

1.2.2 An experimentally supported example: the Casimir Effect

Where we see an experimentally supported example of a classical energy condition violation within the usual approach of Quantum Field Theory.

The Casimir effect is the most notorious among the examples of classical energy conditions violations. In the last section, we learned that positivity of the energy-momentum tensor is inconsistent with Local Quantum Field Theory and we proved it mathematically. In this section, we study the Casimir effect for three reasons. First, the Casimir effect has strong experimental support, so those who were not convinced by the mathematical proof of the last section will feel more comfortable in accepting we must consider negative energy if we take Quantum Field Theory into account. Second, we do the calculations in the usual approach of Quantum Field Theory, so this section is somewhat more accessible than the previous one. Third, there are those who argue that negative energy is just a technicality and that not even the Casimir effect leads us to consider it—we must, and we do, discuss this.

We start with a general discussion on the the Casimir effect; on which we establish how we interpret its measurement, its connection to the Van der Waals interaction and what does it say about the vacuum energy. Then we compute, within the usual approach of Quantum Field Theory, the energy density for the free neutral massless scalar field and we obtain a negative value. Finally, we see an intuitive argument that shows that we cannot remove this negativeness by rescalement, *i.e.* negative energy is seemingly intrinsic of Quantum Field Theory.

A general discussion on the Casimir effect

Casimir predicted, in 1948, that two neutral conducting plates in vacuum would attract each other. That was not the startling character of his work actually, people had known about Van der Waals interaction for at least 38 years, since Van der Waals was given the Nobel prize in 1910 for his work on that. The remarkable feature is that Casimir justified the attraction between the plates using the concept of zero-point energy, *i.e.* the idea of vacuum quantum fluctuations¹⁷. The original work of Casimir [22] together with the experimental verification in 1997¹⁸ [80] marked the debate on the vacuum concept—in appendix C, one can find a brief overview of the evolution of the *vacuum* concept, from Democritus to Casimir. A nice approachable—for Portuguese-readers—reference for a general understating of the effect is [23].

The measurement of the Casimir effect is generally¹⁹ taken as a verification of the vacuum fluctuations, as an evidence of the non-null zero-point energy. One can argue that there are other ways to explain the attraction of the plates and there have been attempts on doing that, but either the concept of vacuum expectation values is implicitly there (like Milton's

¹⁷Zero-point energy refers to the energy of the ground state and *vacuum fluctuations* are associated to Heisenberg's uncertainty principle and to justify the fact that the zero-point energy is not zero; they are indeed different concepts, but since they are fundamentally connected, we use them as synonyms here.

¹⁸It was measured for the first time at the Phyllips laboratory (where Casimir worked) by Sparnaay, in 1958, yet inconclusively [110].

¹⁹“generally” here is an anecdotal evidence based on the correspondences: always \equiv 100%, usually \equiv 90%, normally/generally \equiv 80%, ..., never \equiv 0%.

approach using Green functions in 1976, as he said in [67]) or it is done in a formalism that is not so general. For example, more recently R. Jaffe showed that the Casimir effect can be calculated in the S-matrix formalism, using diagrams with external legs with no reference to vacuum fluctuations [76, SecI]; however an interesting calculation, we cannot yet describe Quantum Field Theory completely avoiding vacuum expectation values and this formalism cannot be naturally generalized to curved spacetimes²⁰.

One could also say that the attraction is due to the long range dispersive Van der Waals interaction between the plates, but this is not necessarily an *alternative* explanation. Since two neutral plates would not classically attract each other, the Van der Waals interaction is also considered a quantum effect: the net attraction is taken to be due to the polarization fluctuations of the plates and as the computations must take under consideration a finite light velocity, *i.e.* a retarded interaction, we can take the Van der Waals interaction as being in the framework of Quantum Mechanics and Special Relativity—which constitute the framework of Quantum Field Theory. Thus, it is not so easy to separate theoretically the Casimir and Van der Waals interactions²¹. Accordingly, within Quantum Field Theory, we consider that the vacuum fluctuations intermediate the Van der Waals action-at-a-distance interaction and we take the measurement of the Casimir effect as an experimental verification of the vacuum fluctuations.

Let's take a look at the original argument of Casimir. Consider a cubic cavity of perfectly conducting neutral plates of sides L . Now put a perfectly conducting neutral square plate of side L inside the cavity and calculate the zero-point energy for when the plate is close to one side (situation 1), and for when it is far (but closer than $L/2$, situation 2) as illustrated below.

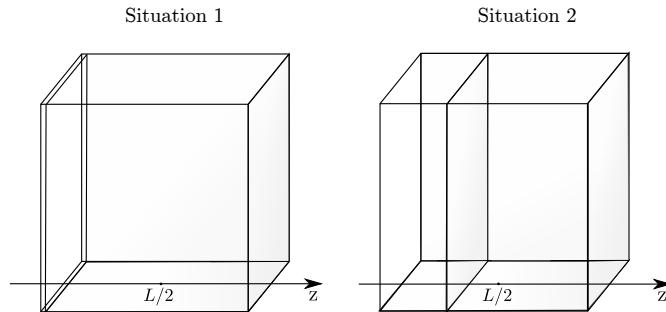


Figure 1.1: Cubic cavity of side L in the situations we compare: in 1, the plate is close to one side and in 2, the plate is at a greater distance $z < L/2$.

For the quantized electromagnetic field, the zero-point energy is given by the sum over all possible frequencies:

$$E_0 = \frac{1}{2} \sum_{\omega} \hbar \omega.$$

²⁰On the other hand, the Casimir effect has been formulated within Algebraic Quantum Field Theory using the functional formalism in Minkowski spacetime [27].

²¹Curiously, when asked (in 1972 and in 1983) “Is the Casimir effect due to the vacuum fluctuations of the electromagnetic field, or is it due to the Van der Waals forces between the molecules in the two media?”, Casimir answer began “I have not made up my mind.”; source: [67]

Since situation 1 and 2 have different configurations, they also have different possible frequencies, *i.e.* different modes of vibration for the vacuum²²; yet, they are both infinite. To compare these different infinities, Casimir introduced a cut-off function f off rapid decay such that:

$$f \rightarrow \begin{cases} 1, & \text{for large } \omega; \\ 0, & \text{for small } \omega. \end{cases}$$

It is a reasonable approximation since we expect the plate not to be an obstacle for the high frequency modes. By considering the energy difference of both situations $E_{0,1} - E_{0,2}$ as the interaction energy between the plate and the closest side of the cavity, Casimir derived and obtained an expression for an attractive force between them.

This is telling us that if we build a system in situation 2, the plate will move towards the closest side of the cavity; if the plate move, there is work and if there is work, there is energy. An interesting question to pose now is: where did that energy come from? Can we justify it by saying that the necessary energy came from the vacuum? To carefully answer, we need to examine what we have idealized in the previous argument. We disconsider every other interaction that is not due to the zero-point energy differences.

Consider the following Gedankenexperiment: imagine we build the perfectly conducting neutral cubic cavity and we create a perfect quantum vacuum inside with our perfect-vacuum pump—like situation 1 before. Now, imagine a plate popping²³ up at distance z from one face, so we have situation 2 from before. Can we do that without introducing energy into the system? Well, imagine that instead of making the plate pop up, it was initially overlapped with one side of the cavity. Then, to put the system in situation 2, we have to drag the overlapping plate to the z position. In order to separate the plate from the side, we must hold the side down: we just learned that they attract each other, so we cannot separate them without introducing energy into the system! We can associate the energy necessary to separate the plate and the side to the energy of the system of when it is in situation 2. When we separate the plate from the side, we are deforming the vacuum inside the cavity; thus, we can also associate the energy of separating them to the energy necessary to *impose that deformation on the vacuum*. Therefore, one can say that the energy the plates use to move is the energy of the vacuum deformation, but keeping in mind that to deform the vacuum we had to separate the plate from the side and with that, we had to spend the same amount of energy.

This Gedankenexperiment tells us that *we cannot steal energy from the vacuum*. If instead of building a system in situation 2 in a laboratory, we just found a system like that in nature; maybe we would be able to use vacuum energy. We can use the gravitational interaction to generate energy, because we know about natural phenomenons that give us systems in the corresponding “situation 2”. For example, the waterfalls we use in hydroelectrics; we do not have to drag the water up there to use the energy from when it falls, “nature puts” the

²²To see that these are in fact different modes let's do a simple computation. Consider only the z direction, then the frequencies are inversely proportional to the separation. For situation 1, $E_{0,1}$ is a sum on $\omega_1 \propto \frac{1}{L}$ and for situation 2, $E_{0,2}$ is a sum on the modes on the smaller region $\omega_2 \propto \frac{1}{z}$ and on the larger region $\omega_2 \propto \frac{1}{L-z}$. Then $E_{0,2} \propto (\frac{1}{z} + \frac{1}{L-z})LE_{0,1}$. Setting, for example, $z = L/4$, we get $E_{0,2} \propto \frac{16}{3}E_{0,1}$.

²³make the plate “pop up”, or *create* the plate, is not in a matterial sense of atoms and molecules; we are considering massless plates, they just represent the other equivalences: plates \equiv boundary conditions \equiv deform the vacuum.

water up there. Yet, so far, we have not seen a natural phenomenon that gives us “separated plates” such that we would be able to use the vacuum energy²⁴. Accordingly, and in analogy with the quark-confinement conception, we can say that the Casimir interaction seems to be of color white.

The plate in Casimir argument seen above represent a boundary condition. We can think of the Casimir effect as the first example of boundary conditions affecting the vacuum with observable effects; this idea is also present, in different levels, in Hawking radiation, quark-binding in Quantum Chromodynamics²⁵ and even, in the cosmological expansion. It is usual to refer as “Casimir effect” the extrapolations of the electromagnetic Casimir effect, seen above, to other fields or using different geometrical configurations²⁶.

In the next section we impose Dirichlet boundary conditions on the space \mathbb{R}^3 and we compute the vacuum expectation value of the energy density for the free neutral massless scalar field. It must be emphasized that the treatment of the next section is informal; for example, we do not consider smeared fields to gain technical simplification and the question of how to impose boundary conditions on distributions will not be addressed.

Vacuum energy for the free neutral massless scalar field

Consider the case of a free neutral massless scalar field ϕ satisfying the Klein-Gordon equation on Minkowski spacetime. With Casimir’s original work in mind, we compare the vacuum energy of when it is defined on the whole \mathbb{R}^3 space with when it is restrained to a region, say $\Omega := \{(x, y, z) \in \mathbb{R}^3 : 0 < z < L\} \subset \mathbb{R}^3$. To restrain the system is to impose boundary conditions, and we consider the so called Dirichlet boundary conditions such that:

$$\text{supp}\phi \in \Omega.$$

The computations are done here in the Fock representation formalism of usual Quantum Field Theory; a good reference for this subject is Schweber’s book [103], and with more mathematical details [59]—let’s quickly recall what it is.

Consider we have a quantum system of particles on Minkowski spacetime. We can write the wave functions ϕ —the solutions of the Klein-Gordon equation—of this system in the Fock space representation $(\mathcal{F}, a^\dagger, a, |0\rangle)$. By constructing the Hilbert space of states of a one-particle system $\mathcal{H}^{(1)}$, which we take it as the space of square-integrable functions \mathcal{L}^2 , we can construct the Hilbert space $\mathcal{H}^{(n)}$ of an n -particle system as the symmetrized (or anti-symmetrized) subspace of the n -tensor product $\mathcal{H}^{(n)} \subset \mathcal{H}^{(1)} \otimes \dots \otimes \mathcal{H}^{(1)} \equiv \mathcal{H}^{(1) \otimes n}$; if one is considering bosonic (or fermionic) statistics. By analyzing these spaces, we find that we can write the wave function $\phi_n(j_1, j_2, \dots, j_n) \in \mathcal{H}^{(n)}$ for an n -particle system, each i -particle in the state j_i , in terms of the $(n+1)$ -particle wave functions or $(n-1)$ -particle wave functions.

²⁴To observe the effect, the separation distance must be of order μm —or less. At 10nm separation, the Casimir effect generates a pressure of order 1 atmosphere—if you do not grasp at how strong that is, I recommend you read about the Magdeburg’s hemispheres in appendix C.

²⁵To read about the connection between bag models and the Casimir effect, two nice references are [93, Chp7,Pg185] and [70, Sec. 6.4]; also for bag models, but including several applications of the Casimir effect, a nice and more recent reference is [15].

²⁶There are some interesting analogue models out there; for example, this one with water [3].

This means we can define operators a_j and a_j^\dagger such that $[a_j, a_j^\dagger] = 1$ (or $\{a_j, a_j^\dagger\} = 1$) and:

$$\begin{aligned} a_j \phi_n(j, j_1, j_2, \dots, j_{n-1}) &= \sqrt{n} \phi_{n-1}(j_2, \dots, j_n), \\ a_j^\dagger \phi_n(j_1, j_2, \dots, j_n) &= \sqrt{n+1} \phi_{n+1}(j, j_1, j_2, \dots, j_n), \\ a_j^\dagger a_j \phi &= n \phi. \end{aligned}$$

By looking at these equations, it makes sense to call a_j the *annihilation operator*, a_j^\dagger the *creation operator* and $a_j^\dagger a_j$ the *number operator*. The Fock space \mathcal{F} is the completion of $\mathcal{F}_0 = \mathbb{C} \oplus \mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)} \oplus \dots \oplus \mathcal{H}^{(n)} \oplus \dots$; here, $\mathbb{C} \equiv a \mathcal{H}^{(1)}$ denotes the scalar field common to all Hilbert spaces $\mathcal{H}^{(i)}$, $i \in \mathbb{N}^*$. Thus, each wave function $\phi \in \mathcal{F}$ can be written as a sequence $\phi = \{\phi_0, \phi_1(j_1), \phi_2(j_1, j_2), \dots, \phi_n(j_1, j_2, \dots, j_n), \dots\}$, up to a limit.

The vector $\{1, 0, \dots, 0, \dots\} \equiv |0\rangle$ is called *vacuum* because it represents a no-particle state that is annihilated by a_j ,

$$a_j^\dagger a_j \{1, 0, \dots, 0, \dots\} = a_j^\dagger \{0, 0, 0, \dots\} = \{0, 0, 0, \dots\} \equiv 0$$

and is uniquely defined, as a ray in the Fock space, by normalization. This summarizes all the ingredients of the Fock representation we need in this section.

We can characterize the system defined in the whole \mathbb{R}^3 with the corresponding Fock representation²⁷:

$$\text{whole system} \equiv (\mathbb{R}^3, \mathcal{F}, a_k^\dagger, a_k, |0\rangle),$$

where \mathcal{F} is the Fock space associated to the creation and annihilation operators a_k^\dagger and a_k defined on points of momentum space²⁸ such that $[a_k, a_{k'}^\dagger] = \delta(k - k')$, and $|0\rangle$ is the vector such that $a_k^\dagger |0\rangle = |k\rangle$ and $a_k |0\rangle = 0$ called *vacuum*. If we impose the boundary conditions (bc) in this whole system we get the restrained system:

$$\text{whole system} \xrightarrow{\text{bc}} \text{restrained system} \equiv (\Omega, \mathcal{F}_L, \tilde{a}_k^\dagger, \tilde{a}_k, |0\rangle_L).$$

When we restrain the space $\mathbb{R}^3 \xrightarrow{\text{bc}} \Omega$, our new system will have a different Fock space $\mathcal{F} \xrightarrow{\text{bc}} \mathcal{F}_L$, since we have different solutions $\phi \xrightarrow{\text{bc}} \phi_L$ and they are associated to different creation and annihilation operators $a_k^\dagger, a_k \xrightarrow{\text{bc}} \tilde{a}_k^\dagger, \tilde{a}_k$ such that $\tilde{a}_k^\dagger |0\rangle_L = |k\rangle_L$ and $\tilde{a}_k |0\rangle_L = 0$ holds for a different vacuum $|0\rangle \xrightarrow{\text{bc}} |0\rangle_L$. However, *this restrained system is just a subsystem of the whole system*.

Given the whole system $(\mathbb{R}^3, \mathcal{F}, a_k^\dagger, a_k, |0\rangle)$, constructed in the usual way described above, we can construct the restrained system as a subsystem in the following way: the Hilbert space of a one-particle system $\mathcal{H}_L^{(1)}$ is taken to be the subset of $\mathcal{H}^{(1)}$ of the solutions that satisfies the boundary conditions $\phi|_{bc}$, *i.e.*

²⁷The creation and anihilation operators and the vacuum vector are defined in respect to a Fock space. The domain of the solutions in the Fock space already gives us information on where the system is defined. Therefore, we can characterize a system simply with \mathcal{F} . The other ingredients, although intrinsic, are highlighted there.

²⁸I changed notation from j to k , because I use j for a general characterization of a quantum state, and k for specifically representing *momentum*.

$$\mathcal{H}_L^{(1)} = \{\psi : \psi = \phi|_{bc}, \phi \in \mathcal{H}^{(1)}\} \subset \mathcal{H}^{(1)},$$

then the Hilbert space of a n -particle system $\mathcal{H}_L^{(n)}$ for $n > 1$ is the symmetrized (or antissymmetrized—let's just consider bosons from now on) subspace of the n -tensor product $\mathcal{H}_L^{(1)} \otimes \dots \otimes \mathcal{H}_L^{(1)} \equiv \mathcal{H}_L^{(1) \otimes n}$. Since $\mathcal{H}_L^{(1)} \subset \mathcal{H}^{(1)}$, we have that $\mathcal{H}_L^{(1) \otimes n} \subset \mathcal{H}^{(1) \otimes n}$ and if we take the symmetrized subspaces, it holds that $\mathcal{H}_L^{(n)} \subset \mathcal{H}^{(n)}$. Thus, for $\mathcal{F}_{0,L} = \mathbb{C} \oplus \mathcal{H}_L^{(1)} \oplus \mathcal{H}_L^{(2)} \oplus \dots \oplus \mathcal{H}_L^{(n)} \oplus \dots$ and \mathcal{F}_0 defined as before, we have that \mathcal{F}_L is a closed subset of \mathcal{F} .

Remark. Explicitly, let $\psi \in \mathcal{F}_L := \overline{\mathcal{F}_{0,L}}$, where $\mathcal{F}_{0,L} = \mathbb{C} \oplus \mathcal{H}_L^{(1)} \oplus \mathcal{H}_L^{(2)} \oplus \dots \oplus \mathcal{H}_L^{(n)} \oplus \dots$, up to a limit we have:

$$\psi = \{\psi_0, \psi_1(j_1), \psi_2(j_1, j_2), \dots, \psi_n(j_1, j_2, \dots, j_n), \dots\},$$

where $\psi_n \in \mathcal{H}_L^{(n)}$ is of the form $\psi_n = (\psi_{n_1} \otimes \dots \otimes \psi_{n_n})$, up to a symmetrization, and each ψ_{n_i} , for $i \in \{n_1, \dots, n_n\}$, is a one-particle solution $\psi_{n_i} \in \mathcal{H}_L^{(1)}$. Thus, there are $\phi_{n_1}, \dots, \phi_{n_n} \in \mathcal{H}^{(1)}$ such that $\phi_{n_i}|_{bc} = \psi_{n_i} \forall i \in \{1, \dots, n\}$. Since $\phi|_{bc} \in \mathcal{H}^{(1)} \forall \phi \in \mathcal{H}^{(1)}$ and then $\phi_n|_{bc} \equiv \phi_{n_1}|_{bc} \otimes \dots \otimes \phi_{n_n}|_{bc} \in \mathcal{H}^{(n)}$, we can write

$$\psi = \{\psi_0, \phi_1|_{bc}(j_1), \phi_2|_{bc}(j_1, j_2), \dots, \phi_n|_{bc}(j_1, j_2, \dots, j_n), \dots\} \in \mathcal{F}.$$

If $\{1, 0, \dots\} \in \mathcal{F}_L \subset \mathcal{F}$, then how can we have different vacua for the whole system and for the restrained system? Well, recall that we call a vector $|0\rangle$ vacuum, in the Fock representation, if it corresponds to a no-particle state—and the operators defined on \mathcal{F}_L are different than those on \mathcal{F} . Thus, let's take a look at the creation and annihilation operators.

The creation and annihilation operators a_k^\dagger and a_k are defined by how they act on the solutions $\phi \in \mathcal{F}$. For an n -particle state $\psi \in \mathcal{F}_L$, the operators \tilde{a}_k and \tilde{a}_k^\dagger such that

$$\begin{aligned} \tilde{a}_k \psi &= \tilde{a}_k \{0, \dots, 0, \psi_n(k, k_1, k_2, \dots, k_{n-1}), 0, \dots\} = \{0, \dots, \sqrt{n} \psi_{n-1}(k_1, k_2, \dots, k_{n-1}), 0, \dots\}, \\ \tilde{a}_k^\dagger \psi &= \tilde{a}_k^\dagger \{0, \dots, 0, \psi_n(k_1, k_2, \dots, k_n), 0, \dots\} = \{0, \dots, 0, 0, \sqrt{n+1} \psi_{n+1}(k, k_1, k_2, \dots, k_{n-1}), 0, \dots\}, \end{aligned}$$

are just a_k and a_k^\dagger restricted to the solutions in \mathcal{F}_L . Therefore, with the canonical projections $P_n : \mathcal{H}^{(n)} \rightarrow \mathcal{H}_L^{(n)}$, we define the projection $P : \mathcal{F}_0 \rightarrow \mathcal{F}_{0,L}$ by

$$P := \bigoplus^n P_n,$$

and we can write $\tilde{a}_k : \mathcal{F}_L \rightarrow \mathcal{F}_L$ and $\tilde{a}_k^\dagger : \mathcal{F}_L \rightarrow \mathcal{F}_L$ as:

$$\begin{aligned} \tilde{a}_k &= P a_k P : P\mathcal{F} \rightarrow P\mathcal{F}, \\ \tilde{a}_k^\dagger &= P a_k^\dagger P : P\mathcal{F} \rightarrow P\mathcal{F}. \end{aligned}$$

Also the restrained solutions $\psi \in \mathcal{F}_L$ can be written in terms of the projection as $\psi = P\phi$ for some $\phi \in \mathcal{F}$, up to a limit. The vacuum for the restrained system is the vector $|0_L\rangle = P|0\rangle$, since

$$\tilde{a}_k |0_L\rangle = P a_k P |0_L\rangle = P a_k P^2 |0\rangle = P a_k |0\rangle = P \{0, 0, \dots\} \equiv 0;$$

that is, even though we can write both vacuums $|0\rangle$ and $|0_L\rangle$ as $\{1, 0, \dots\}$, keep in mind that they are different vectors in different spaces.

In summary, we can see the restrained system $(\Omega, \mathcal{F}_L, \tilde{a}^\dagger, \tilde{a}_k, |0\rangle_L)$ as a subsystem of the whole system $(\mathbb{R}^3, \mathcal{F}, a_k^\dagger, a_k, |0\rangle)$, and we can take $|0\rangle_L$ and $|0\rangle$ as *two states of the same large physical system*. This *large physical system* is just the whole system equipped with the projection $(\mathbb{R}^3, \mathcal{F}, a_k^\dagger, a_k, |0\rangle, P) \equiv (\mathcal{F}, P)$. This implies that it makes sense to consider the energy difference between the two vacuums:

$$\langle 0_L | T_{\mu\nu} | 0_L \rangle - \langle 0 | T_{\mu\nu} | 0 \rangle.$$

Our goal is to discuss negative energy, so we will compute the expectation value for the energy density for the canonical energy-momentum tensor $T_{\mu\nu}$ for the Klein-Gordon field ϕ . $T_{\mu\nu}$ depends on objects like ϕ^2 , which are not well-defined when we consider ϕ as operator-valued distributions. We can regularize it by the two-point splitting procedure²⁹:

$$T_{\mu\nu}(x, x') = \partial_\mu \phi(x) \partial_\nu \phi(x') - \frac{1}{2} \eta_{\mu\nu} \partial_\rho \phi(x) \partial^\rho \phi(x').$$

Then, for the energy density we have:

$$T_{00}(x, x') = \frac{1}{2} \left\{ \partial_0 \phi(x) \partial_0 \phi(x') + \sum_{j=1}^3 \partial_j \phi(x) \partial_j \phi(x') \right\},$$

which we can write³⁰ as:

$$T_{00}(x, x') = \frac{1}{2} \left\{ \left(\partial_0 \partial_{0'} + \sum_{j,j'=1}^3 \partial_j \partial_{j'} \right) \phi(x) \phi(x') \right\};$$

we can renormalized it by computing the difference of the expectation value at some state of interest $|\psi\rangle$ and the vacuum $|0\rangle$. With the identification $T_{\mu\nu}(x) \equiv T_{\mu\nu}(x, x)$ in mind, we can take the coincidence limit, and we get the regularized renormalized expectation value for the energy density at the state ψ :

$$\langle T_{00}(x) \rangle_\psi = \frac{1}{2} \lim_{x' \rightarrow x} \left(\left(\partial_0 \partial_{0'} + \sum_{j,j'=1}^3 \partial_j \partial_{j'} \right) \left(\langle \psi | \phi(x) \phi(x') | \psi \rangle - \langle 0 | \phi(x) \phi(x') | 0 \rangle \right) \right). \quad (1.2.3)$$

Let's compute it for the vacuum of the restrained system $|0_L\rangle$, we will do it analogously to Fulling's calculations for $\langle \phi^2 \rangle_{0_L}$ [59, Chp5]. This will take some pages, but it is crucial that we accept negative energy within Quantum Field Theory to search for a quantum energy inequality in chapter 3.

²⁹which is discussed in more detail in the Hadamard States section in chapter 2.

³⁰by signaling differently the index of the partial derivatives that act on $\phi(x')$ with a '.

Theorem 1.16. *The regularized renormalized expectation value for the energy density at the restrained system vacuum is given by*

$$\langle T_{00} \rangle_{0_L} = -\frac{\pi^2}{1440L^4} - \frac{\pi^2}{48L^4} \frac{3 - 2 \sin^2\left(\frac{\pi z}{L}\right)}{\sin^4\left(\frac{\pi z}{L}\right)} < 0.$$

Let's compute the energy density (1.2.3) for $|\psi\rangle = |0_L\rangle$:

$$\langle T_{00}(x) \rangle_{0_L} = \frac{1}{2} \lim_{x' \rightarrow x} \left(\left(\partial_0 \partial_{0'} + \sum_{j,j'=1}^3 \partial_j \partial_{j'} \right) \left(\langle 0_L | \phi(x) \phi(x') | 0_L \rangle - \langle 0 | \phi(x) \phi(x') | 0 \rangle \right) \right). \quad (1.2.4)$$

Recall that expectation values like $\langle 0_L | \phi(x) \phi(x') | 0_L \rangle$ can be written in terms of the Green functions of the Klein-Gordon equation—in this case, the one called Wightman function, which we will denote as $G_+^L(x, x')$. Imposing the boundary conditions on the canonical solutions of the whole system, we get:

$$\phi(t, x) = \frac{1}{2\pi} \int_{\mathbb{R}^2} dk_1 dk_2 \sum_{n=1}^{\infty} \frac{1}{\sqrt{\omega_k L}} [\tilde{a}_k e^{-i\omega_k t} e^{i(k_1 x + k_2 y)} \sin(k_3 z) + \tilde{a}_k^\dagger e^{i\omega_k t} e^{-i(k_1 x + k_2 y)} \sin(k_3 z)],$$

where $k_3 = \frac{n\pi}{L}$, $\omega_k^2 := k_1^2 + k_2^2 + k_3^2 + m^2$ and $[\tilde{a}_k, \tilde{a}_{k'}^\dagger] = \delta(k_1 - k'_1) \delta(k_2 - k'_2) \delta_{n,n'}$.

Let's denote $x_\perp = (x, y)$ and $k_\perp = (k_1, k_2)$; since

$\tilde{a}_k |0_L\rangle = \langle 0_L | \tilde{a}_k^\dagger = 0$ and $[\tilde{a}_k, \tilde{a}_{k'}^\dagger] = \delta(k_\perp - k'_\perp) \delta_{n,n'}$, we get:

$$\langle 0_L | \tilde{a}_k \tilde{a}_{k'} + \tilde{a}_k \tilde{a}_{k'}^\dagger + \tilde{a}_k^\dagger \tilde{a}_{k'} + \tilde{a}_k^\dagger \tilde{a}_{k'}^\dagger | 0_L \rangle = \langle 0_L | \tilde{a}_k \tilde{a}_{k'}^\dagger | 0_L \rangle = \langle 0_L | \tilde{a}_k \tilde{a}_{k'}^\dagger - \tilde{a}_{k'}^\dagger \tilde{a}_k | 0_L \rangle = \delta(k_\perp - k'_\perp) \delta_{n,n'}.$$

Then, it follows:

$$G_+^L(x, x') = \frac{1}{4\pi^2} \int d^2 k_\perp \sum_{n=1}^{\infty} \frac{1}{\omega_k L} \left\{ e^{-i\omega_k(t-t')} e^{ik_\perp(x_\perp - x'_\perp)} \sin(k_3 z) \sin(k_3 z') \right\}$$

For simplicity, let's impose $x_\perp = x'_\perp$; that is, we will take the coincidence limit not in arbitrary directions, but only in the (t, z) plane. Using that

$$\int_{\mathbb{R}} \frac{|\mathbf{k}_\perp|}{\omega_k} d|\mathbf{k}_\perp| = \int_{k_3}^{\infty} d\omega_k$$

and with usual trigonometric identities, we get:

$$G_+^L(x, x') = \frac{1}{4\pi L} \sum_{n=1}^{\infty} \int_{k_3}^{\infty} d\omega_k \left\{ e^{-i\omega_k(t-t')} \frac{1}{2} [e^{ik_3(z-z')} + e^{-ik_3(z-z')} - e^{ik_3(z+z')} - e^{-ik_3(z+z')}] \right\}. \quad (1.2.5)$$

Proposition 1.17. [adapted from [59, Pg99,Prop1]] *In the distributional sense, modulo terms supported at the origin, it holds:*

$$\begin{aligned}
 a) \int_k^\infty e^{-i\omega\tau} d\omega &= \frac{1}{i\tau} e^{-ik\tau}, & b) \sum_{n=1}^{\infty} e^{-in\lambda} &= \frac{1}{e^{i\lambda}-1} \equiv F(i\lambda), \\
 a') \int_k^\infty \omega^2 e^{-i\omega\tau} d\omega &= \left(\frac{k^2}{(i\tau)^1} + \frac{2k}{(i\tau)^2} + \frac{2}{(i\tau)^3} \right) e^{-ik\tau}, & b') \sum_{n=1}^{\infty} n e^{-in\lambda} &= \frac{e^{i\lambda}}{(e^{i\lambda}-1)^2} = -\dot{F}(i\lambda), \\
 && b'') \sum_{n=1}^{\infty} n^2 e^{-in\lambda} &= \frac{e^{i\lambda}(e^{i\lambda}+1)}{(e^{i\lambda}-1)^3} = \ddot{F}(i\lambda);
 \end{aligned}$$

where dot denotes differentiation with respect to $i\lambda$.

To obtain (1.2.4), we must compute the derivatives of $G_+^L(x, x')$. Note that $G_+^L(x, x')$ does not have any $x_\perp = (x, y)$ dependence, since we already made the simplification $x_\perp = x'_\perp$. The time derivatives just give a multiplying term ω_k^2 in the integral and the derivatives in z and z' just give a multiplying term k_3^2 in the summation and changes the sign of the last two terms; denoting $\tau \equiv (t - t')$,

$$\lambda_1 \equiv (t - t' - z + z'), \quad \lambda_2 \equiv (t - t' + z - z'), \quad \lambda_3 \equiv (t - t' - z - z'), \quad \text{and} \quad \lambda_4 \equiv (t - t' + z + z'),$$

and applying the proposition above, we get that $\partial_0 \partial_{0'} G_+^L(x, x') + \partial_z \partial_{z'} G_+^L(x, x')$ is given by

$$\begin{aligned}
 &= \frac{1}{4\pi L} \left(\frac{1}{(i\tau)^1} \frac{\pi^2}{L^2} \right) \left[\ddot{F}\left(i\frac{\pi}{L}\lambda_1\right) + \ddot{F}\left(i\frac{\pi}{L}\lambda_2\right) \right] + \\
 &+ \frac{1}{4\pi L} \left(\frac{1}{(i\tau)^2} \frac{\pi}{L} \right) \left[-\dot{F}\left(i\frac{\pi}{L}\lambda_1\right) - \dot{F}\left(i\frac{\pi}{L}\lambda_2\right) + \dot{F}\left(i\frac{\pi}{L}\lambda_3\right) + \dot{F}\left(i\frac{\pi}{L}\lambda_4\right) \right] + \\
 &+ \frac{1}{4\pi L} \left(\frac{1}{(i\tau)^3} \right) \left[F\left(i\frac{\pi}{L}\lambda_1\right) + F\left(i\frac{\pi}{L}\lambda_2\right) - F\left(i\frac{\pi}{L}\lambda_3\right) - F\left(i\frac{\pi}{L}\lambda_4\right) \right].
 \end{aligned} \tag{1.2.6}$$

The following proposition gives us all terms in λ_1 and λ_2 of the above.

Proposition 1.18. (adapted from [59, Prop2, Pg100]) *In the distributional sense, it holds:*

$$\begin{aligned}
 F(i\lambda) &= \sum_{m=0}^{\infty} \frac{B_m}{m!} (i\lambda)^{m-1}, \\
 \dot{F}(i\lambda) &= \sum_{m=0}^{\infty} (m-1) \frac{B_m}{m!} (i\lambda)^{m-2}, \\
 \ddot{F}(i\lambda) &= \sum_{m=0}^{\infty} (m-2)(m-1) \frac{B_m}{m!} (i\lambda)^{m-3};
 \end{aligned}$$

where B_m are the Bernoulli numbers $B_0 = 1, B_1 = -\frac{1}{2}, B_2 = \frac{1}{6}, B_3 = 0, B_4 = -\frac{1}{30}, \dots$

The terms in λ_1 and λ_2 depend on $(t - t')$ and $(z - z')$, this means we could expand them directly and consider the coincidence limit to forget about the terms $O(\lambda_j^4), O(\lambda_j^3)$ and

$O(\lambda_j^2)$, respectively in the above—since they will go to zero faster than the terms τ^3 , τ^2 and τ^1 of expression (1.2.6).

On the other hand, the terms on λ_3 and λ_4 depend on $(t - t')$ and $(z + z')$; thus, we need a different approach. Define $\delta \equiv \frac{\pi}{L}(t - t')$ and $\zeta \equiv \frac{\pi}{L}(z + z')$, these new variables will help us work with these distributions. We have:

$$F\left(i\frac{\pi}{L}\lambda_3\right) = F(i\delta - i\zeta) \text{ and } F\left(i\frac{\pi}{L}\lambda_4\right) = F(i\delta + i\zeta).$$

If we consider that we only smear fields with analytics functions, it makes sense to expand in Taylor for small $(t - t')$:

$$\begin{aligned} F(i\delta \pm i\zeta) &= F(\pm i\zeta) + (i\delta)F(\pm i\zeta) + \frac{1}{2}(i\delta)^2 \ddot{F}(\pm i\zeta) + \frac{1}{6}(i\delta)^3 \ddot{\ddot{F}}(\pm i\zeta) + O(\delta^4) \Rightarrow \\ F\left(i\frac{\pi}{L}\lambda_3\right) + F\left(i\frac{\pi}{L}\lambda_4\right) &= F(i\delta - i\zeta) + F(i\delta + i\zeta) \\ &= 1[F(-i\zeta) + F(i\zeta)] + (i\delta)[\dot{F}(-i\zeta) + \dot{F}(i\zeta)] + \frac{1}{2}(i\delta)^2[\ddot{F}(-i\zeta) + \ddot{F}(i\zeta)] \\ &\quad + \frac{1}{6}(i\delta)^3[\ddot{\ddot{F}}(-i\zeta) + \ddot{\ddot{F}}(i\zeta)] + O(\delta^4), \end{aligned} \quad (1.2.7)$$

and analogously for $\dot{F}\left(i\frac{\pi}{L}\lambda_3\right)$ and $\dot{F}\left(i\frac{\pi}{L}\lambda_4\right)$. For real λ , we have:

$$\begin{aligned} F(i\lambda) &= \frac{1}{e^{i\lambda} - 1} = -\frac{1}{2} - i\frac{\sin \lambda}{2(1 - \cos \lambda)} = F(i\lambda)^* = F(-i\lambda), \\ \dot{F}(i\lambda) &= +\frac{1}{4} \csc^2\left(\frac{\lambda}{2}\right) = \dot{F}(i\lambda)^* = \dot{F}(-i\lambda), \\ \ddot{F}(i\lambda) &= -\frac{1}{4} \csc^2\left(\frac{\lambda}{2}\right) \cot\left(\frac{\lambda}{2}\right) = \ddot{F}(i\lambda)^* = -\ddot{F}(-i\lambda), \\ \ddot{\ddot{F}}(i\lambda) &= +\frac{1}{8} \csc^4\left(\frac{\lambda}{2}\right) \{3 - 2\sin^2 \lambda\} = \ddot{\ddot{F}}(i\lambda)^* = \ddot{\ddot{F}}(-i\lambda). \end{aligned}$$

Using the expressions above we get all terms in λ_3 and λ_4 .

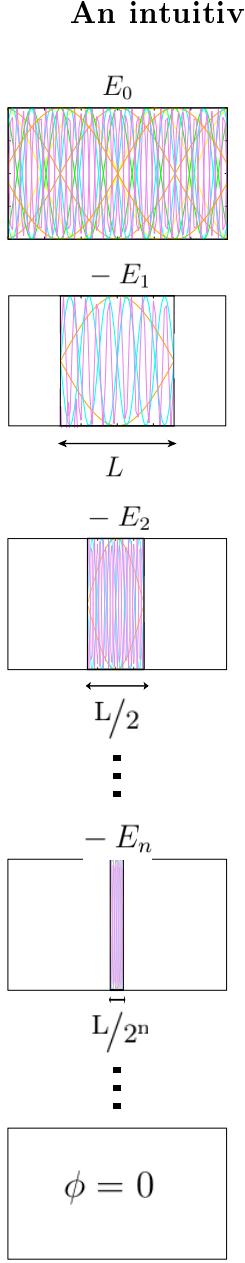
To renormalize, we subtract the following. For the whole system vacuum, the massless case: let $G_+(x, x') \equiv \langle 0 | \phi(x)\phi(x') | 0 \rangle$, from Bogoliubov and Shirkov's work [13, AppI] we know that $G_+(x, x') = \frac{-1}{4\pi^2[(t-t')^2 - (z-z')^2]}$; then, in the limit $z' \rightarrow z$:

$$\partial_0 \partial_0' G_+(x, x') + \partial_z \partial_z' G_+(x, x') = \frac{2}{\pi^2(t-t')^4}. \quad (1.2.8)$$

Therefore, the regularized renormalized expectation value for the energy density in the restrained system vacuum is given by the sum of terms in λ_1 , λ_2 , λ_3 and λ_4 minus (1.2.8):

$$\langle T_{00} \rangle_{0_L} = -\frac{\pi^2}{1440L^4} - \frac{\pi^2}{48L^4} \frac{3 - 2\sin^2\left(\frac{\pi z}{L}\right)}{\sin^4\left(\frac{\pi z}{L}\right)}.$$

One could say that this negative energy is just a technicality; in the next section, we see that we cannot remove it by rescaling the zero energy—in fact, a negative energy density is intrinsic of the framework of Quantum Field Theory established here.



Consider we have a quantum system on Minkowski spacetime satisfying the Klein-Gordon equation just as before $(\mathbb{R}^3, \mathcal{F}, a, a^\dagger, |0\rangle)$. We can equip it with a projection $P : \mathcal{F}_0 \rightarrow \mathcal{F}_{0,L}$ and construct the subsystem $(\Omega, \mathcal{F}_L, \tilde{a}, \tilde{a}^\dagger, |0\rangle_L)$ and we just learned that the expectation value of the energy density at $|0_L\rangle$ is negative in respect to $|0\rangle$, *i.e.* if we set $\langle T_{00} \rangle_0 \equiv E_0 \rightarrow 0$, we get, say $\langle T_{00} \rangle_{0_L} = -E_1$. One could think that this negativeness is arbitrary and if we just translated the energy scale by $+E_1$ we would obtain $\langle T_{00} \rangle_{0_L} = 0$, $\langle T_{00} \rangle_0 = E_1$ and no negative energy.

“Translate the scale” corresponds to redefine the renormalization process; we would have to rewrite equation (1.2.3) as:

$$\langle T_{00}(x) \rangle_\psi = \frac{1}{2} \lim_{x' \rightarrow x} \left(\left(\partial_0 \partial_{0'} + \sum_{j,j'=1}^3 \partial_j \partial_{j'} \right) \left(\langle \psi | \phi(x) \phi(x') | \psi \rangle - \langle 0_L | \phi(x) \phi(x') | 0_L \rangle \right) \right).$$

The above is not a good renormalization process—for the general context of Quantum Field Theory—since the state $|0_L\rangle$ is not translation invariant. Yet, let’s consider this rescalement just to see that it does not remove the negativeness of this particular problem—the Casimir effect in the Fock representation.

Note that $\langle T_{00} \rangle_{0_L}$ depends on L , as in Theorem 1.16; then, what if we consider the projection $P_2 : \mathcal{F}_0 \rightarrow \mathcal{F}_{0,L/2}$? A projection that restrain the whole system to a smaller region, say

$$\Omega_2 = \{(x, y, z) : 0 < z < L/2\} \subset \Omega \subset \mathbb{R}^3,$$

gives, by Theorem 1.16—considering just the first term, for simplicity— $\langle T_{00} \rangle_{0_{L/2}} \equiv -E_2 = 2^4 \langle T_{00} \rangle_0 = -2^4 E_1$ —which is negative in respect to both $|0_L\rangle$ and $|0\rangle$. Then we would have to translate the scale by $+E_2$ to get rid of the negative energy. We can do this over and over again: take the projection P_n , compute the vacuum energy density $\langle T_{00} \rangle_{0_{L/2^n}} \equiv -E_n = 2^{4n} \langle T_{00} \rangle_0$ and translate the energy scale by $+E_n$. The problem is: we *cannot take the limit* $n \rightarrow \infty$. If we repeat this procedure until we obtain an overlap of the plates, this will correspond to a system for which $\phi = 0$ everywhere! Thus, the limit of this sequence of states is not a physical state.

This is consistent with quantum mechanics: absolute nothing does not exist, even the vacuum—the no-particle state—has a non-zero energy. Even if you try to consider a zero wave function, in the next second you would realize that there would be a zero probability of finding a system in that state. So we never get to this limit, it *is not a physical state*.

We cannot define energy differences in respect to this limit, we cannot measure the energy of this limit, we cannot set it to zero. This means we have to cut off this subsystem construction at some point and set the zero somewhere before this limit. Suppose we stop at subsystem n , then the state $|0_{L/2^{n+1}}\rangle$ has negative energy in respect to $|0_{L/2^n}\rangle$. Therefore, even though we only measure energy differences, negative energy is intrinsic here: if we cannot define an absolute zero energy state, we must take into account negative energy states.

1.2.3 Quantum Energy Inequalities

Where we understand what are these quantum energy inequalities and the role they play here.

By accepting that we must take negative energy into account, the question of whether it could be arbitrarily negative naturally arises. Ford was the first to approach this problem, in 1978, and he showed that negative energy fluxes lead to a violation of the second law of Thermodynamics [49]; he also introduced the concept of a quantum inequality: a restriction on the magnitude and the duration of negative energy; thus, also called *quantum energy inequality* (QEI).

Beyond the violation of the second law, some other possible—more exotic—macroscopic effects that could result if arbitrarily negative quantum energy densities were allowed to exist for extended periods of time have been studied; for example, Alcubierre’s warpdrive [4] and its “unphysical” character [92], as well as traversable wormholes and time machines—two nice references for this subject are [53, 114]. QEIs are relevant to study exotic effects, yet, in this dissertation they play a more conservative role; in the context of Singularity Theorems under the light of Quantum Physics, quantum energy inequalities enter as a weakened substitute of the classical energy conditions.

The problem of weakening the classical energy conditions does not have a unique nor canonical solution; a first attempt was to consider averages along geodesics [112] instead of the classical pointwise characterization. Let us take the null energy condition (NEC) as an example; instead of imposing the classical pointlike form

$$T_{\mu\nu}k^\mu k^\nu \geq 0 \text{ for all null } k^\mu,$$

we could consider an average null energy condition (ANEC)

$$\int_{\gamma} T_{\mu\nu} \gamma'^\mu \gamma'^\nu d\lambda \geq 0 \left\{ \begin{array}{l} \text{for a complete (or half-complete) null} \\ \text{geodesic } \gamma \text{ with affine parametrization.} \end{array} \right.$$

Remark 1.19. To make sense out of this integral we have to regularize it somehow: we can interpret it as a \liminf of integrals over a finite interval (as done by Roman in [100]) or we can introduce a mollifying function (as done by Wald and Yurtsever in [116])—in this case, we would take it as a *weighted average*.

The study of Singularity Theorems under weakened energy conditions is also dated to the 70’s; in particular, Singularity Theorems were proven using average energy conditions also by Ford in [112] and the discussion perpetuated, for example in the later works [16, 100, 116]. Yet, ANEC was also shown to be violated by scalar fields (even *classical* scalar fields). In fact, the average energy conditions—which were constructed as the classical ones, *i.e. assumed*—are not free from violations as well.

On the other hand, QEIs are derived *within* Quantum Field Theory. The bound derived by Ford in 1978 was based in the uncertainty principle, but since the 90’s, QEIs have been derived directly from QFT formalism, without other assumptions, as in [100, 91] for example. As Ford said in [53]: “The same laws of physics that allow the existence of this ‘negative energy’ also appear to limit its behaviour”.

As an example of a QEI, consider the Klein-Gordon field in Minkowski spacetime—it was found [51, 52] a bound of the form:

$$\int_{-\infty}^{+\infty} f(t) \langle T_{00} \rangle_\psi dt \geq -\frac{C}{t_0^4},$$

where $\langle T_{00} \rangle_\psi$ is the expected energy density at the state ψ smeared with a sampling function f , which is smooth, vanishes at infinity and integrate to 1; C is a constant that depends on $\langle T_{00} \rangle_\psi$ and f . The parameter t_0 is a sampling time; in the limit $t_0 \rightarrow \infty$, the bound above reduces to an average weak energy condition (with a smearing function) and in the limit $t_0 \rightarrow 0$, there is no bound—the energy density can be arbitrarily negative. This example illustrate the nature of a quantum energy inequality.

To summarize: quantum energy inequalities are bounds, within quantum field theories, on the magnitude and duration of negative energy; they are lower bounds satisfied by the expectation value—weighted averages—of the energy-momentum tensor and we can see them as a generalization of the classical pointwise energy conditions.

1.3 The Transition from Flat to Curved Spacetime

Where we answer the questions: if Quantum Field Theory has problems on Minkowski spacetime, why should we go to curved ones? It should be worst, right?

We can benefit from the discussion on Singularity Theorems of section 1.1 using it to illustrate two reasons for pursuing an axiomatic formulation of any theory, since Hawking and Penrose theorems:

1. do not rely on symmetry hypothesis on the matter content or on counting solutions of Einstein equations \Rightarrow *within a more general formalism, one has the chance to obtain stronger results.*
2. set the ground for the definition of singularity as geodesic incompleteness; in spite of having its subtleties, this definition is clear and enabled us to better comprehend the nature of singularities in General Relativity \Rightarrow *within a well-defined formalism, one has the chance of a better understanding of fundamental concepts.*

The study of an axiomatic formulation of Quantum Field Theory on Curved Spacetimes has, at least, two particular reasons:

3. it allows the study of the interaction between gravity and other fields in regions of high curvature, like near a collapsing star; which has been shown interesting by the Hawking effect, for example.
4. it allows the study of quantum energy inequalities, which is motivated by Singularity Theorems in this dissertation, but is also interesting to study possible macroscopic effects of negative energy—as shown in the last section.

Considering reasons 1-4 above, we can also see an axiomatic formulation of Quantum Field Theory on curved spacetimes as a preliminary work towards a fully quantized theory of gravity.

The framework of Wightman Axioms, as seen in section 1.2.1, constitutes an axiomatization of Quantum Field Theory on Minkowski spacetime. In the same year of Wightman's publication, 1964, R. Haag and D. Kastler established another axiomatic approach: they showed that a purely algebraic formulation of QFT is possible and they explicitly gave a set of axioms based on the concept of local net of observables [68]. Both of them are axiomatizations of QFT, both can be referred to as Local QFT and, in fact, both deal with algebras, but what is often called Axiomatic QFT is Wightman's version and, Algebraic or Local QFT is the formalism based on Haag-Kastler Axioms.

Some levels of equivalence between the two frameworks have been developed; for example, that we can obtain Wightman Fields within an adapted and generalized Haag-Kastler framework [56] and the other way around with some extra assumptions [14]. Furthermore, even though both works [118, 68] are from the same year, Haag and Kastler were familiar with other previous works of Wightman [117]; also of Araki [6] and of Segal [105]—whose work was in the context of searching for an algebraic approach. Therefore, we can consider the Haag-Kastler approach as a generalization of the Wightman framework, in the sense that it takes the algebra of observables, implicit in Wightman's, and elevate it to *fundamental object*.

For completeness, I will state now the Haag-Kastler Axioms; and for convenience, I will state them for Minkowski spacetime—this also allows direct comparison with the Wightman framework stated in section 1.2.1. Even though they listed explicitly their framework in [68], one can find several adaptations, simplifications or generalizations in literature also referred to as H-K axioms. The following is basically Fredenhagen's version as in [54].

Let \mathcal{O} be a region in the Minkowski spacetime, \mathcal{O}' its causal complement and $\mathcal{U}(\mathcal{O})$ its assigned algebra of observables labeled by a family K of regions and satisfying the isotony property. The correspondent Haag-Kastler axioms for the local structure are:

Principle of Locality: if $\mathcal{O}_1 \subset \mathcal{O}'_2 \Rightarrow \mathcal{U}(\mathcal{O}_1) \subset \mathcal{U}(\mathcal{O}'_2)$. This is saying that algebras of spacelike separated regions are independent, which corresponds to Einstein causality and introduce the relativistic character of the system.

Covariance: the symmetry operations map $\mathcal{U}(\mathcal{O})$ into the algebra of the mapped region \mathcal{O} . Usually, the symmetry consider is associated to the Poincaré group \mathcal{P}_+^\uparrow , and we can state this axiom then, equivalently as: exists a family of isomorphisms $\alpha_{\mathcal{L}}^{\mathcal{O}} : \mathcal{U}(\mathcal{O}) \rightarrow \mathcal{U}(\mathcal{L}\mathcal{O})$ such that for $\mathcal{O}_1 \subset \mathcal{O}_2$, we have $\alpha_{\mathcal{L}}^{\mathcal{O}_2} \upharpoonright_{\mathcal{U}(\mathcal{O}_1)} = \alpha_{\mathcal{L}}^{\mathcal{O}_1}$ and such that: $\alpha_{\mathcal{L}'}^{\mathcal{L}\mathcal{O}} \circ \alpha_{\mathcal{L}}^{\mathcal{O}} = \alpha_{\mathcal{L}'\mathcal{L}}^{\mathcal{O}}$ for the Poincaré transformations $\mathcal{L}, \mathcal{L}'$. Sometimes this axiom is also simplified to a statement on the translations only.

Time-slice: the algebra of a neighborhood of a Cauchy surface of a given region coincides with the algebra of the full region. This means we can construct the entire algebra by finding the observables, of an initial value problem, at a small time interval.

Stability Condition: it exists a strongly continuous unitary representation U of the translation group, and a representation π of $U(K)$ on some Hilbert space such that:

$U(a)\pi U(a)^{-1} = \pi(\alpha_a(A))$, $a \in \mathbb{R}^4$, $A \in U(K)$ and the joint spectrum of the generator of U is contained in the closed forward light cone.³¹

The above axioms exhibit the representative property of Algebraic QFT:

The fundamental concepts of the theory, as locality, causality, commutations relations and even, the dynamics one is considering, are introduced in the algebra of observables.

In chapter 2, we study the algebraic approach of QFT for the Klein-Gordon field. We consider the notion of *fields* as operator-valued distributions, as introduced in 1964 by Wightman and we explicitly construct the algebra of observables with the solutions of the Klein-Gordon equation—this procedure has support on the Haag-Kastler framework and the subsequent prosperity of algebraic QFT. A nice reference for a generalization of Haag-Kastler framework to curved spacetimes is [57, 4.2].

The crucial advantage of the algebraic approach is the possibility of generalizing it to curved spacetimes³². Without Poincaré symmetries we lose the notion of particles, of Hamiltonian, of vacuum, for example. Yet, in the algebraic formalism, we have Hadamard states, Radzikowski Theorem, thus the powerful tool of Microlocal Analysis that substitutes the Fourier transforms and other Fock space techniques. The figure below highlight the basic differences between the standard and the algebraic approaches.

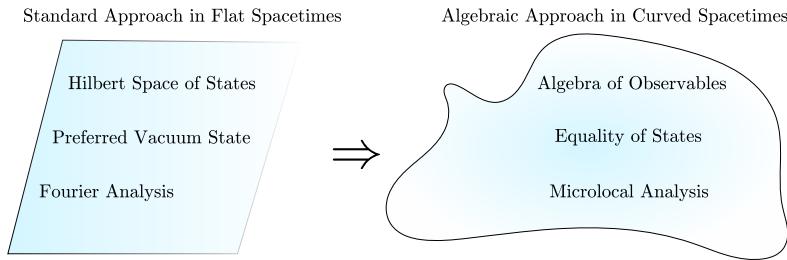


Figure 1.1: The transition from flat to curved spacetimes.

Furthermore, the fundamental object of a quantum field theory is a *field*, thus, to lose the notion of particle when considering curved spacetimes should not withhold us from formalizing QFT in a curved spacetime. Given that, to lose the notion of a preferred vacuum is natural since, in the Fock representation, it is directly related to the notion of particle. To corroborate this idea, a nice quote from R. Wald [115, Pg60] comparing the transition from flat to curved spacetimes with the transition from Special Relativity to General Relativity:

“Indeed, I view the lack of an algorithm for defining a preferred notion of ‘particles’ in quantum field theory in curved spacetime to be closely analogous to the lack of an algorithm for defining a preferred system of coordinates in classical general relativity. (Readers familiar only with presentations of special relativity based upon the use of global inertial coordinates might well find this alarming).”

³¹It is common to say that this axiom is intuitively stating that “energy is positive”, which is reasonable, but one must keep in mind that the positivity here is associated to the support of the generators U , and not to the energy-momentum tensor or Wick products.

³²There are “generalizations of Wightman Axioms”, such as the work of Isham in 1978 and also by Wald and Hollands in 2008; but they are, in essence, the algebraic approach.

2

A FRAMEWORK: KLEIN-GORDON FIELD IN ALGEBRAIC QUANTUM FIELD THEORY

Where we see how we can characterize a quantum system determined by the Klein-Gordon dynamics in a general curved spacetime within the algebraic approach of Quantum Field Theory.

The algebraic approach of Quantum Field Theory (QFT) allows us to formalize QFT on curved spacetimes without the particular concepts that arise naturally in flat spacetimes due to Poincaré symmetries, such as the notion of particles, of a preferred vacuum state and of Hamiltonian, for example. In fact, it allows us to formalize QFT using only local concepts, and we can see it as a preliminary work towards a theory of quantum gravity. In Algebraic QFT (AQFT), the fundamental object is an algebra and, notably, we can introduce all information regarding locality, causality, commutation relations and the dynamics of the model in the algebra of observables. The so called Hadamard states - normalized positive linear functionals on the algebra that satisfy the Hadamard condition - are considered physically reasonable states since they give a well-defined expectation value for the energy-momentum tensor (up to local curvature terms). On the other hand, for fields as distributions, and given Radzikowski Theorem, we have the powerful mathematical tool of Microlocal Analysis, which can be seen as a replacement of the Fourier analysis done in the usual Fock space representation. AQFT is a general, well-defined formalism which has shown to be fruitful and powerful for fundamental topics of Quantum Field Theory on curved spacetimes and for cosmological applications¹.

In this chapter we see how we can formulate quantum field theory for the Klein-Gordon field in the algebraic approach with the goal of understanding the framework in which we derive a general quantum energy inequality in the next chapter.

An ambiguity arises at the starting point: posing the problem. We must choose the *form* of the generalized Klein-Gordon equation and *where* will it be defined; this choice of an equation that couples the Klein-Gordon field with gravity in a curved spacetime is restrained by the condition that it must reduce to the usual equation in flat spacetime.

Consider a free hermitean scalar field ϕ that satisfies the following Klein-Gordon equation:

¹There are references for these applications in section Wind-up of chapter 3.

$$P\phi \doteq (-\square + m^2 + \xi R)\phi = 0 \quad \text{where} \quad \begin{cases} \square = \nabla_\mu \nabla^\mu & \text{is the D'Alembert operator;} \\ m & \text{is the mass;} \\ R & \text{is the Ricci curvature;} \\ \xi & \text{is the coupling parameter.} \end{cases} \quad (2.0.1)$$

The equation above is the simplest generalization of the Klein-Gordon equation to a curved spacetime. Of course we could add other terms to it and still get a functional that reduces to the Klein-Gordon one in flat spacetimes, but we should also find a good reason to do that². Fulling gives, in [59, Pg119], two reasons to include the ξR term: conformal invariance and interaction. First, let n be the dimension of the spacetime, when $m = 0$ and $\xi = \frac{n-2}{4(n-1)}$ the equation is conformally invariant. This means that we could work with rescaled solutions, possibly with simpler calculations. The second and more physical reason is that it is known that the renormalization of an interacting theory, for example Yukawa, will impose a counterterm proportional to $R\phi^2$ in the Lagrangian and thus a term like ξR in the equations of motion. Therefore, we have a mathematical and a physical reason to include the term ξR in the generalization of the Klein-Gordon equation.

Although not the most general background, here, we will pose the problem on globally hyperbolic spacetimes for three reasons:

1. Particular justification: the goal of this dissertation is to approach Singularity Theorems through the energy condition, so we can keep the causality condition on the spacetime as being “global hyperbolicity”;
2. Physical intuition: for the well-posedness of Einstein equations as an initial value problem, spacetime should be predictable from initial data and, thus, globally hyperbolic;
3. Technical convenience: it is well-known that normally hyperbolic operators constitutes a well-posed Cauchy Problem in globally hyperbolic spacetimes.

In appendix B, one can walk towards the spacetime definition—an n -dimensional connected time-orientable Lorentzian manifold—and recall some properties of Lorentzian Geometry.

The generalized problem we face in this chapter is then Equation (2.0.1) on globally hyperbolic spacetimes. We study first the Classical Dynamics of it, in section 2.1; we see that it is, indeed, a well-posed Cauchy problem and we determine the Poisson bracket on which we apply Dirac quantization when constructing the quantized algebra of observables in section 2.2. This algebra admits too many states, so in section 2.3 we analyse properties we would expect states to satisfy to say they are *physically reasonable*. In this last section we also review basic tools of Microlocal Analysis crucial to derive a quantum energy inequality in chapter 3.

Let's set some notation first; let M be a globally hyperbolic spacetime, then:

²A fancy name for this argument is “Occam's razor”: “Numquam ponenda est pluralitas sine necessitate”. There are, for example, models for graviton or inflation, which do include other terms.

- $C^\infty(M, \mathbb{R})$ denotes the collection of smooth real-valued functions on M equipped with the usual locally convex topology, *i.e.* $f_n \rightarrow f$ in $C^\infty(M, \mathbb{R})$ if the derivatives of f_n converge uniformly to the derivatives of f on all compact subsets of M .
- $C_0^\infty(M, \mathbb{R})$ denotes the collection of smooth real-valued functions on M with compact support equipped with the usual locally convex topology, *i.e.* $f_n \rightarrow f$ in $C^\infty(M, \mathbb{R})$ if there is a compact set $K \subset M$ which contains the supports of all f_n and of f and such that the derivatives of f_n converge uniformly to the derivatives of f on K .
- $C_{SC}^\infty(M, \mathbb{R})$ denotes the collection of spacelike-compact support functions in $C^\infty(M, \mathbb{R})$, *i.e.* for all $f \in C_{SC}^\infty(M, \mathbb{R})$ and all Cauchy surfaces Σ on (M, g) we have $\text{supp } f \cap \Sigma$ is compact.
- $C_{tC}^\infty(M, \mathbb{R})$ denotes the collection of timelike-compact support functions in $C^\infty(M, \mathbb{R})$, *i.e.* for all $f \in C_{tC}^\infty(M, \mathbb{R})$ there exists two Cauchy surfaces Σ_1 and Σ_2 on (M, g) such that $\text{supp } f \subset J^-(\Sigma_1) \cap J^+(\Sigma_2)$.
- $\mathcal{D}'(M, \mathbb{R})$ denotes the topological dual of $C^\infty(M, \mathbb{R})$. That is, the space of distributions which consists of continuous linear functionals $C^\infty(M, \mathbb{R}) \rightarrow \mathbb{R}$.
- $\mathcal{D}'_0(M, \mathbb{R})$ denotes the topological dual of $C_0^\infty(M, \mathbb{R})$. That is, the space of distributions which consists of continuous linear functionals with compact support $C_0^\infty(M, \mathbb{R}) \rightarrow \mathbb{R}$.
- $\langle \cdot, \cdot \rangle$ denotes (until said otherwise) the dual pairing of $f \in C^\infty(M, \mathbb{R})$ and $u \in \mathcal{D}'_0(M, \mathbb{R}) \supset C^\infty(M, \mathbb{R}) \supset C_0^\infty(M, \mathbb{R})$ with compact overlapping support given by: $\langle u, f \rangle := \int_M d\text{vol}_g(x) u(x) f(x)$.

Solutions of a partial differential equation do not have to be compactly supported, here they will be generally functions in $C^\infty(M, \mathbb{R})$. Yet, measurements are made at a finite spacial extent region for a finite time interval and we can introduce this information by restraining the analysis to smooth compactly supported functions. These functions, in $C_0^\infty(M, \mathbb{R})$, are called *test functions* and, accordingly, we will interpret them as functions which employ the localisation of the observables in spacetime. In particular, if a solution is time-compactly supported, this means that the initial data gets lost somewhere—which seems unreasonable—thus, within the compactly supported solutions, we will further restrain the construction to the spacelike-compactly supported ones, *i.e.* functions in $C_{SC}^\infty(M, \mathbb{R})$.

2.1 Classical Dynamics

Where we establish that the Klein-Gordon equation constitutes a well-posed Cauchy problem in globally hyperbolic spacetimes and we find a natural Poisson Bracket.

Since we study a scalar field, we consider an operator P acting on a space of functions on the spacetime. In [10, Chp3], one can find more general statements, for P acting on sections of a vector bundle, and their proofs. Yet, keeping this in mind, we can later “trivially complexify” the results here by considering P acting on $C^\infty(M, \mathbb{R}) \otimes iC^\infty(M, \mathbb{R})$. We start with the classical part, and the construction of the Poisson bracket for classical observables,

so it is somewhat more intuitive to remain with the real-valued functions for now. Eventually, we will complexify the solutions, for convenience, and then apply Dirac quantization. This section is a simplified review of [69, Pg18-25] and [79, Sec2]; another nice reference for the subjects treated here is [8], and a more compact one is [33].

Let's start by recognizing that the Klein-Gordon operator, of equation (2.0.1), is a normally hyperbolic operator. The idea is that we can write a linear differential operator by replacing each partial derivative by a new variable, *i.e.* in terms of *symbols*; the highest order terms of the symbols is called *principal symbol*. On a Lorentzian manifold, a normally hyperbolic operator is an operator whose principal symbol is given by the corresponding metric tensor on the manifold. The d'Alembertian is the canonical example of a normally hyperbolic operator, and it is easy to see then that the Klein-Gordon operator is of this kind. Let's formalize this idea. Let α be an n -dimensional multi-index $\alpha = (\alpha_1, \dots, \alpha_n)$, so that $\partial^\alpha = \partial_1^{\alpha_1} \dots \partial_n^{\alpha_n}$, where $\partial_i^{\alpha_i} := \frac{\partial^{\alpha_i}}{\partial x_i^{\alpha_i}}$ and $|\alpha| = \alpha_1 + \dots + \alpha_n$.

Definition 2.1. (Principal symbol) For the linear differential operator $P = \sum_{|\alpha| \leq m} a_\alpha(x) \partial^\alpha$, $P(\xi) = \sum_{|\alpha| \leq m} a_\alpha(x)(i\xi)^\alpha$ is called the *full symbol* of P . The homogeneous term with degree m , $\sigma_P(x, \xi) = \sum_{|\alpha|=m} a_\alpha(x)(i\xi)^\alpha$, is called the *principal symbol* of P .

Definition 2.2. (Normally hyperbolic operator) A second-order differential operator whose principal symbol is a Lorentzian metric is called a *normally hyperbolic operator* (or a *generalized d'Alembert operator*, for example in [8], or even a *wave operator*, for example in [9]). In local coordinates, P can be expressed as $P = -g^{\mu\nu} \partial_\mu \partial_\nu + A^\mu \partial_\mu + B$, with smooth functions A^μ , B and the metric principal symbol $-g^{\mu\nu} \partial_\mu \partial_\nu$.

Evidently, the Klein-Gordon operator is normally hyperbolic. The connection between a metric principal symbol and this “normal hyperbolic” character is due to the fact that the zeros of the principal symbol are the *characteristics* of the associated equation and they give us information about the solutions and the singularities of it.

It is a well-posed Cauchy Problem

From now on, and until said otherwise, let $P : C^\infty(M, \mathbb{R}) \rightarrow C^\infty(M, \mathbb{R})$ be a normally hyperbolic operator on a globally hyperbolic spacetime M . The results of this subsection are simplified from [10, Chp3].

Theorem 2.3. [10, Pg85](The Cauchy Problem) *Let $f \in C_0^\infty(M, \mathbb{R})$, Σ a Cauchy surface on M , $(u_0, u_1) \in C_0^\infty(\Sigma, \mathbb{R}) \times C_0^\infty(\Sigma, \mathbb{R})$, and let \mathbf{n} be the future directed timelike unit vector field of Σ . Then the Cauchy Problem:*

$$Pu = f \quad u|_\Sigma = u_0 \quad \nabla_{\mathbf{n}} u|_\Sigma = u_1$$

has a unique solution $u \in C^\infty(M, \mathbb{R})$. Moreover, the solution depends continuously on the data and

$$\text{supp}(u) \subset J(K), \text{ where } K := \text{supp}(u_0) \cup \text{supp}(u_1) \cup \text{supp}(f).$$

Then, given initial conditions, say data $\equiv (f, \Sigma, u_0, u_1)$, we can evolve this data continuously, causally and uniquely. So the Klein-Gordon equation describes the dynamics of a system in the entire spacetime.

Theorem 2.4. [10, Pg87]($\exists!$ Fundamental operators solutions) *There exist unique—in the distributional sense—advanced E_A and retarded E_R Green operators for P . That is, there are continuous linear maps:*

$$E_{A,R} : C_0^\infty(M, \mathbb{R}) \rightarrow C^\infty(M, \mathbb{R}) \text{ with } \begin{cases} P \circ E_{A,R} = E_{A,R} \circ P = id_{C_0^\infty(M, \mathbb{R})}; \\ \text{supp } E_{A,R} f \subset J^\pm(\text{supp } f) \quad \forall f \in C_0^\infty(M, \mathbb{R}). \end{cases}$$

Corollary 2.5. *Let $f, g \in C_0^\infty(M, \mathbb{R})$. If P is formally self-adjoint, i.e. $\langle f, Pg \rangle = \langle Pf, g \rangle$, then $E_{A,R}$ are formally self-adjoint and E is formally skew-adjoint, i.e. $\langle f, Eg \rangle = -\langle Ef, g \rangle$.*

Claim 2.6. The Klein-Gordon operator is formally self-adjoint, thus the above Corollary is interesting for us.

Theorem 2.4 tells us that exist inverses of P in certain regions of spacetime, i.e. the Green operators for P ; Corollary 2.5 is a crucial property we use later. We can look at E_A and E_R as “fundamental operator solutions”: for $f \in C_0^\infty(M, \mathbb{R})$ we have an advanced solution $E_A f$ with support in the causal future of the support of f and a retarded solution $E_R f$, with support in the causal past. With them, we define the causal propagator E in Theorem 2.7 and state its properties (i-iv).

Theorem 2.7. *The causal propagator of P defined as $E := E_A - E_R$ is a continuous map:*

$$E : C_0^\infty(M, \mathbb{R}) \rightarrow C_{SC}^\infty(M, \mathbb{R}) \text{ such that}$$

- (i) for all solutions u of $Pu = 0$ with compact-supported initial conditions on a Cauchy surface there is an $f \in C_0^\infty(M, \mathbb{R})$ such that $u = Ef$;
- (ii) If $Ef = 0$, then $\exists g \in C_0^\infty(M, \mathbb{R})$ such that $f = Pg$;
- (iii) $EC_0^\infty(M, \mathbb{R})$ and $C_0^\infty(M, \mathbb{R})/PC_0^\infty(M, \mathbb{R})$ are isomorphic;
- (iv) $0 \rightarrow C_0^\infty(M, \mathbb{R}) \xrightarrow{P} C_0^\infty(M, \mathbb{R}) \xrightarrow{E} C_{SC}^\infty(M, \mathbb{R}) \xrightarrow{P} C_{SC}^\infty(M, \mathbb{R})$ is exact.

Proof.

item (i): Let $u \in C_{SC}^\infty(M, \mathbb{R})$ such that $Pu = 0$ and take a cutoff function χ , i.e. $\chi \equiv 0$ in the causal future of some Cauchy surface Σ_2 and $\chi \equiv 1$ in the causal past of some Cauchy surface Σ_1 , such that $\Sigma_2 \subset I^+(\Sigma_1)$. Let $f \equiv -P\chi u$, since f has compact support in $I^+(\Sigma_2) \cap I^-(\Sigma_1)$ and:

- $\text{supp } \chi u \subset I^-(\Sigma_2)$, which is compact, then $\chi u = E_R f$;
- $\text{supp } (1 - \chi) u \subset I^+(\Sigma_1)$, also compact, then $(1 - \chi) u = -E_A f$.

Hence, $u = Ef$ for some $f \in C_0^\infty(M, \mathbb{R})$.

item (ii): $Ef = 0 \Rightarrow E_A f = E_R f$. Then, $\text{supp} E_{A,R} f \in J^+(\text{supp} f) \cap J^-(\text{supp} f)$, which is compact, so $E_{A,R} f \in C_0^\infty(M, \mathbb{R})$. Therefore:

$$f = P \circ E_{A,R} f \in PC_0^\infty(M, \mathbb{R}).$$

item (iii): $\ker E = \text{Ran} P$ since:

$$f \in \ker E \xrightarrow{\text{(ii)}} \exists g : f = Pg \Rightarrow f \in \text{Ran} P;$$

for $f \in C_0^\infty(M, \mathbb{R})$, we have $E \circ Pf = E_A \circ Pf - E_R \circ Pf = f - f = 0$ (*), then:

$$f \in \text{Ran} P \Rightarrow \exists g : f = Pg \xrightarrow{(*)} f \in \ker E.$$

Then, by the first theorem of isomorphism:

$$EC_0^\infty(M, \mathbb{R}) \simeq C_0^\infty(M, \mathbb{R}) / PC_0^\infty(M, \mathbb{R}).$$

item (iv): an exact sequence is one such that the image of each map is the kernel of the next map, it holds since:

- The first arrow says P is injective: let $f \in C_0^\infty(M, \mathbb{R})$, since $f = E_{A,R} \circ Pf$ then $f = 0 \iff Pf = 0 \therefore \ker P = \{0\}$.
- The second arrow is due to item (iii).
- The third arrow corresponds to $\text{Ran} E = \ker P$, which holds since:

$$u \in \ker P \xrightarrow{\text{(i)}} \exists f : u = Ef \Rightarrow u \in \text{Ran} E;$$

for $f \in C_0^\infty(M, \mathbb{R})$, we have $E \circ Pf = E_A \circ Pf - E_R \circ Pf = f - f = 0$ (**), then:

$$u \in \text{Ran} E \Rightarrow \exists f : u = Ef \xrightarrow{(**)} u \in \ker P.$$

□

Proposition 2.7 yields a well-defined causal propagator that maps test functions onto solutions with spacelike-compact support.

Let the space of complex test functions be denoted as $C_0^\infty(M) := C_0^\infty(M, \mathbb{R}) \oplus iC_0^\infty(M, \mathbb{R})$ and $\mathcal{D}'_0(M)$ its dual space; we can extend by \mathbb{C} -linearity the operators $E_{A,R}$ and E seen as linear maps $E_{A,R} : C_0^\infty(M, \mathbb{R}) \rightarrow C^\infty(M, \mathbb{R})$ and $E : C_0^\infty(M, \mathbb{R}) \rightarrow C_{SC}^\infty(M, \mathbb{R}) \subset C^\infty(M, \mathbb{R})$ to continuous linear maps $C_0^\infty(M) \rightarrow \mathcal{D}'_0(M)$, which define—by the Schwartz Nuclear Theorem—the bidistributions, also denoted $E_{A,R}$ and E :

$$\begin{aligned} E_{A,R}(f, g) &:= \langle f, E_{A,R}g \rangle = \int_{M \times M} d\text{vol}_g(x) d\text{vol}_g(y) E_{A,R}f(x)g(y), \\ E(f, g) &:= \langle f, Eg \rangle = \int_{M \times M} d\text{vol}_g(x) d\text{vol}_g(y) Ef(x)g(y) \text{ for } f, g \in C_0^\infty(M, \mathbb{R}). \end{aligned}$$

Since the Klein-Gordon operator is formally self-adjoint, by Corollary 2.5, the bidistribution E is skew-symmetric:

$$E(f, g) := \langle f, Eg \rangle = -\langle Ef, g \rangle = -\langle g, Ef \rangle = -E(g, f);$$

hence, if the supports of f and g are causally separated, then $E(f, g)$ vanishes. We can rewrite Theorem 2.4 in terms of integral kernels:

$$P_x E_{A,R}(x, y) = \delta(x, y), E_A(x, y) = E_R(y, x) \text{ and } E(x, y) = -E(y, x),$$

and if x and y are causally separated, then $E(x, y)$ vanishes. Accordingly, $E(x, y)$ has the nature of a commutator function. Indeed, we can use E to define a Poisson bracket in a suitable space associated to classical observables; that's the subject of the next section.

A natural Poisson Bracket

Let Sol (Sol_{SC}) denotes the space of real-valued (spacelike-compact) solutions to the Klein-Gordon equation:

$$\text{Sol} := \{\phi \in C^\infty(M, \mathbb{R}) : P\phi = 0\} \quad \text{and} \quad \text{Sol}_{SC} := \text{Sol} \cap C^\infty_{SC}(M, \mathbb{R}).$$

Consider the quotient space $\mathcal{E} := C_0^\infty(M, \mathbb{R})/PC_0^\infty(M, \mathbb{R})$. For each equivalence class $[f]$ in \mathcal{E} , we can define an observable on the space of solutions Sol through the map:

$$\text{Sol} \ni \phi \mapsto \mathcal{O}_{[f]}(\phi) := \langle f, \phi \rangle.$$

It is well-defined since, for $f \in C_0^\infty(M, \mathbb{R})$, we have $\langle f + Pg, \phi \rangle = \langle f, \phi \rangle \forall g \in C_0^\infty(M, \mathbb{R}) \Rightarrow$

$$\mathcal{O}_{[f]}(\phi) \text{ is independent of the representative of } [f].$$

We can interpret it as the *smeared classical field* $\phi(f) \equiv \mathcal{O}_{[f]}(\phi)$ and setting $f = \delta_x$ we recover the notion of an observable on configuration points $\phi(x)$. Thus, Sol can be seen as the space of pure states in the classical context. This means that, using \mathcal{E} , we have $[f]$ -labeled classical observables or *classical fields smeared with the test function f*: $\mathcal{O}_{[f]}(\phi) \sim \phi(f) \sim \langle f, \phi \rangle$. Then, \mathcal{E} is the space of linear on-shell observables of the free neutral Klein-Gordon field.

Remark 2.8. In fact, there is a one-to-one correspondence between compactly supported solutions of the Klein-Gordon equation and initial data on an arbitrary but fixed Cauchy surface on Σ on the globally hyperbolic spacetime M which implies³ that the algebra $\mathcal{A}(M)$ satisfies the Time-Slice Axiom of the Haag-Kastler framework discussed in section 1.3.

Using the causal propagator E from Theorem 2.7, we can naturally equip \mathcal{E} with a symplectic form $\tau : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{R}$, as in the following proposition.

Proposition 2.9. (Symplectic Space) *Let $\tau : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{R}$ defined by $\tau([f], [g]) := \langle f, Eg \rangle$, then (\mathcal{E}, τ) is a symplectic space.*

³For proofs, check out [11, 19].

Proof. τ is a symplectic form, since:

τ is bilinear: since $\langle \cdot, \cdot \rangle$ is bilinear;

τ is well-defined: any element $f \in [f]$ can be written as $f = h_{[f]} + Ph_f$, where $h_{[f]} \in C_0^\infty(M, \mathbb{R})$ is fixed for $[f]$ and $h_f \in C_0^\infty(M, \mathbb{R})$ depends on the chosen representative f . Since $E \circ P = 0$, we have

$$\begin{aligned} \langle f, Eg \rangle &= \langle h_{[f]} + Ph_f, E(h_{[g]} + Ph_g) \rangle \\ &= \langle h_{[f]}, h_{[g]} \rangle + \langle h_{[f]}, E(Ph_g) \rangle + \langle Ph_f + E(Ph_{[g]}) \rangle + \langle Ph_f + E(Ph_g) \rangle \\ &= \langle h_{[f]}, Eh_{[g]} \rangle \text{ which does not depends on the representatives } f \text{ and } g \text{ chosen; } \end{aligned}$$

τ is antisymmetric: $\langle f, Eg \rangle = -\langle Ef, g \rangle = -\langle g, Ef \rangle$ since E is skew-symmetric;

τ is weakly non-degenerate: If $\tau([f], [g]) = 0 \forall [g] \in \mathcal{E}$, then

$$\langle f, Eg \rangle = -\langle Ef, g \rangle = 0 \forall g \in C_0^\infty(M, \mathbb{R});$$

but $\langle \cdot, \cdot \rangle$ is non-degenerate, so $Ef = 0$. Thus $f \xrightarrow{E} [f] = 0$;

τ is alternating: since E is skew-symmetric and $\langle \cdot, \cdot \rangle$ is symmetric

$$\tau([f], [f]) = \langle f, Ef \rangle = -\langle Ef, f \rangle = -\langle f, Ef \rangle = 0;$$

\therefore the pair (\mathcal{E}, τ) is a symplectic space. \square

Proposition 2.10. *The causal propagator $E : C_0^\infty(M, \mathbb{R}) \rightarrow C_{SC}^\infty(M, \mathbb{R})$ descends to a bijective map $E : \mathcal{E} \rightarrow \text{Sol}_{SC}$.*

Proof. Let $E : C_0^\infty(M, \mathbb{R}) \rightarrow C_{SC}^\infty(M, \mathbb{R})$ and define $\tilde{E} : C_0^\infty(M, \mathbb{R})/PC_0^\infty(M, \mathbb{R}) \rightarrow \text{Sol}_{SC}$ as

$$[f] \mapsto \tilde{E}([f]) = \tilde{E}(h_{[f]} + Ph_f) := Eh_{[f]}.$$

Since $Eh_{[f]} \in C_{SC}^\infty(M, \mathbb{R})$ and $P(Eh_{[f]}) = 0$, we have that $Eh_{[f]} \in \text{Sol}_{SC}$. Furthermore, $\tilde{E}([0]) = \tilde{E}(0 + Ph_0) = E.0 = 0$ and every $\phi \in \text{Sol}_{SC}$ can be written as $\phi = Ef$ for some $f \in C_0^\infty(M, \mathbb{R})$, then $\tilde{E} : \mathcal{E} \rightarrow \text{Sol}_{SC}$ is bijective; which will also be referred to as E . \square

Definition 2.11. (Future and past part) Let χ be a *cutoff* function, *i.e.* $\chi \equiv 0$ in the future of some Cauchy surface Σ_2 and $\chi \equiv 1$ in the past of some Cauchy surface Σ_1 , such that $\Sigma_2 \subset I^+(\Sigma_1)$. The *future and past part* of $f \in C^\infty(M, \mathbb{R})$ are, respectively:

$$f^+ := (1 - \chi)f \quad \text{and} \quad f^- := \chi f.$$

Proposition 2.12. *Let $\langle \cdot, \cdot \rangle_{\text{Sol}}$ be defined on solutions with compact overlapping support by:*

$$\text{Sol} \times \text{Sol} \ni (\phi_1, \phi_2) \mapsto \langle \phi_1, \phi_2 \rangle_{\text{Sol}} := \langle P\phi_1^+, \phi_2 \rangle,$$

then $\langle \cdot, \cdot \rangle_{\text{Sol}}$ is well-defined and antisymmetric.

Proof. Let $\langle \cdot, \cdot \rangle_{\text{Sol}}$ as above, then it is:

well-defined: let $\phi_1, \phi_2 \in \text{Sol}$ and let α and β be two different cutoff functions. Then

$$\phi_{1,\alpha}^+ = (1 - \alpha)\phi_1 \text{ and } \phi_{1,\beta}^+ = (1 - \beta)\phi_1,$$

$$\begin{aligned} \langle \phi_1, \phi_2 \rangle_{\text{Sol},\alpha} - \langle \phi_1, \phi_2 \rangle_{\text{Sol},\beta} &= \langle P\phi_{1,\alpha}^+, \phi_2 \rangle - \langle P\phi_{1,\beta}^+, \phi_2 \rangle \\ &= \langle P(\beta - \alpha)\phi_1, \phi_2 \rangle = \langle (\beta - \alpha)\phi_1, P\phi_2 \rangle = 0 \end{aligned}$$

because $(\beta - \alpha)\phi_1$ is a smooth function with compact support. Thus $\langle \phi_1, \phi_2 \rangle_{\text{Sol}}$ is independent of the cutoff function.

antisymmetric: note that the dual pairing $\langle u, f \rangle$ is defined for $f \in C^\infty(M, \mathbb{R})$ and $u \in \mathcal{D}'_0(M, \mathbb{R})$. Furthermore, $\langle Pf, \phi \rangle = \langle f, P\phi \rangle = 0$ if f has compact support. Also, if $\text{supp}\phi_1$ or $\text{supp}\phi_2$ is compact, then $\langle \phi_1, \phi_2 \rangle_{\text{Sol}}$ is zero. Let $\phi_1, \phi_2 \in \text{Sol}$ with compact overlapping support, *i.e.* $\text{supp}\phi_1 \cap \text{supp}\phi_2$ is non-empty and compact, yet not necessarily $\text{supp}\phi_1$ or $\text{supp}\phi_2$ is compact, then: $\langle \phi_1, \phi_2 \rangle_{\text{Sol}} := \langle P\phi_1^+, \phi_2 \rangle =$

$$\begin{aligned} &= \langle P(\phi_1^+ + \phi_2^+), \phi_2 \rangle - \langle P\phi_2^+, \phi_2 \rangle \\ &= \langle P(\phi_1^+ + \phi_2^+), \phi_1 + \phi_2 \rangle - \langle P\phi_2^+, \phi_2 \rangle - \langle P(\phi_1^+ + \phi_2^+), \phi_1 \rangle \\ &= \langle P(\phi_1^+ + \phi_2^+), \phi_1 + \phi_2 \rangle - \langle P\phi_2^+, \phi_2 \rangle - \langle P(\phi_1^+ + \phi_2^+), \phi_1 \rangle - \langle P\phi_2^+, \phi_1 \rangle + \langle P\phi_2^+, \phi_1 \rangle \\ &= \langle P(\phi_1^+ + \phi_2^+), \phi_1 + \phi_2 \rangle - \langle P\phi_2^+, \phi_2 - \phi_1 \rangle - \langle P(\phi_1^+ + \phi_2^+), \phi_1 \rangle - \langle P\phi_2^+, \phi_1 \rangle. \end{aligned}$$

Since $\text{supp}(\phi_1 \pm \phi_2) = \text{supp}\phi_1 \cap \text{supp}\phi_2$ is compact, the first three terms on the RHS are zero.

\therefore the pair $(\text{Sol}_{SC}, \langle \cdot, \cdot \rangle_{\text{Sol}})$ is a symplectic space. \square

Corollary 2.13. Let $f \in C_0^\infty(M, \mathbb{R})$ and $\phi \in \text{Sol}$, then $\langle f, \phi \rangle = \langle Ef, \phi \rangle_{\text{Sol}}$.

Proof. Let $f \in C_0^\infty(M, \mathbb{R})$ and $\phi \in \text{Sol}$. There is a cutoff function such that $(Ef)^+ = E_R f \Rightarrow$

$$\langle Ef, \phi \rangle_{\text{Sol}} = \langle P(E_R f), \phi \rangle = \langle \text{id}_{C_0^\infty(M, \mathbb{R})}(f), \phi \rangle = \langle f, \phi \rangle.$$

\square

Proposition 2.14. Let $f, g \in C_0^\infty(M, \mathbb{R})$, then $\tau([f], [g]) = \langle Ef, Eg \rangle_{\text{Sol}}$. Thus (\mathcal{E}, τ) and $(\text{Sol}_{SC}, \langle \cdot, \cdot \rangle_{\text{Sol}})$ are symplectically isomorphic through E .

Proof. If $\phi \in \text{Sol}$, $f \in C_0^\infty(M, \mathbb{R})$, let $g \in C_0^\infty(M, \mathbb{R})$ such that $\phi = Eg$. Thus:

$$\tau([f], [g]) := \langle f, Eg \rangle = \langle f, \phi \rangle \stackrel{2.13}{=} \langle Ef, \phi \rangle_{\text{Sol}} = \langle Ef, Eg \rangle_{\text{Sol}};$$

\therefore the bijection $E : \mathcal{E} \rightarrow \text{Sol}_{SC}$ is then a symplectic isomorphism $(\mathcal{E}, \tau) \xrightarrow{E} (\text{Sol}_{SC}, \langle \cdot, \cdot \rangle_{\text{Sol}})$. \square

What the results above show is that through the causal propagator E , we have the symplectic isomorphism $(\mathcal{E}, \tau) \xrightarrow{E} (\text{Sol}_{SC}, \langle \cdot, \cdot \rangle)$ that enable us to look at $\mathcal{O}_u(\phi)$ as the *classical field symplectically smeared with a test solution u* :

$$\begin{aligned}\mathcal{O}_{[f]}(\phi) &\sim \mathcal{O}_u(\phi) = \langle u, \phi \rangle_{\text{Sol}} \text{ for some } u \in \text{Sol}_{SC} \text{ and} \\ (\mathcal{E}, \tau) &\cong (\text{Sol}_{SC}, \langle \cdot, \cdot \rangle_{\text{Sol}}) \equiv \text{classical phase space.}\end{aligned}$$

We can associate to τ a Poisson bracket⁴:

$$\{\phi(f), \phi(g)\} \cong \tau([f], [g]) = \langle f, Eg \rangle = E(f, g). \quad (2.1.1)$$

Note, however, that (2.1.1) is written in a covariant form. Let's rewrite it in the *equal-time* version of usual QFT, *i.e.* $\{\phi(x), \phi(y)\} = E(x, y)$ has the equal-time equivalent Poisson brackets of the field $\phi(x)$ and its canonical momentum $\nabla_{\mathbf{n}}\phi(x)$:

$$\{\nabla_{\mathbf{n}}\phi(x)|_{\Sigma}, \phi(y)|_{\Sigma}\} = \nabla_{\mathbf{n}}E(x, y)|_{\Sigma \times \Sigma} = \delta_{\Sigma}(x, y) \text{ and } \{\phi(x)|_{\Sigma}, \phi(y)|_{\Sigma}\} = E(x, y)|_{\Sigma \times \Sigma} = 0.$$

Proposition 2.15. *Let Σ be a Cauchy surface on (M, g) with unit future-pointing normal vector field \mathbf{n} and canonical measure $d\Sigma$ induced by $d\text{vol}_g(x)$. Let $\phi_1, \phi_2 \in \text{Sol}$ with spacelike-compact overlapping support, then:*

$$\langle \phi_1, \phi_2 \rangle_{\text{Sol}} = \int_{\Sigma} d\Sigma \mathbf{n}^{\mu} (\phi_1 \nabla_{\mu} \phi_2 - \phi_2 \nabla_{\mu} \phi_1).$$

Proof. Let $f \in C_0^{\infty}(M, \mathbb{R})$ such that $\phi_1 = Ef$, we have:

$$\langle \phi_1, \phi_2 \rangle_{\text{Sol}} = \langle Ef, \phi_2 \rangle_{\text{Sol}} = \langle f, \phi_2 \rangle = \int_M d\text{vol}_g f \phi_2 = \int_{\Sigma^+} d\text{vol}_g f \phi_2 + \int_{\Sigma^-} d\text{vol}_g f \phi_2.$$

By Stokes theorem and using

$$0 = \int_M d\text{vol}_g Ef P \phi_2 = \int_M d\text{vol}_g (E_A - E_R) f P \phi_2 = \int_{\Sigma^+} d\text{vol}_g E_A f P \phi_2 + \int_{\Sigma^-} d\text{vol}_g E_R f P \phi_2,$$

one can easily conclude the proof. \square

Note that $\langle \phi_1, \phi_2 \rangle_{\text{Sol}} = E(f_1, f_2) = \tau([f_1], [f_2])$.

Proposition 2.16. *Let $f \in C_0^{\infty}(\Sigma, \mathbb{R})$, then $\nabla_{\mathbf{n}}Ef|_{\Sigma} = f$, $Ef|_{\Sigma} = 0$. In terms of level of distributions kernels:*

$$\nabla_{\mathbf{n}}E(x, y)|_{\Sigma \times \Sigma} = \delta_{\Sigma}(x, y) \text{ and } E(x, y)|_{\Sigma \times \Sigma} = 0.$$

Proof. This is a sketch of the proof based on the carefully commented reference [29, Cor1.2]. Let $u_0, u_1 \in C_0^{\infty}(\Sigma, \mathbb{R})$, $f \in C_0^{\infty}(M, \mathbb{R})$ and Σ be a Cauchy surface on (M, g) such that:

$$Pu = f, u|_{\Sigma} = u_0, \nabla_{\mathbf{n}}u|_{\Sigma} = u_1.$$

⁴One can justify this identification of the Poisson bracket with symplectic geometry arguments, as done by Fewster in [34, Pg20].

Define ρ_0 and ρ_1 as the operators: $\rho_0 u = u_0$ and $\rho_1 u = u_1$ with adjoints $\bar{\rho}_0$ and $\bar{\rho}_1$. From Proposition 2.15: $\langle f, u \rangle = \int_{\Sigma} d\Sigma u \nabla_{\mathbf{n}} (Ef) - \int_{\Sigma} d\Sigma Ef \nabla_{\mathbf{n}} u$, which can now be written as:

$$\begin{aligned} \langle f, u \rangle &= \langle u|_{\Sigma}, \nabla_{\mathbf{n}} (Ef) \rangle - \langle Ef|_{\Sigma}, \nabla_{\mathbf{n}} u \rangle = \langle \rho_0 u, \rho_1 Ef \rangle - \langle \rho_0 Ef, \rho_1 u \rangle = -\langle E\bar{\rho}_1 \rho_0 u, f \rangle + \langle f, E\bar{\rho}_0 \rho_1 u \rangle \\ &\Rightarrow \langle f, u \rangle = -\langle f, E\bar{\rho}_1 \rho_0 u \rangle + \langle f, E\bar{\rho}_0 \rho_1 u \rangle. \end{aligned}$$

Thus, in the distributional sense $u = E\bar{\rho}_0 u_1 - E\bar{\rho}_1 u_0$. Therefore:

- Applying ρ_0 : $\rho_0 u = \rho_0 E\bar{\rho}_0 u_1 - \rho_0 E\bar{\rho}_1 u_0 \Rightarrow \rho_0 E\bar{\rho}_0 = 0$ and $-\rho_0 E\bar{\rho}_1 = 1$.
- Applying ρ_1 : $\rho_1 u = \rho_1 E\bar{\rho}_0 u_1 - \rho_1 E\bar{\rho}_1 u_0 \Rightarrow \rho_1 E\bar{\rho}_0 = 1$ and $-\rho_1 E\bar{\rho}_1 = 0$.

$$\therefore \nabla_{\mathbf{n}} Ef|_{\Sigma} = \rho_1 E\bar{\rho}_0 f = f \quad \text{and} \quad Ef|_{\Sigma} = E\bar{\rho}_0 = \rho_0 E\bar{\rho}_0 = 0.$$

□

The above can be compactified in the following sentence:

The space of observables ($\{\phi(f) : f \in C_0^{\infty}(M, \mathbb{R})\}, \{\cdot, \cdot\}$) provides a complete dynamical description of the underlying system since it is also a copy of the phase space.

Now that we have classical observables, we can construct the quantized algebra of observables as the unital $*$ -algebra generated by $\{\phi(f) : f \in C_0^{\infty}(M)\}$ and impose the (expected) relations on it. For convenience, we allow smearings with complex functions $f \in C_0^{\infty}(M) \equiv C^{\infty}(M, \mathbb{R}) \otimes iC^{\infty}(M, \mathbb{R})$, defined by:

$$\phi(f) := \mathcal{O}_{[\text{Ref}]}(\phi) + i\mathcal{O}_{[\text{Im}f]}(\phi).$$

Let's see how this is done.

2.2 Algebra of Observables

Where we construct the quantized algebra of observables. One familiar with the Borchers-Uhlmann algebra will notice the same essence here.

In this section, we construct the quantized algebra $\mathcal{A}(M)$ of linear hermitean observables that satisfies the Klein-Gordon(KG) equation and the canonical commutation relations(CCR) from the classical observables we studied in the last section by taking the quotient of the unital $*$ -algebra generated by $\{\phi(f) : f \in C_0^{\infty}(M)\}$ with the desired relations:

$$\mathcal{A}(M) \equiv \frac{\text{unital } *-\text{algebra generated by the classical observables } \{\phi(f) : f \in C_0^{\infty}(M)\}}{\text{Linearity} + \text{Hermiticity} + \text{KG} + \text{CCR}}$$

For a review on basic definitions—algebra, homeomorphism, involution, ideal, *etc*—the reader can check chapter 1 of [8]. For a deeper understanding of operator algebras, there are Kadison's books, like [77]. Intuitively, we can generate an algebra \mathcal{A}_G given a set G , whose elements we call *generators*, by taking the smallest algebra that contains the elements of G , products among them and linear combinations. We can define this algebra with a universal property, as below.

Definition 2.17. (Freely generated algebra) An algebra \mathcal{A}_G is said to be *freely generated by the set G* if there is a map $\gamma : G \rightarrow \mathcal{A}_G$ such that, for any other algebra \mathcal{B} and map $\beta : G \rightarrow \mathcal{B}$, there exists a unique algebra homomorphism $h : \mathcal{A}_G \rightarrow \mathcal{B}$ such that $\beta = h \circ \gamma$.

Remark 2.18. \mathcal{A}_G is uniquely determined by G —any two algebras freely generated by G are isomorphic—and for every set G , there does exist such a pair (\mathcal{A}_G, γ) ; thus, the above is a good definition. Actually, we need a $*$ -algebra to define adjoints through the involution operation $(\phi(f)\phi(g))^* = \phi(\bar{g})\phi(\bar{f})$; for a $*$ -algebra freely generated by G , just replace “algebra” for “ $*$ -algebra” everywhere in the definition above—which gives a total of three replacements. For convenience, we will omit the word *freely* from now on.

Let \mathcal{A}_G be the unital $*$ -algebra generated by: $G = \{\phi(f) : f \in C_0^\infty(M)\}$. For all $f, g \in C_0^\infty(M)$ and $a, b \in \mathbb{C}$, let R be the following set of relations:

$$\begin{aligned} \text{Linearity} \quad & 0 = \phi(af + g) - a\phi(f) - \phi(g); \\ \text{Hermiticity} \quad & 0 = \phi(f)^* - \phi(\bar{f}); \\ \text{Klein-Gordon} \quad & 0 = \phi((- \square + m^2 + \xi R)f); \\ \text{CCR} \quad & 0 = [\phi(f), \phi(g)] - E(f, g)\mathbb{1}. \end{aligned}$$

To impose this set of relations R on \mathcal{A}_G is to make sure that the right-hand side of the relations are zero, *i.e.* “ $R = 0$ ”; since we are not dealing with C^* or Banach algebras and we have an explicit set of relations, it suffices to take the quotient⁵, symbolically “ $\mathcal{A}(M) = \mathcal{A}_G/R$ ”. Formally, each relation $r \in R$ corresponds to an ideal \mathcal{I}_r of the algebra, so if we take the intersection of them $\mathcal{I}_R = \bigcap_{r \in R} \mathcal{I}_r$, then:

$$\mathcal{A}(M) := \mathcal{A}_G/\mathcal{I}_R.$$

Remark 2.19. The above also specify that R is the *only* set of relations satisfied by the elements of $\mathcal{A}(M)$ —it is *simple*: we can not impose any further relation to it without it collapsing to a trivial algebra[79, Pg19]. Fortunately, $\mathcal{A}(M)$ is *not trivial*: it is, in fact, isomorphic to the symmetric tensor vector space $\bigoplus_{n=0}^{\infty} \text{Sol}(M)^{\odot n}$ [33, Pg41].

A physical theory always determines measurements

In the algebraic approach, states are normalized positive linear functionals on the algebra $\mathcal{A}(M)$ and the expectation value of an observable a in a state ω is given by $\omega(a) \in \mathbb{C}$.

Definition 2.20. (State and expectation value) A *state* ω on $\mathcal{A}(M)$ is a linear functional

$$\omega : \mathcal{A}(M) \rightarrow \mathbb{C}, \text{ satisfying } \begin{cases} \text{positivity} & \omega(a^*a) \geq 0 \forall a \in \mathcal{A}(M); \\ \text{normalization} & \omega(\mathbb{1}) = 1. \end{cases}$$

and $\omega(a)$ is called the *expectation value* of the observable $a \in \mathcal{A}(M)$ at the state ω .

⁵[2] is a really nice reference that illuminates this construction; it is about tensor products and it helps in understanding quotient spaces taken with relations.

Remark 2.21. Note that the set of states on $\mathcal{A}(M)$ is a convex body, that is: if ω_1 and ω_2 are states, then the convex linear combination $\lambda\omega_1 + (1 - \lambda)\omega_2$, for $\lambda \in (0, 1)$, is also a state on $\mathcal{A}(M)$.

Definition 2.22. (Pure and mixed states) A state ω is called a *pure state*, or *extremal state*, if $\omega = \lambda\omega_1 + (1 - \lambda)\omega_2$, for $\lambda \in (0, 1)$, implies $\omega_1 = \omega_2 = \omega$; that is, it cannot be written as a convex linear combination. A state that is not pure is called a *mixed state*.

Let's see some properties of states, that will be useful in the next section.

Proposition 2.23. (Properties of states) Let ω be a state on $\mathcal{A}(M)$, and $a, b \in \mathcal{A}(M)$, then:

$$(a, b) \mapsto \omega(b^*a) \text{ is a positive semi-definite, hermitean, sesquilinear form; } \quad (2.2.1)$$

$$|\omega(b^*a)|^2 \leq \omega(a^*a)\omega(b^*b) \text{ (Cauchy-Schwarz inequality); } \quad (2.2.2)$$

$$\omega(a^*) = \overline{\omega(a)}; \quad (2.2.3)$$

$$\omega(a^*a) = 0 \iff \omega(ca) = 0 \forall c \in \mathcal{A}(M). \quad (2.2.4)$$

Proof. By construction, $(a, b) \mapsto \omega(b^*a)$ is positive, semi-definite sesquilinear form. Now, let $c = za + b$ for $z \in \mathbb{C}$, $a, b \in \mathcal{A}(M)$, then:

$$\omega(c^*c) = \bar{z}z\omega(a^*a) + \bar{z}\omega(a^*b) + z\omega(b^*a) + \omega(b^*b) \geq 0 \Rightarrow \text{Im}[\bar{z}\omega(a^*b) + z\omega(b^*a)] \geq 0;$$

setting $z = 1$ and then $z = i$ we get $\omega(a^*b) = \omega(b^*a)$, that is, the form in (2.2.1) is hermitean. For $z = -\omega(a^*b)/\omega(a^*a)$ in the above, it follows Cauchy-Schwarz inequality. (2.2.3) holds because $\mathcal{A}(M)$ is unital: $\omega(a^*) = \omega(a^*1) \stackrel{2.2.1}{=} \overline{\omega(1^*a)} = \overline{\omega(a)}$. Regarding the last property, we have that if $\omega(ba) = 0 \forall b \in \mathcal{A}(M)$, of course it holds $\omega(a^*a) = 0$, since $\mathcal{A}(M)$ is closed under the involution operation. Now suppose $\omega(a^*a) = 0$. By the Cauchy-Schwartz inequality:

$$\forall b \in \mathcal{A}(M) : |\omega(ba)|^2 \leq \omega(a^*a)\omega(b^*b) = 0 \Rightarrow \omega(ba) = 0.$$

□

By analysing the general form of an element $a \in \mathcal{A}(M)$ we obtain a crucial symmetry property of states. Recall that an algebra is a vector space $(X, +, \cdot)$, over a field \mathbb{K} , closed under a binary operation \circ distributive over $+$:

$$(a + b) \circ c = a \circ c + b \circ c \quad \text{and} \quad c \circ (a + b) = c \circ a + c \circ b$$

for a, b and c in X ; and compatible with scalar multiplication:

$$(\alpha A) \circ (\beta B) = (\alpha\beta)(a \circ b) \forall \alpha, \beta \in \mathbb{K}.$$

Thus, our algebra $\mathcal{A}(M)$, being generated by $\{\phi(f)\}$ and the unit, will contain sums and products and scalar multiplications of the objects $\phi(f)$, for $f \in C_0^\infty(M)$ ⁶, i.e. an element $a \in \mathcal{A}(M)$ is a *finite polynomial* of the form:

$$a = c_0 \mathbb{1} + \sum_{i_1} c_{(1)}^{i_1} \phi(f_{i_1}^{(1)}) + \sum_{i_1, i_2} c_{(2)}^{i_1 i_2} \phi(f_{i_1}^{(2)}) \phi(f_{i_2}^{(2)}) + \cdots + \sum_{i_1 \dots i_n} c_{(n)}^{i_1 \dots i_n} \phi(f_{i_1}^{(n)}) \dots \phi(f_{i_n}^{(n)}); \quad (2.2.5)$$

where $c_{(k)}^{i_1 \dots i_k} \in \mathbb{C}$, $f_k^{(j)} \in C_0^\infty(M)$ and all sums are finite. From (2.2.5), follows two remarks:

⁶Note that the adjoints are included in this, since we imposed the hermiticity property.

1. If ω is a state, then $\omega(A)$ is completely characterized by its n -point functions:

$$C_0^\infty(M) \times \dots \times C_0^\infty(M) \ni (f_1, \dots, f_n) \mapsto \omega(\phi(f_1) \dots \phi(f_n)) =: \omega_n(f_1, \dots, f_n).$$

This means that if two states have the same n -point functions, they necessarily coincide. For a continuous ω_n , by the Schwartz kernel theorem, we can write the n -point function in terms of its distribution kernel:

$$\omega_n(f_1, \dots, f_n) = \int_{M^n} \omega_n(x_1, \dots, x_n) d\text{vol}_{M^n}.$$

2. $\mathcal{A}(M)$ is a *filtered* algebra: $\mathcal{A}(M) = \bigcup_{n=0}^{\infty} \mathcal{A}_n(M)$, where each linear subspace $\mathcal{A}_n(M)$ contains polynomials of at most n generators $\phi(f_i)$, $i \in \{1, \dots, n\}$. Since the canonical commutation relations holds for $\mathcal{A}(M)$, permutations of generators $\phi(f_1), \dots, \phi(f_n)$ will not all be independent.

Regarding item 2, let's consider a simple example: a permutation that swap only $1 \leftrightarrow 2$. Let ω be a state, and consider its n -point function on the two observables $\phi(f_1)\phi(f_2) \dots \phi(f_n)$, $\phi(f_2)\phi(f_1) \dots \phi(f_n) \in \mathcal{A}_n(M)$, then:

$$\begin{aligned} \omega(\phi(f_1)\phi(f_2) \dots \phi(f_n)) - \omega(\phi(f_2)\phi(f_1) \dots \phi(f_n)) &= \omega([\phi(f_1), \phi(f_2)] \dots \phi(f_n)) \\ &= iE(f_1, f_2)\omega(\phi(f_3) \dots \phi(f_n)) \\ \Rightarrow \omega_n(f_1, f_2, \dots, f_n) - \omega_n(f_2, f_1, \dots, f_n) &= iE(f_1, f_2)\omega_{n-2}(f_3, \dots, f_n). \end{aligned}$$

This means that the n -point functions of $\phi(f_1), \dots, \phi(f_n)$ and $\phi(f_{\sigma(1)}) \dots \phi(f_{\sigma(n)})$ at ω coincide up to $(n-2)$ -order terms for any permutation of two indices, hence, for any permutation σ . Equivalently, the n -point functions coincide at the quotient $\mathcal{A}_n(M)/\mathcal{A}_{n-2}(M)$. Herewith, for any permutation of the indices i_1, \dots, i_k , the k -point function coincides at k -order, thus for the k^{th} -order term in the general element form (2.2.5):

$$\sum_{i_1 \dots i_k} c_{(k)}^{i_1 \dots i_k} \phi(f_{i_1}^{(k)}) \dots \phi(f_{i_k}^{(k)}),$$

we can take $c_{(k)}^{i_1 \dots i_k}$ to be fully symmetric coefficients, *i.e.*

The symmetric part of the n -point functions completely specify a state.

Since we are particularly interested in the energy-momentum tensor, we can focus on the two-point function, defined as the bilinear functional:

$$\begin{aligned} \omega_2 : C_0^\infty(M) \otimes C_0^\infty(M) &\rightarrow \mathbb{C} \\ (f, g) \equiv f \otimes g &\mapsto \omega_2(f, g) \equiv \omega_2(f \otimes g). \end{aligned}$$

Proposition 2.24. (Properties of the two-point function). Consider a state ω on $\mathcal{A}(M)$, P the Klein-Gordon operator as before and $f, g \in C_0^\infty(M)$. Then, ω_2 satisfies:

$$\omega_2(Pf, g) = \omega_2(f, Pg) = 0; \quad (2.2.6)$$

$$\omega_2(f, g) - \omega_2(g, f) = iE(f, g); \quad (2.2.7)$$

$$\overline{\omega_2(f, g)} = \omega_2(\bar{g}, \bar{f}); \quad (2.2.8)$$

$$\omega_2(f, g) = \frac{1}{2}(\omega_2(f, g) + \omega_2(g, f)) + \frac{i}{2}E(f, g). \quad (2.2.9)$$

Proof. We have that identity

(2.2.6) holds since ω is linear:

$$\omega_2(Pf, g) := \omega(\phi(Pf)\phi(g)) = \omega(0) = 0 = \omega(\phi(f)\omega(Pg)) =: \omega_2(f, Pg);$$

(2.2.7) holds since ω is a state:

$$\begin{aligned} \omega_2(f, g) - \omega_2(g, f) &= \omega(\phi(f)\phi(g)) - \omega(\phi(g)\phi(f)) = \omega([\phi(f), \phi(g)]) = \omega(iE(f, g)\mathbb{1}) \\ &= iE(f, g)\omega(\mathbb{1}) = iE(f, g); \end{aligned}$$

(2.2.8) holds because of the hermiticity property:

$$\overline{\omega_2(f, g)} = \overline{\omega(\phi(f)\phi(g))} = \omega((\phi(f)\phi(g))^*) = \omega(\phi(g)^*\phi(f)^*) = \omega(\phi(\bar{g})\phi(\bar{f})) = \omega_2(\bar{g}, \bar{f});$$

(2.2.9) follows directly from (2.2.7):

$$\frac{1}{2}\omega_2(f, g) = \frac{1}{2}\omega_2(g, f) + \frac{i}{2}E(f, g) \Rightarrow \omega_2(f, g) = \frac{1}{2}(\omega_2(f, g) + \omega_2(g, f)) + \frac{i}{2}E(f, g).$$

In the case f and g are real functions we have $\omega_2(g, f) = \omega_2(\bar{g}, \bar{f})$, then the symmetric part on the expression above is real and $\text{Im}(\omega_2(f, g)) = \frac{1}{2}E(f, g)$. \square

Although implicit in the previous discussion on the general form of an observable, given identity (2.2.9) it is manifest that:

All two-point functions have a symmetric state-dependent part and an antisymmetric common (state-independent) part.

The property above will be crucial in the quantum energy inequality derivation of next chapter. Now that we are familiar with algebraic states and we saw that, in the algebraic approach, the expectation value of an observable a of a system at the state ω is simply $\omega(a)$, we should ask ourselves: how this association connects with the usual approach of QFT? Moreover, if we do measure $\omega(a)$, how do we introduce the information that the measurement was realized? In the next section we state the connection between the algebraic approach and the usual approach of QFT. A good reference to understand this connection is Wald's book [115, Chap1-4], where one can find all of the subtleties of the subject highlighted and a nice discussion on the measurement question.

The connection with standard QFT

The Gelfand-Naimark-Segal Theorem establishes a connection between the algebraic formalism and the usual approach of QFT. It guarantees that for each state ω on a C^* -algebra \mathfrak{A} there is a $*$ -representation π_ω acting on a Hilbert space \mathcal{H}_ω with a cyclic vector Ψ_ω such that $\pi_\omega(\mathfrak{A})\Psi_\omega = \mathcal{H}_\omega$ and $\omega(a) = \langle \Psi_\omega, \pi_\omega(a)\Psi_\omega \rangle \forall a \in \mathfrak{A}$. Furthermore, for a fixed state ω , the so called GNS triple $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ is unique up to unitary equivalences. Consider a system at a state ω , the probability of a measurement of the self-adjoint observables $a_1, \dots, a_n \in \mathfrak{A}$, respectively at times t_1, \dots, t_n , to yield values inside the intervals $I_1, \dots, I_n \subset \mathbb{R}$ is defined by:

$$p := \lim_{i_1, \dots, i_n \rightarrow \infty} \omega((q_1)_{i_1} \dots (q_n)_{i_n} (q_n)_{i_n} \dots (q_1)_{i_1}), \quad (2.2.10)$$

where $\{(q_k)_{i_k}\}_{k \in \mathbb{N}}$ is a sequence of polynomials in a_k such that $(q_k)_{i_k}(x)$ are uniformly bounded on the spectrum of a_k and converges pointwise to the characteristic function of the interval I_k . Let $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ be the GNS representation for the state ω , with a simple computation, we get:

$$\begin{aligned} \omega((q_1)_{i_1} \dots (q_n)_{i_n} (q_n)_{i_n} \dots (q_1)_{i_1}) = \\ \text{tr} \{ (q_n)_{i_n} [\pi_\omega(a_n)] \dots (q_1)_{i_1} [\pi_\omega(a_1)] \rho (q_1)_{i_1} [\pi_\omega(a_1)] \dots (q_n)_{i_n} [\pi_\omega(a_n)] \}. \end{aligned}$$

Where we defined $\rho := |\Psi_\omega\rangle\langle\Psi_\omega|$. It is easy to see that the intuition behind the definition (2.2.10) above is the procedure in the standard formalism of considering the projections P_k of a_k on the interval I_k and defining the probability of a measurement at the state $|\Psi\rangle$ as $\frac{P|\Psi\rangle}{\|P|\Psi\rangle\|}$, which give us in the Heisenberg picture: $p := \text{tr}\{P_n \dots P_1 \rho P_1 \dots P_n\}$, where ρ is the density matrix associated to $|\Psi\rangle$. For details, proofs and references, one can check [115, Sec4.5]. Here, the goal is to illustrate that with the GNS Theorem we can recover the usual Hilbert space representation and the usual probability formalism.

Note that we defined the algebra of observables $\mathcal{A}(M)$ as a $*$ -algebra, not as a C^* -algebra—working with bounded or unbounded observables is arbitrary since both should yield the same experimental results: one can measure with a usual ruler r or with its hyperbolic tangent ruler $\tanh r$. For the argument on the probabilities above, it was technically convenient to consider C^* -algebras, but for many analysis, we do not even need a norm. To derive a quantum energy inequality, for example, we can remain with the more general $*$ -algebra structure. In addition, there is a generalized version for the GNS Theorem, given in [79].

Theorem 2.25. [79, Thm1](The GNS construction for a $*$ -algebra) *Let ω be a state on the unital $*$ -algebra \mathcal{A} . Then, there exists a quadrupole $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ such that:*

- (i) \mathcal{H}_ω is a complex Hilbert space;
- (ii) $\pi_\omega : \mathcal{A} \rightarrow \mathcal{L}(\mathcal{D}_\omega)$ is a $*$ -representation of \mathcal{A} on \mathcal{H}_ω with domain \mathcal{D}_ω ;
- (iii) $\pi_\omega(\mathcal{A})\Psi_\omega = \mathcal{D}_\omega$;
- (iv) $\omega(a) = \langle \Psi_\omega, \pi_\omega(a)\Psi_\omega \rangle \forall a \in \mathcal{A}$.

Furthermore, if $(\mathcal{H}'_\omega, \mathcal{D}'_\omega, \pi'_\omega, \Psi'_\omega)$ also satisfies (i-iv), then there exists $U : \mathcal{H}_\omega \rightarrow \mathcal{H}'_\omega$ surjective, isometric and such that:

- (v) $U\Psi_\omega = \Psi'_\omega$;
- (vi) $U\mathcal{D}_\omega = \mathcal{D}'_\omega$;
- (vii) $U\pi_\omega(a)U^{-1} = \pi'_\omega(a) \forall a \in \mathcal{A}$.

Proof. The proof of the existence of $(\mathcal{H}_\omega, \mathcal{D}_\omega, \pi_\omega, \Psi_\omega)$ is analogous to the usual GNS theorem: define $N := \{a \in \mathcal{A} : \omega(a^*a) = 0\}$ and then define \mathcal{D}_ω as the quotient \mathcal{A}/N ; we can equip \mathcal{D}_ω with the well-defined inner product $\langle [a], [b] \rangle := \omega(a^*b)$ and take \mathcal{H}_ω as the completion of $(\mathcal{D}_\omega, \langle \cdot, \cdot \rangle)$. The representation is defined by $\pi_\omega(a)[b] := [ab]$, which is well-defined since N is a left ideal by Proposition 2.23. Finally, Ψ_ω is defined as the equivalence class [1], thus $\pi_\omega(a)[1] := [a]$, then:

$$\omega(a) = \omega(1.a) = \langle [1], [a] \rangle = \langle \Psi_\omega, \pi_\omega(a)\Psi_\omega \rangle$$

and the above implies $\pi_\omega(a)^\dagger = \pi_\omega(a^*)$. For the second part, (v-vii), define $U : \mathcal{H}_\omega \rightarrow \mathcal{H}'_\omega$ by:

$$U\pi_\omega(a)\Psi_\omega := \pi'_\omega(a)\Psi'_\omega \quad \forall a \in \mathcal{A}. \quad (2.2.11)$$

Property (iii) implies that U is well-defined and surjective since, respectively, any $\Psi \in \mathcal{H}_\omega$ can be approximated by elements like $\pi_\omega(a)\Psi_\omega$ and (iii) also holds for $(\mathcal{H}'_\omega, \mathcal{D}'_\omega, \pi'_\omega, \Psi'_\omega)$; together with the definition (2.2.11), Property (vi) follows immediately. Moreover, since $\pi_\omega(1) = 1$, we have that (v) holds. For Property (vii), we analogously define $U' : \mathcal{H}'_\omega \rightarrow \mathcal{H}_\omega$, which is easily checked to be the inverse of U , thus:

$$U\pi_\omega(a)\Psi_\omega = U\pi_\omega(a)U^{-1}U\Psi_\omega \stackrel{(v)}{=} U\pi_\omega(a)\Psi'_\omega = \pi'_\omega(a)\Psi'_\omega \Rightarrow U\pi_\omega(a)U^{-1} = \pi'_\omega(a) \quad \forall a \in \mathcal{A}.$$

Finally, U is isometric since $\langle \Psi_\omega, \pi_\omega(a)\Psi_\omega \rangle \stackrel{(vii)}{=} \langle \Psi_\omega, U^{-1}\pi'_\omega(a)U\Psi_\omega \rangle = \langle \Psi'_\omega, \pi'_\omega(a)\Psi'_\omega \rangle$. This easy proof show the interesting fact that Properties (v-vii) follow directly from the definition of U , that is: U is completely determined by (2.2.11). \square

The theorem above guarantees that different GNS representations for the *same state* are unitarily equivalent. However, that is not true when we consider GNS representations for *different states* ω and ω' : it does not exist, in general, a surjective isometric operator $U : \mathcal{H}_\omega \rightarrow \mathcal{H}_{\omega'}$ such that $U\pi_\omega(a)\Psi_\omega := \pi_{\omega'}(a)\Psi_{\omega'} \forall a \in \mathcal{A}$. The great advantage of this approach is that, even though there are unitarily inequivalent Hilbert space representations for different states, the algebra allows us to not choose a representation: “the algebra has state-equality”.

In this section 2.2, we defined our quantized algebra of observables $\mathcal{A}(M)$ and studied properties of its states. We saw that states are determined by their n -point functions and that the two-point function has a common antisymmetric part determined by the causal propagator and a state-dependent symmetric part. Finally, by the GNS theorem we saw that we can recover the Hilbert space formalism associated to a fixed state ω on $\mathcal{A}(M)$. As it happens, the class of states acting on the algebra of observables is too large, in the next section we analyse which states are physically reasonable in the context of this dissertation, that is, for which states we can define the energy-momentum tensor⁷.

⁷Yet, note that the algebra of observables $\mathcal{A}(M)$ is not complete: the energy-momentum tensor itself is not an element of it.

2.3 Hadamard States

Where we name the physically allowable states as Hadamard states and we characterize them in two different ways, equivalent ways by the Radzikowski theorem.

The smeared field ϕ is a distribution and thus, for the Klein-Gordon field, $T_{\mu\nu}$ has products of distributions at the same spacetime point, which is not well-defined mathematically. To deal with this, we apply the two-point splitting procedure to consider the well-defined object $\phi(x)\phi(x')$ for x, x' distinct spacetime points.

Let ω and ω_0 be algebraic states acting on $\mathcal{A}(M)$. If $F(x, x') := \omega(\phi(x)\phi(x')) - \omega_0(\phi(x)\phi(x'))$ is a smooth function, then we can define the regularized renormalized expectation value for the energy-momentum tensor at a state ω as:

$$\langle T_{\mu\nu} \rangle_{\omega} := \lim_{x' \rightarrow x} \{ \nabla_{\mu} \nabla_{\nu'} F(x, x') - \frac{1}{2} g_{\mu\nu} ((\nabla_l \nabla^{l'} + m^2) F(x, x')) \}. \quad (2.3.1)$$

This procedure, however, does not make sense for all the states on the algebra. To start with, $F(x, x')$ has to be smooth. Furthermore, equation (2.3.1) does not suffice as a prescription for a physically meaningful expectation value for $T_{\mu\nu}$. A good expectation value for the energy-momentum tensor must be conserved, must be consistent with the local character of the algebraic approach and, to be consistent with the flat case, must vanish at the Poincaré vacuum state in Minkowski. These three considerations, plus expression (2.3.1) constitute the set of axioms given by Wald in [115, Pg89]. In the first section we see that $\langle T_{\mu\nu} \rangle_{\omega}$ is well-defined for states ω that satisfy the Hadamard condition, thus the physically reasonable states in this context are called Hadamard states.

The Hadamard condition restricts the singularity structure of the bidistributions $\phi(x)\phi(x')$ and imposes that it is like the *UV*-behavior of Minkowski vacuum. On the other hand, recall that the pointwise product of distributions is only well-defined if they somehow “balance each other”. At the points where their restrictions are smooth, we can, of course, take their product straightforwardly; but if one is not smooth at x for some direction k , but the other decays at exponential speed at the opposite direction $-k$ at the same point x , then they balance each other in such a way that we can also take their product at x . This is known as *Hörmander condition* and it is written in terms of the wavefront set, an object that compactify the information of points and directions of non-smoothness of a distribution and is defined in the formalism of Microlocal Analysis. In section 2.3.2, we review some definitions and results concerning distributions and Microlocal Analysis to understand how we associate the Hadamard condition to the Hörmander condition.

From one side, we get a condition on states being physically reasonable from the process of defining the energy-momentum tensor on curved spacetimes. From the other side, we have that states are distributions and for distributions we have Microlocal Analysis. Notably, Radzikowski theorem, which we see in section 2.3.3, allows us to translate the Hadamard condition to the formalism of Microlocal Analysis, providing us with a powerful mathematical tool to work with. In fact, this formalism we will use to derive a quantum inequality.

2.3.1 Hadamard condition from $T_{\mu\nu}$ -considerations

Where we accept that to obtain a regularized renormalized expectation value for the quantized $T_{\mu\nu}$ we must consider only Hadamard states.

The process of defining the energy-momentum tensor in Minkowski spacetime already has its subtleties. We can directly substitute the classical fields with the quantum field operators and obtain, straightforwardly, a quantized version of the energy-momentum tensor, symbolically $T_{\mu\nu}(\phi_{\text{classical}}) \rightarrow T_{\mu\nu}(\hat{\phi}_{\text{quantum}})$, but two complications emerge here. First, the zero-point energy is infinite. This is standardly solved by the regularization process called *normal ordering*, which is an *ad hoc* procedure for “subtracting the vacuum energy”. The other complication is that fields cannot be defined at points of spacetime, by Wightman’s work of 1964 [118], thus we consider smeared fields ϕ , that are, in fact, distributions. Henceforth, $T_{\mu\nu}$, for the Klein-Gordon field, has products of distributions at the same spacetime point, which is ill-defined in general.

In order to deal with the second complication we apply the *two-point splitting procedure*: even though $\phi^2(x)$ is not well-defined in general, the bidistribution $\phi(x)\phi(x')$ is. Furthermore, we can reformulate *normal-ordering* in a literal way that can be naturally generalized to curved spacetimes. Let’s see how this is done to understand how we can generalize the idea of “subtracting the vacuum energy”; for convenience, let’s consider $\phi(x)\phi(x')$ instead of $T_{\mu\nu}$, we can then introduce appropriately the derivatives in the expression.

Consider the standard Fock space representation in Minkowski spacetime with creation and annihilation operators $a_{\vec{k}}^\dagger$ and $a_{\vec{k}}$; we can write in momentum space:

$$\phi(x) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d\vec{k}}{\sqrt{2k_0}} (a_{\vec{k}}^\dagger e^{ikx} + a_{\vec{k}} e^{-ikx}).$$

Then:

$$\phi(x)\phi(x') = \frac{1}{(2\pi)^3} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d\vec{k}}{\sqrt{2k_0}} \frac{d\vec{k}'}{\sqrt{2k'_0}} (a_{\vec{k}}^\dagger e^{ikx} + a_{\vec{k}} e^{-ikx})(a_{\vec{k}'}^\dagger e^{ik'x'} + a_{\vec{k}'} e^{-ik'x'}).$$

The normal-ordered product $:\phi(x)\phi(x'):$ is defined by replacing $a_{\vec{k}} a_{\vec{k}'}^\dagger$ by $a_{\vec{k}'}^\dagger a_{\vec{k}}$ on the above expression, which *literally* corresponds to:

$$:\phi(x)\phi(x'):= \phi(x)\phi(x') - \frac{1}{(2\pi)^3} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d\vec{k}}{\sqrt{2k_0}} \frac{d\vec{k}'}{\sqrt{2k'_0}} (a_{\vec{k}} a_{\vec{k}'}^\dagger - a_{\vec{k}'}^\dagger a_{\vec{k}}) e^{-ikx} e^{ik'x'}.$$

Since $[a_{\vec{k}}, a_{\vec{k}'}^\dagger] = \delta^3(\vec{k} - \vec{k}')$ and $\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d\vec{k}}{\sqrt{2k_0}} e^{-ik(x-x')}$ is the two-point function $\omega_2^\Omega(x, x')$ of the vacuum state Ω in Minkowski spacetime, we have that normal-ordering is equivalent “to subtracting the vacuum energy”:

$$:\phi(x)\phi(x'):= \phi(x)\phi(x') - \omega_2^\Omega(x, x').$$

The point is that, although there is no straightforward generalization for normal ordering and fields cannot be defined at spacetime points, we can apply two-point splitting and we

can consider *differences with respect to a reference state*. Let's use this idea to define the regularized renormalized energy-momentum tensor in Minkowski spacetime; the following discussion is basically a short review of [115, Chp4]. The goal is to illustrate that we can, indeed, find a well-defined $\langle T_{\mu\nu} \rangle$ in a general curved spacetime.

Consider states ω of finite number of particles in the usual Fock space; those are considered physically reasonable in the standard formalism and they all share the same singular character that of Minkowski vacuum Ω . Thus, $F(x, x') := \langle \phi(x)\phi(x') \rangle_\omega - \langle \phi(x)\phi(x') \rangle_\Omega$ is a smooth function and we can take the coincidence limit to define the regularized renormalized expectation value $\langle \phi^2(x) \rangle_\omega$ as:

$$\langle \phi^2(x) \rangle_\omega = \lim_{x' \rightarrow x} F(x, x').$$

Then, we can define the regularized renormalized expectation value of the energy-momentum tensor at the state ω by:

$$\langle :T_{\mu\nu}: \rangle_\omega := \lim_{x' \rightarrow x} \{ \nabla_\mu \nabla_{\nu'} F(x, x') - \frac{1}{2} g_{\mu\nu} ((\nabla_l \nabla^{l'} + m^2) F(x, x')) \}. \quad (2.3.2)$$

The above discussion shows that we can define $\langle :T_{\mu\nu}: \rangle_\omega$ by the two-point splitting process in a way equivalent to "subtracting the vacuum energy" and that expression (2.3.2) is well-defined only if $F(x, x')$ is sufficiently differentiable. Even though in general curved spacetime we no longer have a preferred vacuum state, we can choose a reference state ω_0 to consider

$$F(x, x') := \langle \phi(x)\phi(x') \rangle_\omega - \langle \phi(x)\phi(x') \rangle_{\omega_0},$$

and, for distincts algebraic states ω and ω_0 that have a common singular part, we can define $\langle :T_{\mu\nu}: \rangle_\omega$ by the equation above.

Remark 2.26. We should identify the tangent spaces at x and at x' before taking the coincidence limit. This is done by parallel transport through the unique geodesic joining x and x' . For it to make sense at general spacetimes, x' must be close enough to lie in a causal convex normal neighborhood of x .

If we consider further physical conditions on the energy-momentum tensor, we can guarantee its uniqueness up to local curvature terms. Wald sets up the following four axioms.

Wald's axioms on the energy-momentum tensor:

1. If $\langle \phi(x)\phi(x') \rangle_{\omega_1} - \langle \phi(x)\phi(x') \rangle_{\omega_2}$ is smooth, then $\langle T_{\mu\nu} \rangle$ is given by (2.3.2).
2. Locality: Let (M, g) and (M', g') be two globally hyperbolic spacetimes and let Σ and Σ' be Cauchy surfaces for M and M' , respectively. Suppose there are globally hyperbolic, open neighborhoods $\mathcal{O} \subset M$ of $p \in M$, with Cauchy surface of the form $\mathcal{O} \cap \Sigma$, and $\mathcal{O}' \subset M'$, with Cauchy surface of the form $\mathcal{O}' \cap \Sigma'$. Suppose there is an isometry $i : \mathcal{O} \rightarrow \mathcal{O}'$ and denote $p' \equiv i(p)$. This isometry allows us to identify the subalgebras $\mathcal{A}_\mathcal{O} \subset \mathcal{A}$ for M and $\mathcal{A}_{\mathcal{O}'} \subset \mathcal{A}'$ for M' . If the states ω on \mathcal{A} and ω' on \mathcal{A}' such that their restrictions onto the subalgebras, respectively $\mathcal{A}_\mathcal{O}$ and $\mathcal{A}'_{\mathcal{O}'}$, are equal, then, we require that $\langle T_{\mu\nu} \rangle_\omega$ at p equals $\langle T_{\mu\nu} \rangle_{\omega'}$ at p' .

3. Conservation: $\nabla^\mu \langle T_{\mu\nu} \rangle = 0$ for all states.
4. Minkowski: $\langle T_{\mu\nu} \rangle_\Omega = 0$ at Minkowski vacuum state Ω .

Axiom 1 is just the previous discussion. Axiom 2 is to guarantee the consistency with the local character of the algebraic approach and axiom 4 is to guarantee that it reduces consistently to the flat case. Axiom 3 is the usual conservation law required. Notably, these axioms guarantees the following theorem.

Theorem 2.27. [115, Thm4.6.1] *Let $\langle T_{\mu\nu} \rangle$ and $\langle \tilde{T}_{\mu\nu} \rangle$ denote two prescriptions for the expectation value of the energy-momentum tensor which satisfies axioms above. Then $t_{\mu\nu} = \langle T_{\mu\nu} \rangle - \langle \tilde{T}_{\mu\nu} \rangle$ is a conserved local curvature term, i.e. $t_{\mu\nu}$ is independent of the state ω , satisfies $\nabla^\mu t_{\mu\nu} = 0$, and its value at any given event p depends only upon the spacetime geometry in an arbitrarily small neighborhood of p —with $t_{\mu\nu}(p) = 0$ if the geometry in a neighborhood of p is flat.*

If there is a prescription for $\langle T_{\mu\nu} \rangle$, Theorem 2.27 guarantees it is unique up to conserved local curvature terms. Fortunately, a suitable prescription does exist due to Hadamard's work on constructing local bidistributional solutions of elliptic and hyperbolic equations in the beginning of last century. In fact, only axioms 1 and 2 are needed for the proof of the theorem above to guarantee uniqueness of $\langle T_{\mu\nu} \rangle$; axioms 3 and 4, by the *Hadamard algorithm*, restrain the singularity structure of the states for which $\langle T_{\mu\nu} \rangle$ makes sense.

Recall that for the free neutral scalar Klein-Gordon field, the two-point function at Minkowski's vacuum is:

$$\langle \Omega | \phi(x) \phi(x') | \Omega \rangle = \frac{1}{4\pi^2 \sigma^2} + \frac{m^2}{16\pi^2} \log m^2 \sigma^2 + \dots$$

Based on this singular character and by the Hadamard algorithm, we can construct the local bidistribution⁸:

$$H(x, x') = \frac{U(x, x')}{4\pi^2(\sigma^2 + 2i\epsilon(t - t') + \epsilon^2)} + V(x, x') \ln(\sigma^2 + 2i\epsilon(t - t') + \epsilon^2) + W(x, x'),$$

where U, V, W are smooth functions on (x, x') and $U(x, x) = 1$. These functions are determined by imposing that $H(x, x')$ satisfies the Klein-Gordon equation both at x and x' .

In Minkowski spacetime $H(x, x')$ has the same *UV*-behavior of the vacuum; by requiring that $\langle \phi(x) \phi(x') \rangle$ have the same *UV*-behavior of $H(x, x')$, then

$$F(x, x') := \langle \phi(x) \phi(x') \rangle - H(x, x')$$

is smooth and axioms 3 and 4 holds. Thus, it follows the definition below.

Definition 2.28. (Hadamard States) The states ω acting on $\mathcal{A}(M)$ whose two-point function are of the form

$$\omega_2(x, x') = \frac{U(x, x')}{4\pi^2(\sigma^2 + 2i\epsilon(t - t') + \epsilon^2)} + V(x, x') \ln(\sigma^2 + 2i\epsilon(t - t') + \epsilon^2) + W(x, x'), \quad (2.3.3)$$

with the functions as explained above, are called *Hadamard states*. We say they satisfy the Hadamard condition (2.3.3) and they are the ones for which we can use the prescription above to define $\langle T_{\mu\nu} \rangle$.

⁸One should introduce a parameter inside the logarithm, for dimensional reasons.

2.3.2 Distributions and the Wavefront Set

Where we review Microlocal Analysis to be able to translate the Hadamard condition into a condition on the wavefront set of the two-point function in the next section.

We learned that considerations on the energy-momentum tensor induce a condition on the singularity structure of the quantum states—the Hadamard condition. In this section, we review Microlocal Analysis: the study of distributions and their singular character. We see only the necessary definitions and results to understand and invoke Radzikowski theorem in the next section, and derive a quantum energy inequality in the next chapter. For a detailed study on distributions and Microlocal Analysis, the capital reference is [74], on which the following review is based.

The concept of a distribution arose to extend the notion of differentiable functions with the motivation of establishing the existence of solutions to differential equations; they evolved from the notion of *weak solutions* and the first rigorous formalization was done by Sergey Sobolev in 1936 and later developed and highlighted by Schwartz in the 40's, 50's. Distributions are defined as continuous linear functionals acting on a space of functions, which is called *test functions*. If we take the infinitely differentiable compactly-supported functions C_0^∞ equipped with the usual topology as said in page 43 as the test functions space, the distributions acting on it are the *standard distributions*. If we take the Schwartz space, the distributions acting on it are called *tempered distributions*—these are the ones for which the Fourier transform is always well-defined. The duality between smoothness of functions and decay of its Fourier transform seen in Fourier analysis plays a crucial role in this section; this duality equipped with the local characterization of distributions gives us Microlocal Analysis.

Let's first review the formalism on \mathbb{R}^n , and then we extend it to smooth manifolds.

Definition 2.29. (Distribution on \mathbb{R}^n) Let X be an open set in \mathbb{R}^n . A distribution in X is a linear form $u : C_0^\infty(X) \rightarrow \mathbb{C}$ that satisfies the continuity condition, *i.e.* for every compact $K \subset X$ there are constants C and k such that:

$$|u(\phi)| \leq C \sum_{|\alpha| \leq k} \sup |\partial^\alpha \phi| \quad \forall \phi \in C_0^\infty(K). \quad (2.3.4)$$

Moreover:

- The set of all distributions in X is denoted $\mathcal{D}'(X)$ ⁹ and is the topological dual of $C_0^\infty(X)$: the subspace of continuous linear functions in the algebraic dual of C_0^∞ .
- The condition (2.3.4) is equivalent to the usual continuity condition:

$$\lim_{k \rightarrow \infty} u(\phi_k) = u(\lim_{k \rightarrow \infty} \phi_k) \text{ for any convergent sequence } \{\phi_k\}_{k \in \mathbb{N}} \text{ in } C_0^\infty.$$

- If $f \in C^\infty(X)$ and $\phi \in C_0^\infty(X)$, then $f\phi \in C_0^\infty(X)$ and we can naturally define the product of a distribution by a smooth function as:

$$fu(\phi) = u(f\phi).$$

⁹Because Laurent Schwartz denoted $C_0^\infty(X)$ by $\mathcal{D}(X)$.

Example 2.30. To every locally integrable function u on \mathbb{R}^n , we can associate the distribution

$$u(\phi) = \int u(x)\phi(x)d^n x, \text{ for any } \phi \in C_0^\infty(X).$$

By integration by parts, and since ϕ is compactly supported, we have

$$u(\phi') = \int u(x)\phi'(x)d^n x = - \int u'(x)\phi(x)d^n x \equiv -u'(\phi).$$

Inspired by the example above, we define the derivative of $u \in \mathcal{D}'(X)$ with respect to a differential operator D^α of order $|\alpha|$ by

$$D^\alpha u(\phi) = (-1)^{|\alpha|} u(D^\alpha \phi), \phi \in C_0^\infty(X).$$

Let $u \in \mathcal{D}'(X)$ and let N be an open set in X , the distribution $u|_N$ defined as the restriction of u to N is given by

$$u|_N(\phi) = u(\phi), \phi \in C_0^\infty(N).$$

If every point in X has a neighborhood on which $u|_N = 0$, then $u = 0$. This means that, although not pointwisely defined, distributions do have a local nature since we can characterize a distribution on X by its restrictions on an open covering of X . With this in mind, we define the *support of a distribution* $u \in \mathcal{D}'(X)$ as the set of points in X on which there is no neighborhood $N \subset X$ such that $u|_N = 0$; we denote it by $\text{supp } u$ and, clearly, its definition implies that u vanishes at $X \setminus \text{supp } u$.

Remark 2.31. a family of distributions u_i defined in an open covering of $X = \cup X_i$ such that they are compatible in the intersections, *i.e.* $u_i = u_j$ at $X_i \cap X_j$, have a unique distribution $u \in \mathcal{D}'(X)$ compatible with it; this validates the discussion above and one can find a proof here: [74, Thm2.2.4].

Furthermore, since, intuitively, distributions are generalizations of smooth functions, and given their local nature, it makes sense to consider the following definition.

Definition 2.32. (Singular support) Let $X \subset \mathbb{R}^n$ be an open set. The *singular support* of a distribution $u \in \mathcal{D}'(X)$ is the set of points in X having no neighborhood to which the restriction of u is a smooth function and its denoted by $\text{sing supp } u$. Note that this means that $u|_{X \setminus \text{sing supp } u}$ is a smooth function.

Let's now review the duality between smoothness and decay we see in Fourier Analysis, mentioned in the beginning of this section, to understand how we can characterize the singular structure of distributions by it. We choose the non-symmetric convention for the Fourier transform, so for an integrable function $f : \mathbb{R} \rightarrow \mathbb{C}$ it is given by:

$$\hat{f}(k) = \int e^{ik \cdot x} f(x) d^n x. \quad (2.3.5)$$

Let $\mathcal{E}'(\mathbb{R}^n)$ denotes the subset of $\mathcal{D}'(\mathbb{R}^n)$ of the compactly supported distributions and $\mathcal{S}'(\mathbb{R}^n)$ denotes the space of tempered distributions. It holds that $\mathcal{E}' \subset \mathcal{S}' \subset \mathcal{D}'$. Although the Fourier transform is not defined for any distribution in \mathcal{D}' , it is a linear isomorphism on the Schwartz space into itself, thus it is always well-defined there and the following definition makes sense.

Definition 2.33. (Fourier Transform) For tempered distributions $u \in \mathcal{S}'(\mathbb{R}^n)$, the Fourier transform of u is simply $\hat{u}(f) := u(\hat{f})$, where \hat{f} is the Fourier transform of f as defined in equation (2.3.5). For a compactly supported distribution $u \in \mathcal{E}'(\mathbb{R}^n)$ and setting $e_k \equiv \chi e^{ik \cdot x}$ for a function $\chi \in C_0^\infty(\mathbb{R}^n)$ which is 1 at $\text{supp } u$, the Fourier transform of u is:

$$\hat{u}(k) := u(e_k).$$

If u originated from a smooth compactly supported function, which we will also denote u , the above reduces to the standard form (2.3.5):

$$\hat{u}(k) = \int u(x) e^{ik \cdot x} d^n x.$$

To illustrate the idea of the duality, let's see two examples. For the Dirac delta distribution on \mathbb{R} defined by

$$\int \phi(x) \delta(x - x_0) dx = \phi(x_0) \text{ for } \phi \in C_0^\infty(\mathbb{R}),$$

its Fourier transform at x_0 —where it is not smooth—is $\hat{\delta}(k) = \frac{1}{\sqrt{2\pi}} e^{-2\pi i k x_0}$ which shows no decay at ∞ . Furthermore, it is known that

$$f \in C_0^\infty(\mathbb{R}^n) \Rightarrow \text{ for each } N \in \mathbb{N}, \exists C_N : |\hat{f}(k)| \leq \frac{C_N}{1 + |k|^N} \text{ as } k \rightarrow \infty, \quad (2.3.6)$$

where \hat{f} is the Fourier transform of f . Equation (2.3.6) is telling us that a compactly supported function is smooth only if its Fourier transform decays as rapidly as indicated by the inequality of the right hand side of the implication above. This inspire defining a *rapid decay* Fourier transform of f , which is intuitively saying “rapidly enough for f to be smooth”. The wavefront set contains this kind of information: which relates the smoothness and decay duality illustrated above. It combines the location of the singularities—given by the singular support—with the directions of the high frequencies causing them—given by the singular directions set. Let's formalize this idea.

Definition 2.34. (Cone) A *cone with apex at zero* is a subset $V \subset \mathbb{R}^n$ such that: if $k \in V$ then $\lambda k \in V$ for all $\lambda \geq 0$.

Definition 2.35. (Rapid decay) Let $X \subset \mathbb{R}^n$ be an open set and $u \in \mathcal{D}'(X)$. If there is a function $\phi \in C_0^\infty(\mathbb{R}^n)$ such that $\phi(x) \neq 0$ and if there is a cone $V \subset \mathbb{R}^n$ such that

$$\exists C_N \in \mathbb{R} : |\widehat{\phi u}(k)| \leq \frac{C_N}{1 + |k|^N}, \forall k \in V, \forall N \in \mathbb{N},$$

then k is said to be a *direction of rapid decay* for u .

Definition 2.36. (Singular directions) Let $X \subset \mathbb{R}^n$ be an open set. The *singular directions set* of a distribution $u \in \mathcal{D}'(X)$ is the complement in $\mathbb{R}_*^n \equiv \mathbb{R}^n \setminus \{0\}$ of the set of directions of rapid decay, *i.e.*

$$\Sigma(u) := \{\eta \in \mathbb{R}_*^n : \nexists \text{ a conic neighborhood } V \text{ such that } \hat{u}(\eta) \text{ is of rapid decay for } \eta \in V\}.$$

It does not increase under the product by a smooth function:

$$\Sigma(\phi u) \subset \Sigma(u), \text{ for } \phi \in C^\infty(X), \quad (2.3.7)$$

so we can define the singular directions of u at a point x , using compactly supported functions:

$$\Sigma_x(u) := \bigcap_{\substack{\phi \in C_0^\infty(X) \\ \phi(x) \neq 0}} \Sigma(\phi u).$$

It is easy to see that $\Sigma(\phi u) \rightarrow \Sigma_x(u)$ if $\phi \in C_0^\infty$, $\phi(x) \neq 0$ and $\text{supp } \phi \rightarrow \{x\}$. Hence $\Sigma_x(u) = \emptyset \iff \phi u$ is smooth for some $\phi \in C_0^\infty$ with $\phi(x) \neq 0$ —that is, if $x \notin \text{sing supp } u$.

Now we can compactify the above in the wavefront set.

Definition 2.37. (wavefront set of a distribution on \mathbb{R}^n) Let $X \subset \mathbb{R}^n$ be an open set. The *wavefront set* of a distribution $u \in \mathcal{D}'(X)$ is the closed subset of $X \times \mathbb{R}_*^n$:

$$WF(u) := \{(x, k) \in X \times \mathbb{R}_*^n : k \in \Sigma_x(u)\}.$$

The definition above does compactify the information on the singularity structure of the distribution u , since the projection of $WF(u)$ in the first variable is $\text{sing supp } u$, and on the second variable is $\Sigma(u)$.

Remark 2.38. By the definition above, we have that $WF(u) = \emptyset \iff u \in C^\infty(X)$. Recall that for Hadamard states differences between their two-point functions are smooth functions, thus, when we define the wavefront set on manifolds, this property (which still holds) implies that, for all states, the wavefront sets of the two-point functions are equal.

Example 2.39. For the Dirac delta distribution at x_0 on \mathbb{R} , $WF(\delta) = \{(x_0, k) : k \in \mathbb{R}_*\}$.

Example 2.40. Consider the Heaviside distribution on \mathbb{R} , defined by:

$$\int_{\mathbb{R}} \phi(x) \Theta(x) dx = \int_{\mathbb{R}^+} \phi(x) dx;$$

It is equivalent to the principal value: $\Theta(x) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{e^{i\lambda x}}{x-i0^+} d\lambda$. So, for $T(\phi) = \int_{-\infty}^{+\infty} \frac{\phi(x)}{x-i0^+} dx$, we have $\hat{T}(k) = 2\pi i \Theta(k)$. Hence: $WF(\Theta) = \{(0, k) : k > 0\}$.

The wavefront set also does not increase under taking partial derivatives. Let $u \in \mathcal{D}'(X)$ and $\chi \in C_0^\infty(X)$. Since $\chi u \in \mathcal{S}'(X)$, the Fourier transform of $\partial_j \chi u$ is simply the Fourier transform of χu multiplied by a factor (ik_j) ; this means that if $k \in \Sigma(D^\alpha \chi u)$, then $k \in \Sigma(\chi u)$, *i.e.*

$$\Sigma(D^\alpha \chi u) \subset \Sigma(\chi u). \quad (2.3.8)$$

By the definition of the singular directions set at a point:

$$\Sigma_x(D^\alpha u) \subset \Sigma(\tilde{\chi} D^\alpha u) \text{ for } \tilde{\chi} \in C_0^\infty(X), \text{ with } \tilde{\chi}(x) \neq 0. \quad (2.3.9)$$

Choosing $\tilde{\chi} \in C_0^\infty(X)$ with $\tilde{\chi} = 1$ at a neighborhood of x and $\chi \in C_0^\infty(X)$ such that $\chi = 1$ at the support of $\tilde{\chi}$, it holds:

$$\Sigma_x(D^\alpha u) \stackrel{(2.3.9)}{\subset} \Sigma(\tilde{\chi} D^\alpha u) = \Sigma(\tilde{\chi} D^\alpha \chi u) \stackrel{(2.3.7)}{\subset} \Sigma(D^\alpha \chi u) \stackrel{(2.3.8)}{\subset} \Sigma(\chi u).$$

Taking $\text{supp}\chi \rightarrow \{x\}$, then $\Sigma(\chi u) \rightarrow \Sigma_x(u)$, i.e. $\Sigma_x(D^\alpha u) \subset \Sigma_x(u)$ and thus

$$WF(D^\alpha u) \subset WF(u).$$

For a partial differential operator with smooth coefficients P , since

$$WF(\alpha u + \beta v) \subset WF(u) \cup WF(v) \text{ for } v \in \mathcal{D}'(X), \alpha, \beta \in \mathbb{C},$$

it follows from the above that:

$$WF(Pu) \subset WF(u).$$

In fact, for the operator P as above, it holds:

$$WF(Pu) \subset WF(u) \subset WF(Pu) \cup \text{Char}P, \quad (2.3.10)$$

where $\text{Char}P$ is the characteristic set of P defined by

$$\text{Char}P := \{(x, k) \in \mathbb{R}^n \times \mathbb{R}_*^n : p_m(x, k) = \sum_{|\alpha|=m} a_\alpha(x) k^\alpha = 0\}. \quad (2.3.11)$$

For a proof, one can check [74, Thm8.3.1]. This result is crucial for our understanding of the microlocal spectral condition.

We have all ingredients of Microlocal Analysis necessary for the next section, we just have to take them onto a general manifold. This is naturally possible due to the local characterization of distributions on \mathbb{R}^n and the behaviour of it, and of the wavefront and the characteristic sets, under coordinate changes. Given a diffeomorphism $\varphi : U \rightarrow \tilde{U}$ between open sets of \mathbb{R}^n and a function f on \tilde{U} , then we define φ^*f such that, at p , it gives the value of f at $\varphi(p)$ by $\varphi^*f = f \circ \varphi$. If we have a distribution $u \in \mathcal{D}'(U)$, we define φ^*u by $\varphi^*u(f) = u(f \circ \varphi)$ and thus

$$WF(u) = \{(x, kD\varphi|_x) : (\varphi(x), k) \in WF(\varphi^*u)\};$$

where $kD\varphi|_x$ is the action of the dual map to $D\varphi|_x$ on k (which is the composition of k and $D\varphi|_x$ as linear maps). That is, the wavefront set transforms as a subset of the cotangent bundle under coordinate changes.

Definition 2.41. (Distribution on manifolds) Let M be an n -dimensional smooth manifold equipped with the differentiable structure $\mathcal{A} = \{(U_\alpha, \varphi_\alpha)\}_{\alpha \in \Lambda}$, where $\varphi_\alpha : M \supset U_\alpha \rightarrow \tilde{U}_\alpha \subset \mathbb{R}^n$ are the homeomorphisms between the open sets U_α and \tilde{U}_α . If for every parametrization φ_α we have a distribution $u_\alpha \in \mathcal{D}'(\tilde{U}_\alpha)$ and if $\forall \alpha, \beta \in \Lambda$ it holds that $u_\beta = u_\alpha \circ (\varphi_\alpha \circ \varphi_\beta^{-1})$ on $U_\alpha \cap U_\beta$ then the family of local representatives u_α defines a distribution u on M through: $u_\alpha = u \circ \varphi_\alpha^{-1}$.

The proof that this is a consistent definition can be found in [74, Thm6.3.4], that is: u is unique in the distributional sense and it falls back to Definition 2.29 when M is an open set X in \mathbb{R}^n . Let's see an example that shows that a distribution defined as above, at least, exists in spacetimes.

Example 2.42. Every spacetime (M, g) has a natural density defined through its metric $\rho = \sqrt{|\det g|}$ and there is canonical way of defining a distribution on an n -dimensional smooth manifold M with a smooth density ρ . For any $u \in C^\infty(M)$:

$$u(\phi) = \int d^n x \rho(x) \phi(x) u(x) \quad \text{for any } \phi \in C_0^\infty(M).$$

This is well-defined because if we consider ρ with different chart expressions $\rho_\alpha(x)$ for $x \in \varphi_\alpha(U_\alpha)$ and $\rho_\beta(x)$ for $x \in \varphi_\beta(U_\beta)$, supported on $U_\alpha \cap U_\beta$, it holds that

$$\int_{\varphi_\alpha(U_\alpha)} \rho_\alpha(x) d^n x = \int_{\varphi_\beta(U_\beta)} \rho_\beta(x) d^n x.$$

If there is a smooth map $\varphi : X \rightarrow Y$ between the smooth manifolds X and Y , there is a corresponding linear map between the cotangent bundles $\varphi^* : T^*Y \rightarrow T^*X$, which is called *pullback*. Since the wavefront set of a distribution $u \in \mathcal{D}'(\mathbb{R}^n)$ is a subset of the cotangent bundle $T^*\mathbb{R}^n$, we can use the pullback to define the wavefront set of a distribution on a smooth manifold.

Definition 2.43. (Wavefront set of a distribution on a manifold) Let $(U_\alpha, \varphi_\alpha)$ be a chart of an n -dimensional smooth manifold M . Let $u \in \mathcal{D}'(M)$, then $u \circ \varphi_\alpha^{-1}$ is a distribution on \mathbb{R}^n . Hence, the wavefront set of u is defined as the following subset of the cotangent bundle:

$$WF(u) := \varphi_\alpha^* WF(u \circ \varphi_\alpha^{-1}) := \{(x, (D\varphi_\alpha(x))^t k) : (\varphi_\alpha(x), k) \in WF(u \circ \varphi_\alpha^{-1})\},$$

where $(D\varphi_\alpha(\cdot))^t$ is the transpose of the derivative of φ_α .

Let $\varphi : X \rightarrow Y$ be a smooth map between the smooth manifolds X and Y . The *pullback of a smooth function* $f : Y \rightarrow \mathbb{R}^n$ by φ is given by $\varphi^* f := f \circ \varphi : X \rightarrow \mathbb{R}^n$. For $u \in \mathcal{D}'(X)$, we can also define the *pullback of the distribution* u if a condition on the wavefront set of u and the set of normals of φ ,

$$N_\varphi := \{(\varphi(x), k) \in Y \times \mathbb{R}^n : (D\varphi(x))^t k = 0\},$$

is satisfied. This is due to the following theorem.

Theorem 2.44. [73, Thm2.5.11'] Let $\varphi : X \rightarrow Y$ be a smooth function between manifolds X and Y , with set of normals N_φ . Let $u \in \mathcal{D}'(Y)$. If $N_\varphi \cap WF(u) = \emptyset$, we can uniquely define the pullback $\varphi^* u$ such that: if u is continuous, then $\varphi^* u = u \circ \varphi$; and $\varphi^* : \mathcal{D}'_c(Y) \rightarrow \mathcal{D}'(X)$ is sequentially continuous for any closed cone $\Gamma \subset T^*(Y) \setminus \{0\}$ with $\Gamma \cap N_\varphi = \emptyset$. Moreover,

$$WF(\varphi^* u) \subset \varphi^* WF(u) = \{(x, (D\varphi(x))^t k) : (\varphi(x), k) \in WF(u)\}.$$

Those are almost all ingredients we need to invoke Radzikowski Theorem and to show that the quantized energy density is well-defined in chapter 3; we only need one more crucial result regarding distributions of positive type.

Theorem 2.45. [32, Thm2.2] *Let X and Y be smooth manifolds equipped with smooth positive densities σ_X and σ_Y , and suppose $\gamma : Y \rightarrow X$ is smooth. If $u \in \mathcal{D}'(M \times M)$ is of positive type and $N_\varphi \cap WF(u) = \emptyset$, where $\varphi(y, y') = (\gamma(y), \gamma(y'))$, then φ^*u is of positive type.*

To see that the result above is indeed useful to us, recall that every spacetime has the natural energy density given by $\sqrt{|\det g|}$ and note that, since states ω on $\mathcal{A}(M)$ are positive hermitean functionals, their two-point functions satisfy $\omega_2(\bar{f}, f) \geq 0 \forall f \in C_0^\infty(M)$ —then the distribution ω_2 is said to be of *positive type*.

2.3.3 Radzikowski's Theorem

We take the simplest path to understand how to translate the Hadamard condition into a condition on the wavefront set, following the argument of the lecture notes [33]. First, we discuss the wavefront set of the bisolutions of the Klein-Gordon operator. Then, by comparing it with the wavefront set of the two-point function for the Minkowski vacuum, we generalize the Hadamard condition by invoking Radzikowski Theorem.

Let P be the Klein-Gordon operator defined on a globally hyperbolic spacetime (M, g) . Since its principal symbol is $p_2(x, k) = -g^{\mu\nu}(x)k_\mu k_\nu$, its characteristic set, defined by (2.3.11), is just the bundle of non-zero null covectors on M :

$$\text{Char } P = \mathcal{N} := \{(x, k) \in T^*M : k \text{ is non-zero null at } x\}.$$

Then, for any solution $u \in \mathcal{D}'(M)$ of the Klein-Gordon equation, $Pu = 0$, by property (2.3.10) we have $WF(u) \subset \mathcal{N}$. Since we are particularly interested in the two-point function, let's consider bisolutions $U \in \mathcal{D}'(M \times M)$:

$$(P \otimes 1)U = (1 \otimes P)U = 0.$$

Let $\mathbf{0}$ denotes the zero-section of T^*M , that is $\mathbf{0} := \{(x, 0) \in T^*M : x \in M\}$. The principal symbol of $(P \otimes 1)$ is $p_2(x, k; x', k') = -g^{\mu\nu}(x)k_\mu k_\nu$, hence

$$\text{Char}(P \otimes 1) = \mathcal{N}_0 \times (T^*M \setminus \mathbf{0});$$

analogously, we have

$$\text{Char}(1 \otimes P) = (T^*M \setminus \mathbf{0}) \times \mathcal{N}_0.$$

Therefore,

$$WF(U) \subset \text{Char}(P \otimes 1) \cap \text{Char}(1 \otimes P) \subset \mathcal{N}_0 \times \mathcal{N}_0. \quad (2.3.12)$$

For the Minkowski's vacuum state Ω , (2.3.12) implies $WF(\omega_2^\Omega) \subset \mathcal{N}_0 \times \mathcal{N}_0$. Consider $\phi(x, x') = \phi_1(x)\phi_2(x')$, for $\phi_1, \phi_2 \in C_0^\infty$, then

$$\phi\omega_2^\Omega(x, x') = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d^3k}{2k_0} e^{-ik(x-x')} \phi_1(x)\phi_2(x')$$

and, taking the Fourier transform in both variables:

$$\mathcal{F}(\phi\omega_2^\Omega(x, x'))(l, l') = \int_{\mathbb{R}^3} \frac{d^3k}{2k_0} \frac{1}{2\omega} \hat{\phi}_1(l - k) \hat{\phi}_2(l' + k). \quad (2.3.13)$$

Since both functions ϕ_1 and ϕ_2 are in C_0^∞ , $\hat{\phi}_1$ and $\hat{\phi}_2$ are of rapid decay—recall the duality given in expression (2.3.6). Then, the greater contributions to $\mathcal{F}(\phi\omega_2^\Omega(x, x'))(l, l')$ corresponds to simultaneous small values of $(l - k)$ and $(l' + k)$; where “small” here corresponds to a scale determined by the functions.

The integral is only on the spatial components, so if we fix $k_0 \leq 0$, then the argument $(l_0 - k_0) \rightarrow \infty$ when $l_0 \rightarrow \infty$. In this case, the contribution of $\hat{\phi}_1$ goes to zero rapidly and $\mathcal{F}(\phi\omega_2^\Omega(x, x'))(l, l') \rightarrow 0$ independently of l' . This is illustrated in the figure below, which is a clone of [34, Pg35, Fig4].

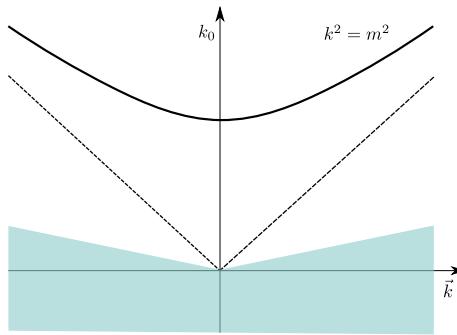


Figure 2.1: : If $l_0 \rightarrow \infty$ in the shaded region, then $\mathcal{F}(\phi\omega_2^\Omega)(l, l') \rightarrow 0$ rapidly.

Note that the shaded region in the figure above does not correspond only to negative values for k_0 , that's because we only need the argument $(l - k)$ to be “big”, so “small” positive values for k_0 are still ok. On the other hand, if we fix $k_0 \geq 0$, the contribution of $\hat{\phi}_2$ goes to zero for $l'_0 \rightarrow \infty$.

Accordingly, $(x_1, k_1; x_2, k_2)$ is a regular direction for (2.3.13) if $(k_1)_0 \leq 0$ or $(k_2)_0 \geq 0$. Since the wavefront set of the two-point function of the vacuum is in $\mathcal{N}_0 \times \mathcal{N}_0$, we have that

$$WF(\omega_2) \subset \mathcal{N}^+ \times \mathcal{N}^-, \quad (2.3.14)$$

where $\mathcal{N}^{+(-)} = \{(x, k) \in \mathcal{N} : k \text{ is future(past) directed}\}$. This condition on the wavefront set is more than a property satisfied by the Minkowski vacuum, it defines the *microlocal spectrum condition*, as follows.

Definition 2.46. (μSC) Let \mathcal{N} be the bundle of nonzero null covectors of M . A state ω is said to satisfy the *microlocal spectrum condition* (μSC) if

$$WF(\omega_2) \subset \mathcal{N}^+ \times \mathcal{N}^-.$$

Recall that it was necessary that differences between expectation values were smooth functions, to provide us a well-defined energy-momentum tensor. In fact, the μSC suffices to guarantee it: if ω and ω' obeys the μSC , then

$$\omega_2 - \omega'_2 \in C^\infty(M \times M);$$

which means that all two-point functions that satisfies the μSC have equal wavefront sets. Moreover, given that all two-point functions have a common antisymmetric part, $\frac{i}{2}E$, we obtain that

$$WF(\omega_2) = WF(E) \cap WF(\mathcal{N}^+ \times \mathcal{N}^-);$$

this last property allows us to write the wavefront set of ω_2 as

$$WF(\omega_2) = \{((x_1, k_1), (x_2, -k_2)) \in T^*M \setminus \mathbf{0} \times T^*M \setminus \mathbf{0} : (x_1, k_1) \sim (x_2, k_2), k_1 \in \mathcal{N}^+\},$$

where the equivalence relation above is defined by: $(x_1, k_1) \sim (x_2, k_2) \iff (x_1, k_1) = (x_2, k_2)$ for null k_1 or there is a null geodesic γ connecting x_1 and x_2 such that k_1 is cotangent to γ at x_1 and k_2 is the parallel transport of k_1 from x_1 to x_2 along γ .

The following is a simplified version of Radzikowski's Equivalence Theorem [94, Thm5.1].

Theorem 2.47. (Equivalence Theorem) *Let (M, g) be a globally hyperbolic spacetime, P the Klein-Gordon operator, $\mathcal{A}(M)$ the algebra of observables as in section 2.2 and ω a state acting on it. Then*

$$\omega \text{ is Hadamard} \iff \omega_2 \text{ satisfies the } \mu SC.$$

Remark 2.48. Radzikowski used the definition of *Globally Hadamard*, which is in fact weaker than the one we used here; then, his Equivalence Theorem is stronger than the one stated above. Yet, for our purposes, it suffices as it is.

Radzikowski theorem says that a state ω is Hadamard if and only if the two-point function ω_2 satisfy the microlocal spectrum condition. But the Hadamard condition only holds for free theories, while the μSC can be generalized to more general theories; in this sense, Radzikowski theorem is saying that the microlocal spectrum condition is more fundamental than the Hadamard condition.

3

AN ANSWER: QUANTUM ENERGY INEQUALITIES IN SINGULARITY THEOREMS

Where we derive a quantum energy inequality for the Klein-Gordon field within Algebraic Quantum Field Theory and (...) obtain generalizations of Hawking and Penrose Singularity Theorems.

Let's recall what this dissertation is about. In chapter 1, we reviewed the problem to be discussed: we saw that Singularity Theorems are strong results within General Relativity that gives us sufficient conditions on the spacetime for it to be geodesic incomplete; these results relied on a powerful geometric formalism that prevented us of having to impose a particular matter model and yet, they do rely on some consideration on the matter content—the energy condition. Then, we saw that the classical energy conditions are all violated within Quantum Field Theory and we accepted the search for quantum energy inequalities, to enter as weakened substitutes of the classical conditions. Given the need to do this search on general curved spacetimes, in chapter 2 we saw the formalism of Algebraic Quantum Field Theory.

Now we can derive quantum energy inequalities on general curved spacetimes. A nice introduction into the subject is [34] and a recent review is [35]. In section 3.1, by reviewing [32], we derive “a general worldline quantum inequality” for the Klein-Gordon field on globally hyperbolic spacetimes for Hadamard states—a bound satisfied by weighted averages of the energy-momentum tensor along the worldline of observables. This bound, however, cannot be directly applied to Singularity Theorems.

Although there are not quantum energy inequalities analogues for the classical strong and null energy conditions that recovers Hawking and Penrose classical theorems¹, in 2011, Fewster and Galloway showed that Singularity Theorems can be obtained by QEI-inspired hypotheses [37]. The idea is that exponentially damped energy conditions can be obtained from hypotheses inspired by quantum energy inequalities and generalizations of Hawking and Penrose Theorems can be obtained by exponentially damped energy conditions with an extra lower bound consideration. The weakened energy condition imposed is of the form:

¹In fact, there is not a QEI generalization for NEC, as proved by Fewster in [43], not even for Minkowski spacetime.

$$\int_{\gamma} e^{-a\lambda} T_{\mu\nu} \dot{\gamma}^{\mu} \dot{\gamma}^{\nu} d\lambda - b \text{ is finite and "strong enough"²}$$

for some constants $a, b > 0$ and $\gamma : [0, +\infty) \rightarrow M$, a future-complete null geodesic with affine parametrization λ . Note that it combines ideas from two different weakening approaches: it is similar to ANEC with an exponential damping—a mollifying function, as seen in Remark 1.19—with a further imposition of a lower bound³

The goal of this chapter is to clarify three things: how can we derive a quantum energy inequality within Algebraic Quantum Field Theory, how can they inspire energy conditions which also yield Singularity Theorems and in which sense can we say that Singularity Theorems hold under subtle quantum effects; to accomplish it, after the QEI derivation, we review Fewster and Galloway's results of [37] in sections 3.2 and 3.3.

3.1 A general worldline quantum energy inequality

For the free neutral scalar Klein-Gordon field with minimal coupling on a globally hyperbolic spacetime, with dimension greater than 2, (M, g) , such that $(+, -, \dots, -)$ is the metric signature, ∇_a as affine connection compatible with g , and $m \geq 0$ is the mass parameter, the classical energy-momentum tensor is given by⁴:

$$T_{ab} = \nabla_a \phi \nabla_b \phi - \frac{1}{2} g_{ab} g^{cd} \nabla_c \phi \nabla_d \phi + \frac{1}{2} m^2 \phi^2 g_{ab}.$$

Let's write it in a quantization-friendly form; for that, we need the notion of *tubular neighborhood* and thus, of *normal bundle*.

Definition 3.1. (Normal bundle) Let N be a submanifold of M equipped with a metric h and such that $\dim N < \dim M$. Let $\langle \cdot, \cdot \rangle$ be the usual scalar product on N induced by h . The *normal space* at x in N is given by:

$$T_x^\perp N = \{v \in T_x M : \langle v, w \rangle = 0, \forall w \in T_x N\}$$

The disjoint union of all the normal spaces at points in M is called the *normal bundle*, denoted by $T^\perp N$.

Definition 3.2. (Tubular Neighborhood) Let M and N as above. An open set $\Omega \subset M$ containing N is called a *tubular neighborhood* if there is a neighborhood Z of the zero section of $T^\perp N$ and a diffeomorphism $f : Z \rightarrow \Omega$ such that $f(0_x) = x$ for any zero vector 0_x in $T^\perp N$ corresponding to x in N .

²in a sense to be made precise: dominates the initial expansion.

³This other weakening approach can be seen in [16], for example.

⁴I will use latin letter for convenience, they still run through 0 and $n - 1$.

Let's try to understand these two definitions. The normal space at $x \in N$ is the collection of the tangent vectors in $T_x M$ which are orthogonal to all tangent vectors of $T_x N$. The ones which are not included are the ones not orthogonal to all vectors in $T_x N$, thus they are proportional to some vector in $T_x N$. Which means that the normal bundle is defined by the quotient $T_x^\perp N = T_x M / T_x N$ by doing that we are identifying the vectors of $T_x N$ with the zero vector 0_x . Now, to understand the idea behind a tubular neighborhood, let's look at an example. Take a smooth curve on \mathbb{R}^2 , unless it is a straight line, perpendicular curves to it will intersect each other. A tubular neighborhood of it would be a cut of these perpendicular curves close enough to the the curve so that it does not have intersections. It is a way to make sure we can walk on one of the perpendicular curves of the normal bundle further way from the curve and walk back towards the same starting point. Below, one can see a drawing of this.

Consider an observable traveling freely in spacetime, described by a smooth timelike geodesic curve $\gamma(\tau)$, with velocity $u(\tau) \equiv \dot{\gamma}(\tau)$. In a tubular neighborhood Γ of $\gamma(\tau)$, we can define the orthonormal frame $\{v_0^a, \dots, v_{n-1}^a\}$ such that $v_0^a = u^a$ and v_μ^a are mutually orthonormal with respect to the scalar product induced by g , that is, for $\eta^{\mu\nu} := \text{diag}[1, -1, \dots, -1]$, we have $g^{ab} = \eta^{\mu\nu} v_\mu^a v_\nu^b$ in Γ . Then, it holds

$$u^a u^b g_{ab} = u^a u^b \eta_{\mu\nu} v_\mu^a v_\nu^b = v_0^a v_0^b \eta_{\mu\nu} v_\mu^a v_\nu^b = \delta_0^\mu \delta_0^\nu \eta_{\mu\nu} = 1.$$

With these definitions, it is easy to see that the classical energy density measured by the observer along γ , defined as $T(\tau) := u^a u^b T_{ab}(\gamma(\tau))$, is given by:

$$T(\tau) = \frac{1}{2} \left(\sum_{\mu=0}^{n-1} v_\mu^a v_\mu^b \right) \nabla_a \phi \nabla_b \phi + \frac{1}{2} m^2 \phi^2.$$

Explicitly, we have the friendly-form:

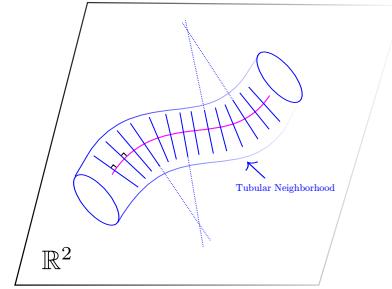
$$T(\tau) = \frac{1}{2} \left(\sum_{\mu=0}^{n-1} v_i^a(\gamma(\tau)) v_i^b(\gamma(\tau)) \right) \nabla_a \phi|_{(\gamma(\tau))} \nabla_b \phi|_{(\gamma(\tau))} + \frac{1}{2} m^2 \phi^2(\gamma(\tau)),$$

and applying two-point splitting on it:

$$T(\tau, \tau') = \frac{1}{2} \left(\sum_{\mu=0}^{n-1} v_i^a(\gamma(\tau)) v_i^b(\gamma(\tau')) \nabla_a \phi|_{\gamma(\tau)} \nabla_b \phi|_{\gamma(\tau')} \right) + \frac{1}{2} \phi(\gamma(\tau)) \phi(\gamma(\tau')), \quad (3.1.1)$$

from which we recover the energy density by taking $\tau' = \tau$ and identifying $T(\tau) = T(\tau, \tau)$.

Let ω be a Hadamard state on the algebra of observables $\mathcal{A}(M)$ associated to the Klein-Gordon field, as defined in chapter 2. The expectation value for the energy density in the state ω is, *intuitively*, given by " $\omega(T(\tau))$ "; $T(\tau)$ is not an element of $\mathcal{A}(M)$. Yet, with this idea and the definition of the two-point function in mind we can define the *quantized energy density*



by associating the first term in (3.1.1) to a sum of elements like $(v_i^a \nabla_a, v_i^{b'} \nabla_{b'}) \omega_2(\gamma(\tau), \gamma(\tau'))$ and the second term, to $\omega_2(\gamma(\tau), \gamma(\tau'))$. In fact,

$$\frac{1}{2} \left(\sum_{i=0}^{n-1} (v_i^a \nabla_a, v_i^{b'} \nabla_{b'}) \omega_2(\gamma(\tau), \gamma(\tau')) + \frac{1}{2} m^2 \omega_2(\gamma(\tau), \gamma(\tau')) \right)$$

defines a bidistribution on $M \times M$. Then, we use the pullback $\varphi^* : \mathcal{D}'(M \times M) \rightarrow \mathcal{D}'(\mathbb{R}^2)$ induced by $\varphi : \mathbb{R}^2 \rightarrow M \times M$ defined by $\varphi(\tau, \tau') := (\gamma(\tau), \gamma(\tau'))$ to take it to \mathbb{R}^2 . Thus, we get the following definition.

Definition 3.3. (Energy density) For a Hadamard state ω , the *quantized energy density* is the bidistribution on \mathbb{R}^2 given by

$$\langle T \rangle_\omega := \frac{1}{2} \sum_{i=0}^{n-1} \varphi^*((v_\mu^a \nabla_a, v_\mu^{b'} \nabla_{b'}) \omega_2) + \frac{1}{2} m^2 \varphi^* \omega_2. \quad (3.1.2)$$

Proposition 3.4. *The quantized energy density above is*

1. *well-defined;*
2. *of positive type;*
3. *of rapid decay as $\alpha \rightarrow \infty$.*

Proof. For the energy-density as in (3.1.2), we have:

1. Given Theorem 2.44, it is enough to show that $N_\varphi \cap WF(\omega_2) = \emptyset$.

For $(k, k') \in T_{(\gamma(\tau), \gamma(\tau'))}^*(M \times M)$, we have:

$$D\varphi(\tau, \tau')^t(k, k') = \begin{bmatrix} \frac{\partial \gamma^1}{\partial \tau} & \dots & \frac{\partial \gamma^n}{\partial \tau} \\ \frac{\partial \gamma^1}{\partial \tau'} & \dots & \frac{\partial \gamma^n}{\partial \tau'} \end{bmatrix} \begin{bmatrix} k_1 & k'_1 \\ \vdots & \vdots \\ k_{n-1} & k'_{n-1} \end{bmatrix} = (\dot{\gamma}^a(\tau) k_a, \dot{\gamma}^{b'}(\tau') k'_{b'})$$

That is, $D\varphi(\tau, \tau')^t$ is a linear map onto \mathbb{R}^2 such that $D\varphi(\tau, \tau')^t(k, k') = (u^a(\tau) k_a, u^{b'}(\tau') k'_{b'})$. Therefore, the set of normals for φ is

$$N_\varphi = \{(\gamma(\tau), k; \gamma(\tau'), k') : k_a u^a(\tau) = k'_{b'} u^{b'}(\tau') = 0\}.$$

Now, let $(x, k; x', k') \in N_\varphi \cap WF(\omega_2)$. Since $(x, k; x', k') \in N_\varphi$, we have that $x = \gamma(\tau)$, $x' = \gamma(\tau')$ for some τ, τ' and $k_a u^a(\tau) = k'_{b'} u^{b'}(\tau') = 0$. Yet, since $(x, k; x', k') \in WF(\omega_2)$, k and k' must be both null.

Those two conditions are incompatible: non-zero timelike and null vectors cannot be orthogonal. Since u^ν is timelike, there is a Lorentz frame where it has zero spatial components and there we can write:

$$g_{\mu\nu} k^\mu u^\nu = k^0 u^0 = 0 \iff k^0 = 0,$$

which contradicts the fact that k^μ is null.

$$\therefore N_\varphi \cap WF(\omega_2) = \emptyset \text{ and } \varphi^* \omega_2 \text{ is well-defined.}$$

2. Since $(v_\mu^a \nabla_a, v_\mu^{b'} \nabla_{b'}) \omega_2(\bar{f}, f) = \omega_2(\overline{\nabla_a(v_\mu^a f)}, \nabla_{b'}(v_\nu^{b'} f))$ and ω_2 is of positive type, then $\varphi^* \omega_2$ is of positive type by Theorem 2.45.
3. Let $(\tau, \xi; \tau', -\xi') \in WF(\varphi^* \omega_2)$, then, by Theorem 2.44 and item 1 here, there are k, k' such that

$$(\xi, -\xi') = (D\varphi(\tau, \tau'))^t(k, k') = (u^a(\tau)k_a, -u^{b'}(\tau')k_{b'}),$$

and $(\gamma(\tau), k; \gamma(\tau'), k') \in WF(\omega_2)$. Also, for a Hadamard state, the microlocal spectrum condition says that $(\gamma(\tau), k) \sim (\gamma(\tau'), k')$, k, k' are future-pointing. Since the velocities are also future-pointing, we have that ξ is positive.

Let $g \in C_0^\infty(\mathbb{R}^n)$, then $WF(g \langle T \rangle_\omega) \subset WF(\langle T \rangle_\omega)$. Then:

$$\Sigma(g \langle T \rangle_\omega) \subset \Sigma(\langle T \rangle_\omega) \subset \{(\xi, -\xi') : \xi, \xi' > 0\}.$$

Therefore, the Fourier transform of $g \langle T \rangle_\omega$, denoted by $[g \langle T \rangle_\omega]^\wedge(-\alpha, \alpha)$, decays rapidly in all directions as $\alpha \rightarrow +\infty$.

□

Given Proposition 3.4, it is simple to prove the following theorem, which is the main result of [32], and states the general worldline quantum energy inequality.

Theorem 3.5. [32, Thm4.1](General-QEI) *Let ω and ω_0 be states on $\mathcal{A}(M)$ with globally Hadamard two-point functions and define the normal ordered energy density relative to ω_0 by $\langle :T:\rangle_\omega = \langle T \rangle_\omega - \langle T \rangle_{\omega_0}$. Then $\langle :T:\rangle_\omega$ is smooth, and the quantum inequality*

$$\int d\tau (g(\tau))^2 \langle :T:\rangle_\omega(\tau, \tau) \geq - \int_0^{+\infty} \frac{d\alpha}{\pi} [(g, g) \langle T \rangle_{\omega_0}]^\wedge(-\alpha, \alpha) \quad (3.1.3)$$

holds for all real-valued $g \in C_0^\infty(M, \mathbb{R})$ (and the right-hand side of (3.1.3) is convergent for all such g).

Proof. We must show that $\langle :T:\rangle_\omega$ is smooth, that the inequality holds and that the right hand side converges to a finite limit. That $\langle :T:\rangle_\omega$ is smooth is trivial, since Hadamard states share the singular part of the two-point function it follows that the energy density is smooth by definition.

The inequality holds, since:

$$\begin{aligned}
\int d\tau (g(\tau))^2 \langle :T: \rangle_\omega(\tau, \tau) &= \int d\tau' \int d\tau g(\tau)g(\tau') \langle :T: \rangle_\omega(\tau, \tau')\delta(\tau, \tau') \\
&= \int_{-\infty}^{+\infty} \frac{d\alpha}{2\pi} \int d\tau \int d\tau' g(\tau)g(\tau') \langle :T: \rangle_\omega(\tau, \tau')e^{-i\alpha(\tau-\tau')} \\
&= \int_{-\infty}^{+\infty} \frac{d\alpha}{2\pi} \langle :T: \rangle_\omega(g_{-\alpha}, g_\alpha) \text{ where } g_\alpha(\tau) = g(\tau)e^{i\alpha\tau} \\
&= \int_0^{+\infty} \frac{d\alpha}{\pi} \langle :T: \rangle_\omega(g_{-\alpha}, g_\alpha) \text{ since } \langle :T: \rangle_\omega \text{ is symmetric} \\
&= \int_0^{+\infty} \frac{d\alpha}{\pi} \langle :T: \rangle_\omega(\bar{g}_\alpha, g_\alpha) \text{ since } g \text{ is real: } \bar{g}_\alpha = g_{-\alpha} \\
&\geq - \int_0^{+\infty} \frac{d\alpha}{\pi} \langle T \rangle_{\omega_0}(\bar{g}_\alpha, g_\alpha) \text{ since } \langle :T: \rangle_\omega \text{ is of positive type.}
\end{aligned}$$

Let $e_{(\alpha, \alpha')}(\tau, \tau') = e^{i(\alpha\tau + \alpha'\tau')}$, then $\langle T \rangle_{\omega_0}(\bar{g}_\alpha, g_\alpha) = \langle T \rangle_{\omega_0}((g, g)e_{(-\alpha, \alpha)}) = [(g, g) \langle T \rangle_{\omega_0}](e_{(-\alpha, \alpha)})$. Hence, by item 3 of Proposition 3.4,

$$\langle T \rangle_{\omega_0}(\bar{g}_\alpha, g_\alpha) \stackrel{\text{def.}}{=} [(g, g) \langle T \rangle_{\omega_0}]^\wedge(-\alpha, \alpha) \quad (3.1.4)$$

does converge for $\alpha \in (0, \infty)$. \square

We can do an analogous derivation considering any partial differential operator Q with smooth coefficients. For the Klein-Gordon field, let's see a sketch of it—this example is from [34]. Let $\gamma(\tau) : \mathbb{R} \rightarrow M$ be a smooth timelike curve, τ the proper time parameter, and Q a partial differential operator with smooth real coefficients. To define the point-split quantity

$$G(\tau, \tau') = \langle Q\phi(\gamma(\tau))Q\phi(\gamma(\tau')) \rangle_\omega$$

for any Hadamard state ω , recall section 2.3.3 and consider φ as in last section (page 74), then the quantity above corresponds to

$$G(\tau, \tau') = (\varphi^*(Q \otimes Q)\omega_2)(\tau, \tau');$$

let G_0 be the above evaluated at the reference Hadamard state ω_0 . The difference $F = G - G_0$ is a smooth function whose diagonal is $F(\tau, \tau) \equiv \langle : (Q\phi)^2 : \rangle_\omega(\gamma(\tau))$. By the same arguments, for any real valued $g \in C_0^\infty$, the positivity of G implies:

$$\int d\tau (g(\tau))^2 \langle : (Q\phi)^2 : \rangle_\omega(\gamma(\tau)) \geq - \int_0^{+\infty} \frac{d\alpha}{\pi} G_0(\bar{g}_\alpha, g_\alpha)_\omega. \quad (3.1.5)$$

From equation (3.1.5), we can obtain bounds on the energy density—like Theorem 3.5—and on any other quantity that depends on finite sums of quantities of the form $\langle : (Q\phi)^2 : \rangle_\omega$. Expression (3.1.5) is completely analogous to expression (3.1.3).

It is important to note that the definition 3.3 of the energy density used depends on the frame chosen; not on the whole tubular neighborhood Γ , but on its restriction to the curve γ .

Thus the bound derived here depends, so far, on the observables worldline γ , the weighting function g and the reference Hadamard state ω_0 ; however, one can get rid of the dependence on the reference state by defining the renormalized energy density in a distinct way: instead of considering differences with respect to a reference state, one can subtract a Hadamard parametrix (2.3.3), which is locally constructed, as described in section 2.3. For a careful description of these “absolute quantum inequalities”, see [44].

By reviewing Fewster’s work [32], we derived the expression (3.1.3)—a lower bound for a weighted average of the energy-momentum tensor expectation value for the Klein-Gordon field on globally hyperbolic spacetimes; from now on, let’s call it “general QEI”, for simplicity. We proved it in the mathematically rigorous formalism of Algebraic Quantum Field Theory without any other assumptions—like the uncertainty principle—and differently from the previous bound for the static case [45], which relied on the positivity of the product of an operator with its adjoint, the derivation of the general QEI relied on the positivity of the pullback of a positive distribution, thus on the “distributional positivity” of the two-point function. The general QEI is indeed a generalization of previous works, since it does reduce to the bounds for the flat [36] and the static [45] cases—the compact form it assumes in the case of stationary spacetimes can be checked also in [32].

Since the bound for the static case [45] is stronger than the bound of [51] by a factor of 4 and Flanagan’s optimal bound of [46] is stronger than [51] by a factor of 6, then the bound in [45] is weaker than Flanagan’s one by a factor of $3/2$.

$$\begin{array}{ccc}
 [51] \text{ Ford and Roman} & \xrightarrow{\text{(General QEI reduces to) Static [45]}} & \text{Flanagan [46]} \\
 \parallel & \times 4 & \parallel \times 3/2 \\
 & \times 6 &
 \end{array}$$

We infer that the general QEI—which does reduce to [45]—is not an optimal bound. Yet, Flanagan’s work [46]—which considered two-dimensional Minkowski spacetime and was later generalized to two-dimensional curved spacetimes [47]—relied on particular properties of the two-dimensional field and, thus, a direct generalization to higher dimensions is not possible. On the other hand, the general QEI holds for globally hyperbolic spacetimes of $n > 2$ dimensions, and even for $n = 2$ with some extra care⁵.

The general QEI, however defined on globally hyperbolic spacetimes, cannot be directly applied in Singularity Theorems; nevertheless, quantum energy inequalities inspire weakened Singularity Theorems, as we see in the next two sections.

3.2 QEI-inspired hypotheses

Where we see how quantum energy inequalities inspire exponentially damped energy conditions.

Recall that Singularity Theorems have a pattern structure, as we saw in section 1.1 by establishing Theorem 1.3; their proofs also have a characteristic structure: they are by contradiction and based on a geometrical argument that relies on Raychaudhuri equation. The

⁵The massless two-dimensional field has well-known pathologies and it does require separate treatment (for example, see [119]).

proofs in [37] of the Singularity Theorems from weakened energy conditions—and from QEI-inspired hypotheses—are also like that, yet, they rely on results regarding the nonexistence of global solutions for initial value problems involving the more general Riccati equations. The thing is that Raychaudhuri equation can be seen as a particular Riccati equation, and we can obtain results of geodesic incompleteness by translating, to the General Relativity context, these results on Riccati equations.

A Riccati equation is of the form:

$$\dot{z}(t) = q_0(t) + q_1(t)z(t) + q_2(t)z^2(t) \quad (3.2.1)$$

where $q_0(t) \neq 0$ and $q_2(t) \neq 0$. If $q_0(t) = 0$, then (3.2.1) is a Bernoulli equation; if $q_2(t) = 0$, it is a first order linear ODE. If we set $q_0(t) = Ric(\gamma', \gamma') + 2\sigma^2$, $q_1(t) = 0$, $q_2(t) = \frac{1}{n-1}$ and $z = -\theta$, we recover Raychaudhuri equation—for an irrotational dust:

$$\dot{\theta} = -Ric(\gamma', \gamma') - 2\sigma^2 - \frac{\theta^2}{n-1}. \quad (3.2.2)$$

Since we are indeed interest in the case of equation (3.2.2), let's simplify the general equation (3.2.1) by setting $q_0(t) = r(t)$, $q_1(t) = 0$, $q_2(t) = s$; we thus consider the following initial value problem (i.v.p.):

$$\left. \begin{aligned} \dot{z} &= \frac{z^2}{s} + r \\ z(0) &= z_0 \end{aligned} \right\} \text{ where } r(t) \text{ is continuous on } [0, \infty) \text{ and } s > 0 \text{ is constant.} \quad (\text{i.v.p.})$$

To obtain geodesic incompleteness, the basic idea is to find conditions that guarantee that the (i.v.p) above has no solution on all of $[0, \infty)$. In fact, the *exponentially damped energy conditions* play exactly this role. First, I sketch how we obtain the QEI-inspired hypotheses from quantum energy inequalities in Minkowski spacetime; then, I illustrate how these exponentially damped energy conditions are obtained from it. In the next section, we study Hawking and Penrose Singularity Theorems generalizations based on the ideas here.

Let's start by writing the general QEI (3.1.3) in the flat case. For the massless Klein-Gordon field ϕ in the four dimensional Minkowski spacetime, the energy density is simply $T_{00} = \frac{1}{2} \sum_{\mu=0}^3 (\partial_\mu \phi)^2$; so just consider $Q = 2^{-1/2} \partial_\mu$, $\mu = 0, \dots, 3$ in the example of expression (3.1.5). Take the standard vacuum state as the reference state ω_0 ; in Fourier representation its two-point function is given by

$$\omega_2(x, x') = \int \frac{d^3 \vec{k}}{(2\pi)^3} \frac{1}{2\omega} e^{-ik(x-x')};$$

along an inertial trajectory $\gamma(\tau) = (\tau, \vec{x})$, we have

$$\langle T_{00} \rangle_{\omega_0}(\tau, \tau') = \int \frac{d^3 \vec{k}}{(2\pi)^3} \frac{|p(k)|^2}{2\omega} e^{-i\omega(\tau-\tau')};$$

where $p(k)$ is given by $Q e^{ikx} = p(k) e^{ikx}$; then

$$\langle T_{00} \rangle_{\omega_0}(\bar{g}_\alpha, g_\alpha) = \int \frac{d^3 \vec{k}}{(2\pi)^3} \frac{|p(k)|^2}{2\omega} \hat{g}(-\omega - \alpha) \hat{g}(\omega + \alpha).$$

By equation (3.1.4), we can substitute the above in the general QEI (3.1.3) and, after a simple computation, we obtain⁶:

$$\int_{-\infty}^{\infty} g(t)^2 \langle :T_{00}: \rangle_{\omega}(\tau, \vec{x}) dt \geq -\frac{1}{16\pi^2} \int_{-\infty}^{+\infty} (g''(t))^2 dt \quad (3.2.3)$$

for any smooth compactly supported real-valued function g and any Hadamard state ω .

We can read expression (3.2.3) as:

The averaged expectation value of the energy density is lower bounded by a term on some L^2 -norm of the second derivative of the weighting function;

That is, using the notation of the (i.v.p.) and using the correspondence between Riccati and Raychaudhuri equations, the bound above reads:

$$\int_{-\infty}^{+\infty} (r(t) - r_0(t)) f(t)^2 dt \geq -Q_2 \|f''\|^2 \quad (\text{QEI-inspired})$$

for some constant $Q_2 \in [0, \infty)$, a test-function f and a fixed continuous function $r_0(t)$ which corresponds—in the QEI analogy—to the quantity $r(t)$ evaluated at a reference Hadamard state; symbolically: " $(r(t) - r_0(t)) \equiv: r(t) :$ ". If we further read (3.2.3), more generally, as:

The averaged expectation value of the energy density is lower bounded by a term that depends on L^2 -norms of derivatives of the weighting function;

then, we can consider imposing on the (i.v.p) the most-inspired bound of:

$$\int_{-\infty}^{+\infty} f(t)^2 (r(t) - r_0(t)) dt \geq -\|f\|^2 \quad (\text{QEI-most-inspired})$$

for any Sobolev semi-norm:

$$\|f\|^2 := \sum_{l=1}^L Q_l \|f^{(l)}\|^2,$$

where $Q_l \in [0, \infty)$, $L \in \mathbb{N}$ and $\|\cdot\|$ is any L^2 -norm.

The bounds (QEI-inspired) and (QEI-most-inspired) above came straightforwardly from the form the quantum energy inequalities assume in four dimensional flat spacetime (3.2.3); by imposing them, we implicitly assume that there is a scale on which averages on general curved spacetimes can be well-approximated by these “flat QEIs”. Indeed, we suppose there is a timescale τ_0 for which they hold for all $f \in C_0^\infty((0, \infty))$ with support of length less or equal to, say, $2\tau_0$; and we can take τ_0 as way smaller than local curvature length scales⁷. Now, in order to regularize the average integral over longer timescales, we will soon introduce a bump function to obtain a partition of unity on \mathbb{R} .

As already mentioned, the interesting feature of these inspired bounds is that they give us exponentially damped energy conditions; accordingly, due to the following lemma.

⁶Note that the rescalement $g_\tau(t) = \tau^{-1/2} g(t/\tau)$ gives us the illustrative bound of section 1.2.3.

⁷This is indeed reasonable—for examples, check out [48].

Lemma 3.6. [37, Lem2.3] *If there exists $c \geq 0$ such that*

$$z_0 - \frac{c}{2} + \liminf_{T \rightarrow +\infty} \int_0^T e^{-2ct/s} r(t) dt > 0 \quad (3.2.4)$$

then (i.v.p.) has no solution on all of $[0, \infty)$.

On the other hand, if we assume (QEI-inspired), we obtain expression (3.2.5), and then we also get a result of the nonexistence of global solutions for the (i.v.p.).

Suppose that $r(t)$ is nonconstant and let r_0 be a fixed continuous function such that (QEI-inspired) holds for any $f \in C_0^\infty((0, \infty))$ supported in an interval of length at most $2\tau_0 > 0$. Let g be a fixed real-valued compactly supported smooth function that is non-increasing on \mathbb{R}^+ and such that $g(t) = 1$ on $[0, 1]$; let $c \geq 0$ and $h \in C^\infty(\mathbb{R})$, such that $\text{supp } h \subset [-\tau_0, \infty)$ and $h(t) = e^{-ct/s}$ on $[0, \infty)$. Then

$$f_\tau(t) = \begin{cases} e^{-ct/s} g(t/\tau) & t > 0 \\ h(t) & t < 0, \end{cases}$$

defines a test function for each τ . Then, for any $c > 0$, it holds

$$\begin{aligned} \liminf_{\tau \rightarrow \infty} \int_0^\infty r(t) g(t/\tau)^2 dt &\geq \liminf_{\tau \rightarrow \infty} \int_0^\infty e^{-2ct/s} r_0(t) g(t/\tau)^2 dt - \int_{-\tau_0}^0 (r(t) - r_0(t)) h(t)^2 dt \\ &\quad - Q \left(\|h''\|^2 + \frac{1}{2} \left(\frac{c}{s} \right)^3 + \frac{\|\psi''\|}{\tau_0^3 (1 - e^{-2c\tau_0/s})} \right), \end{aligned} \quad (3.2.5)$$

where ψ is a bump function from which we obtain a partition of unity on \mathbb{R} . Furthermore, if the previous considerations hold and if, for some $c > 0$, we have

$$z_0 \geq \frac{c}{2} - (\text{RHS of (3.2.5)}), \quad (3.2.6)$$

then (i.v.p.) has no solution on all of $[0, \infty)$.

Regarding the more general (QEI-most-inspired) bound, there is the following analogous result.

Theorem 3.7. [37, Thm4.1] *Let r_0 be a fixed continuous function and suppose $r(t)$ obeys (QEI-most-inspired) and is nonconstant. Suppose there exist $c > 0$ and $h \in C^\infty(\mathbb{R})$ with $\text{supp } h \subset [-\tau_0, \infty)$ and $h(t) = e^{-ct/s}$ on $[0, \infty)$, for which*

$$z_0 - \frac{c}{2} + \liminf_{\tau \rightarrow \infty} \int_0^\infty e^{-2ct/s} r_0(t) g(t/\tau)^2 dt \geq \int_{-\tau_0}^0 h(t)^2 (r(t) - r_0(t)) dt + \|h\|^2 \quad (3.2.7)$$

then (i.v.p.) has no solution on all of $[0, \infty)$.

The proof of Theorem 3.7 is given in details in [37]; for it, a generalization of Wald and Yurtsever's argument [116] of 1991 is given as Lemma [37, Lmm3.1] and then: if there is a solution, there is a contradiction; so the (i.v.p) has no solution on all of $[0, \infty)$.

Note that, as mentioned before, there is a scale τ_0 of relevance and that the dependence on the values of $r(t)$ —which, in the General Relativity context, represents the matter content—is only on $[-\tau_0, 0]$.

In addition, if the initial contraction z_0 is strong enough, there will be a focal point. This is reasonable due to the way the problem is posed. If we look at this with Singularity Theorems in mind, note that we are already assuming Raychaudhuri equation holds, we are implicitly assuming we can use Einstein equations to translate (QEI-inspired) to a condition on the curvature of spacetime and the information regarding the “initial/boundary condition” is already in the condition (3.2.7).

Interesting is to see the consistency of this bound (3.2.7) with the nature of quantum energy inequalities: larger positive energies at some instant allows larger negative energies at some later instant; to compensate this possible future larger violations, a stronger initial contraction is in order—and that is exactly what is going on in (3.2.7): greater values of z_0 are needed for greater positive values of $(r(t) - r_0(t))$;

In this section we saw that exponentially damped energy conditions can be obtained from (QEI-inspired) bounds and, additionally, how these conditions yield Singularity Theorems by looking at Raychaudhuri equation as a particular Riccati equation and using results regarding nonexistence of global solutions. In the next section, we see how generalizations of Hawking and Penrose Singularity Theorems can be derived from exponentially damped energy conditions.

3.3 ..Generalizations of Hawking and Penrose Singularity Theorems

Where we answer the question: do Singularity Theorems hold if we consider quantum effects?

Let's see how exponentially damped energy conditions yield generalizations for Hawking and Penrose Singularity Theorems. First, I sketch the proof for the cosmological context, and then, I state the theorem in the Black Hole context in the end, for completeness.

Let M be a globally hyperbolic spacetime of dimension $n \geq 2$, and let S be a smooth compact spacelike Cauchy surface for M . Suppose along each future complete unit speed timelike geodesic $\gamma : [0, \infty) \rightarrow M$ issuing orthogonally from S , there exists $c \geq 0$ such that,

$$\liminf_{T \rightarrow \infty} \int_0^T e^{-\frac{2ct}{n-1}} r(t) dt > \theta(p) + \frac{c}{2} \quad (3.3.1)$$

where $r(t) := Ric(\dot{\gamma}(t), \dot{\gamma}(t)) = R_{\mu\nu}\dot{\gamma}^\mu\dot{\gamma}^\nu(t)$ and $\theta(p)$ is the expansion (i.e., mean curvature) of S at $p = \gamma(0)$.

Let's prove that under these hypothesis, we get a singular spacetime. The steps we follow are: construct an S —ray, around which Raychaudhuri equation holds, then we show that is has no solution.

We can equip any n —dimensional smooth manifold M with a Riemannian metric h . A canonical way for that is to take the induced metric from \mathbb{R}^{2n} , by Whitney embedding theorem. Of course, the pair (M, h) is not unique—for example, we can embed S^2 into \mathbb{R}^3 as

a sphere or as a cube and that gives us different induced metrics⁸. Moreover, to any smooth Riemannian manifold, there is a complete Riemannian manifold conformally equivalent to it⁹—this follows from a result by Nomizu and Ozeki [85].

With a complete Riemannian background metric, take a sequence of points q_n in $J^+(S)$ such that this Riemannian distance from S to q_n goes to infinity as $n \rightarrow \infty$. Since M is globally hyperbolic, the Lorentzian distance is finite, continuous and satisfies the Avez-Seifert property, *i.e.* for any pair of causally related distinct points p and q , there is a causal geodesic from p to q with length equals to $d(p, q)$. Since S is a Cauchy surface, $p_n \in S$ and $q_n \in I^+(S)$, then there is a timelike geodesic segment γ_n from p_n in S to q_n that realizes the Lorentzian distance from S to q_n .

Since S is compact, we can take γ as the limit of γ_n for $n \rightarrow \infty$, then γ is a future inextendible timelike geodesic emanating from $p \in S$ such that from each of its points, it realizes Lorentzian distance to S , *i.e.* γ is an S —ray and has no focal points and no focal cut points¹⁰; then ρ is smooth in a neighborhood U of γ . Moreover, U can be foliated by geodesics orthogonal to S and the tangent vectors to these geodesics yield a unit timelike smooth vector field given, by the Gauss Lemma, by $u = -\nabla\rho$. Then, Raychaudhuri equation holds in U —for the irrotational case, equation (3.2.2).

To show that it has no solution we just use Lemma 3.6; assuming (3.3.1) holds and setting $z = -\theta$, $r = Ric(\gamma', \gamma') + 2\sigma^2$, $s = n - 1$ and $z(0) = -\theta(p)$, by Lemma 3.6, we get that Raychaudhuri equation has no solution on all of $[0, \infty)$ and thus, γ must be incomplete. That is, we obtain the following theorem.

Theorem 3.8. [37, Thm5.1](Generalized Hawking Singularity Theorem): *Let M be a globally hyperbolic spacetime of dimension $n \geq 2$, and let S be a smooth compact spacelike Cauchy surface for M . Suppose along each future complete unit speed timelike geodesic $\gamma : [0, \infty) \rightarrow M$ issuing orthogonally from S , there exists $c \geq 0$ such that,*

$$\liminf_{T \rightarrow \infty} \int_0^T e^{-\frac{2ct}{n-1}} r(t) dt > \theta(p) + \frac{c}{2} \quad (3.3.2)$$

where $r(t) := Ric(\dot{\gamma}(t), \dot{\gamma}(t)) = R_{\mu\nu}\dot{\gamma}^\mu\dot{\gamma}^\nu(t)$ and $\theta(p)$ is the expansion (*i.e.*, mean curvature) of S at $p = \gamma(0)$. Then M is future timelike geodesically incomplete.

Theorem 3.8 is, indeed, a generalization of Hawking Singularity Theorem 1.2, since (3.3.2) holds if we assume SEC holds. If (3.3.2) holds for $c = 0$:

$$\liminf_{T \rightarrow \infty} \int_0^T r(t) dt > \theta(p),$$

⁸A more interesting example: the flat and the donut torus $\mathbb{R}^2/\mathbb{Z}^2$ with the induced metric from \mathbb{R}^2 and \mathbb{R}^3 , respectively, are diffeomorphic (equals, as smooth manifolds); yet, as Riemannian manifolds, they are not equivalent.

⁹A conformal map is one that preserves angles (and thus, shapes of infinitesimally small things), but not necessarily volume and curvature.

¹⁰The cut locus of a point p , a concept of Riemannian Geometry, is the set in $T_p M$ on which the geodesics defined by the (radial isometries of the) exponential map are minimizing.

then, if $\theta < 0$ on S , $r(t)$ can be globally negative and still satisfy the hypothesis. Now, if we assume the strong energy condition and that S is mean contracting—both Hawking Singularity Theorem hypotheses—then, obviously $r(t) \geq 0 \Rightarrow r(t) \geq \theta(p) \Rightarrow (3.3.2)$ holds and we recover the Cosmological singularity of Hawking's Theorem. The analogous argument holds for the generalized Singularity Theorem in the Black Hole context; although it deals with diverse geometrical objects, for example: an S -ray is not considered, rather affinely parametrized future inextendible null geodesics are constructed by the generators of the achronal boundary $\partial J^+(\Sigma)$; the contradiction argument that concludes the incompleteness is also based on Lemma 3.6. For completeness, the statement of the generalization of Penrose Singularity Theorem 1.1 follows.

Theorem 3.9. [37, Thm5.2](Generalized Penrose Singularity Theorem): *Let M be a spacetime of dimension $n \geq 3$ with a noncompact Cauchy surface S . Let Σ be a smooth compact acausal spacelike submanifold of M of codimension two, with null expansion scalars θ_{\pm} associated to the future directed null normal vector fields l_{\pm} . Suppose along each future complete affinely parameterized null geodesic $\eta : [0, \infty) \rightarrow M$, issuing orthogonally from Σ with initial tangent l_{\pm} , there exists $c \geq 0$:*

$$\liminf_{T \rightarrow \infty} \int_0^T e^{-\frac{2ct}{n-2}} r(t) dt > \theta_{\pm}(p) + \frac{c}{2} \quad (3.3.3)$$

where $r(t) = R_{\mu\nu} \dot{\eta}^{\mu} \dot{\eta}^{\nu}(t)$ and $p = \eta(0)$. Then M is future null geodesically incomplete.

Analogously, Theorem 3.9 is a generalization of Penrose Singularity Theorem, since (3.3.3) holds when Σ is trapped and NEC holds.

It is interesting to point out that the statements of these generalizations, however similar to the Pattern Singularity Theorem 1.3, do not have the same ingredients. Note that there is not an initial/boundary condition—which is compensated by the fact that the own energy conditions includes a term on the expansion (indeed, θ is on the RHS of expressions (3.3.2) and (3.3.3)). Furthermore, there is an extra condition in Theorem 3.8: the compacity of the Cauchy surface S ; yet, if we consider the observable universe, this condition is reasonable.

In addition, in [37], Fewster and Galloway applied to the Einstein-Klein-Gordon theory the results described in the last section; their methods were then used in [18] for the derivation of a “Hawking-like Singularity Theorem” considering the massive non-minimally coupled Klein-Gordon field. Basically, if there is sufficient initial contraction, a singularity is inevitable. But how strong must be the initial contraction? In a recent work [18], Brown, Fewster and Kontou gave a nice discussion regarding this and argued that for a model whose field mass is taken to be of an elementary particle, a teeny tiny initial contraction would be required¹¹.

Now that we understand how quantum energy inequalities inspired Singularity Theorems from weakened energy conditions that generalizes Hawking and Penrose's Theorems, we can finally answer the question posed in chapter 1;

¹¹For the Higgs mass $125\text{GeV}/c^2$, it would be necessary a minimum contraction of 10^{-14}s^{-1} ; also, in the model they considered, this is compatible with a maximum temperature of order 10^{13}K —which corresponds to the Universe temperature at time 0,0001s.

3.4 Wind-up

Where we give an answer to: *do Singularity Theorems hold if we consider quantum effects?*

In this dissertation we deal with the question of whether quantum effects could elude a singularity in General Relativity. If singularities are a disaster for General Relativity is still controversial, an observable singularity would break causality and would leave us without predictive power. Whence, physicists have always been trying to elude them: first, by considering them just a mathematical artifact, then by blaming the (high) symmetry hypothesis of the exact solutions and currently, by either checking if quantum effects could prevent a singularity from arising or working with the cosmic censorship conjecture.

—Do Singularity Theorems hold if we consider quantum effects?

Within a semi-classical analysis, considering “quantum effects” whose manifestations are represented just by the energy condition and using energy bounds that allow global violations of the classical energy conditions, there are generalizations of Hawking and Penrose Singularity Theorems. Hence, an answer is:

—Yes, Singularity Theorems do hold for *subtle* quantum effects; where “subtle” rules out, for example, backreaction effects and interaction effects.

One would now wonder, could backreaction or interaction effects change everything?

This is a tough question and my answer is: I have no idea, yet:

—Maybe, yes. There are bouncing models, for example, one can explicitly construct a quantum state for the universe that is consistent with a bouncing model [89], thus obtaining a non-singular universe. Furthermore, a recent work obtained a quantum No-Singularity Theorem considering geometric flows [5]. Thus, it is reasonable to expect that the inclusion of backreaction or interaction effects could elude a singularity from arising.

—Maybe, no. The energy condition is just a lower bound; it is expected that, with the inclusion of backreaction or interaction effects, we still have a lower bound on averages of the energy density, thus nothing dramatic would happen in the proof showed in this section; thus, for sufficiently strong initial contraction, we still have a singularity.

Even though there is an answer, there are things to be done—I give a brainstorm list of them in the next page.

Things to do, regarding:

- * the concept of singularity in General Relativity: in 1968, the same year of “What is a singularity in General Relativity?”, Geroch wrote another article [60] in which he describes a way to characterize singularities by defining equivalence classes of geodesics and constructing a boundary of singular points—called the g -boundary—which provides a local description and allow us to study topological properties of a singularity. Unfortunately, its construction is difficult and the freedom of the definitions used makes them not so natural. There were some other studies, like the b -boundary of [102] and the a -boundary of [104], on the local characterization of singularities, also based on this idea of defining a spacetime boundary with singular points, but there is still a lot of work to be done in this topic until we obtain a mathematically precise and physically intuitive characterization. In particular, in the study of the topology of these boundaries, there were indicatives of weirdness: non Hausdorff interaction between boundary and interior spacetime points [62];
- * negative energy within quantum field theory—the Casimir effect: it has been formulated in the algebraic approach [27] and I wonder if we can describe the dynamical Casimir effect in this formalism and relate it to analogue moving mirror models for Black Holes. In fact, Black Hole physics is also studied within AQFT; for example, towards a better understand of Hawking radiation, there are rigorous analysis of the Hadamard condition for quantum states on Black Hole spacetimes as [26], and recently [20];
- * quantum energy inequalities: with Singularity Theorems in mind, study the asymptotic behaviour of quantum energy inequalities and the scale on which the ones on curved spacetimes can be well-approximated by the flat ones. In fact, a quantum energy inequality version of the SEC is expected soon [18]. Furthermore, several other QEI’s have been derived considering different fields: for the Electromagnetic field [90] and recently [41], for Dirac fields [38, 28, 109], for spin-one fields [42], for the non-minimally coupled scalar field [39, 40] and for the massive Ising model [17]. One could continue this by searching for quantum inequalities for Rindler, Milner or Schwarzschild spacetimes. Can we relate it with the Hawking-Unruh effect? Check [34, Pgs27-30];
- * other cosmological applications of Algebraic Quantum Field Theory: towards a better understanding of the standard cosmological model and the Cosmological Constant Problem, one can follow the works of K. Fredenhagen and T. Hack [55] and of C. Dappiaggi, T. Hack, J. Möller and N. Pinamonti [25]. Both these references consider a semi-classical analysis, but they consider different averages for the energy-momentum tensor. It would be interesting to study how the free parameter of [55] can be associated to Dark radiation and to pursue a comparison between these two analysis. Furthermore, it would be interesting to consider these formalisms in the regime where interaction must be taken into account. Indeed, the interaction picture has been developed, over the last 20 years, in the perturbative formalism of AQFT by several works of R. Brunetti, K. Fredenhagen, S. Hollands, K. Rejzner, R. Wald and others. To work towards including the interaction picture in cosmological applications of AQFT, one could start by studying the monograph [97].

A

WHAT IS A SINGULARITY IN GENERAL RELATIVITY?

Where we are convinced that a Singularity in General Relativity is different from the usual ones that appear in Physics and we get an idea of why we define it the way we define it.

Singularity is a common word, so that we can say it has three canonical meanings: one used by society, one in the science community in general and another one just for relativists. Something singular is something unique, different, rare, but this is too broad a definition to be useful for us. In Physics and Mathematics usually a singularity is a point where something either goes to infinity or is not well-defined. Relativists say that spacetime is singular if it contains an incomplete geodesic. In this section we will see why relativists had the need to redefine a singularity.

The canonical example of a mathematical singularity is the function $\frac{1}{x}$ at $x = 0$. This type of singularity appears a lot in physics, for example: the electric field of a point charge at the point charge or the velocity of a fluid vortex at the center of it. Yet, this does not startle anyone. Considering the Uncertainty Principle, since we could never get infinitely close to the electron, it does not make sense to say that this singular point actually exists. Classically, we could just say that the electric field is not defined at the charge. And even though we can watch water spiraling into a drain at our homes, we do not observe any catastrophe. Nature has turbulence and cavitation and other effects that weren't considered in that model, thus nothing goes wrong at the center here. Both are mathematical singularities, functions with singular points, yet they do not represent real physical problems¹.

A singularity in General Relativity cannot be a point of spacetime. When dealing with mathematical singularities like the above, one is implicitly using the Minkowski background—the knowledge of which points the respective quantity *could* be defined on. These points where the theory cannot be applied are points of the spacetime and they can be called *singularities of the specific theory* considered on the spacetime background. In General Relativity, we no longer know where the theory could be applied, since the spacetime itself is part of the theory. We need to *define* spacetime and then, on it, deal with peculiar things that arise.

¹The singularities in the context of Microlocal Analysis of this dissertation are also mathematical singularities.

Let's keep in mind that there are two consensuses among physicists : “a singularity is a place where things go bad” and “Minkowski spacetime is non-singular”. It is important to note that “something blowing up” is not a consensus, we will discuss the reason for that in a while. The discussion here is based on [61, 107]. In [61], Geroch argued that there is no perfect definition of singularity in General Relativity after debating the ambiguities of the concept through a nice Galilean dialogue between Sagredo and Salviati—his conclusion still holds. In [107], Senovilla and Garfinkle discussed the types of difficulties one runs into when trying to construct a definition in an extended review of Penrose Singularity Theorem of 1965. Another good reference for this topic is [98].

First, we need to define spacetime²; of course it will be constituted of regular points because regular points are, by definition, those where “physics holds”, where we have enough differentiability to do physics at. That is a restatement for the assertion that a singularity cannot be defined as a point of spacetime.

We have to guarantee that the manifold chosen cannot be extended to another one with only regular points, for we would not have a reason not to consider these other points also as constituents of our spacetime. Then, we try to find if problematic points or regions were excluded by this. Yet, what types of regions could have been excluded and are of physical relevance? Let's see an example.

Consider a spacetime with:

$$ds^2 = -\left(\frac{1}{t}\right)^2 dt^2 + dx^2 \quad \text{defined for } t > 0.$$

The corresponding metric tensor will go to infinity approaching the point $t = 0$, but this is simply a bad choice of coordinates for the Minkowski spacetime (which we do not want to classify as singular). We should just choose another set of coordinates and include the point $t = 0$. In fact, the coordinates of any tensor cannot be used to define a singularity, since they depend on the basis chosen³. Another canonical example of a non-physical singularity caused by this would be the Schwarzschild original solution for the spherically symmetric vacuum universe with the problematic $r = 2m$ surface:

$$ds^2 = -\left(1 - \frac{2m}{r}\right) dt^2 + \left(1 - \frac{2m}{r}\right)^{-1} dx^2 \quad \text{defined for } r > 2m;$$

this $r = 2m$ region is called a *coordinate singularity*.

The natural attempt after realizing that we cannot characterize a singularity through some bad behaviour of the curvature tensors, would be to use curvature scalars, since they are at least independent of basis. Two things need to be considered: first, curvature scalars depend on the point of the manifold, and second, we are considering an indefinite metric. Hence, we should consider their behavior along curves on the manifold, in particular on geodesic curves. Geodesic curves are affinely parametrized and this gives us a notion of distance. What can we say, however, about something that goes to infinity along a geodesic that also goes to infinity? Nothing, actually. But we could call a spacetime singular if some curvature scalar goes to infinity on a finite affine length geodesic. The only question now would

²Take a look at the appendix B for the construction of the definition of spacetime.

³In any spacetime with non-constant curvature we can, for every point x , choose coordinates such that the curvature tensor blows up at x .

be: can we find a collection of curvature scalars to characterize the curvature of a regular metric? Unfortunately, the answer is no. With an indefinite regular metric, we cannot find a collection of curvature scalars that characterizes the curvature and remains finite—so we cannot characterize a singular behavior by curvature scalars blowing up. Furthermore, there are pathological examples of spacetimes with vanishing curvature and incomplete geodesics. In summary: *we cannot characterize a singularity through some bad behavior of curvature scalars.*

So what if we just consider incomplete geodesics as signaling a singularity? An incomplete geodesic also gives an idea of a removed region. Imagine an observer traveling through spacetime reaching the “end” of a geodesic. It seems reasonable to call that a singular behavior. In fact, that is the usual definition in General Relativity:

Definition. A spacetime is singular if it is not geodesically complete, i.e. if the geodesics cannot be extended to arbitrarily large parameter values.

An interesting fact that Geroch shows (also in [61]) is that: null, time and spacelike geodesic completeness are not equivalent. Moreover, he gives an example of a universe complete in all three senses but which contains a timelike curve of bounded acceleration and finite total length.

We often refer to a singular spacetime as a spacetime that “contains a singularity”; so, informally, we associate the existence of an incomplete geodesic with the idea of a “singularity”, even if we did not give an ontology to a “singularity” or a “singular point”.

Note that the relation between a singularity and the curvature of the spacetime is not yet well understood. The conclusion of this topic is that Classical Singularity Theorems, which uses the definition above, do not give us much information, since they do not characterize the singularity: *they only state that there is at least one incomplete geodesic.* Their strength comes from the fact that not much is asked out of the spacetime in the hypothesis. To characterize the nature of the singularity, we would need more details on the matter content of the spacetime.

To end this section, a nice quote from Geroch’s PhD thesis:

“What a strange little object is the singularity with its strange properties and nonexistent definition. Yet the singularity promises to remain one of the most intriguing and disturbing aspects of gravitation theory for a long time to come. Here is a problem with which we must someday come to grips—at least if we are ever to understand this phenomenon called gravitation.” [64, Pg145]

B

TOWARDS THE DEFINITION OF A CURVED GENERAL SPACETIME

Where we recall the necessary definitions to understand the definition of a curved general spacetime.

A first glance at pure mathematics gives the idea that it is a collection of abstract general concepts apart from the real world. Whereas every definition was inspired by some property observed in the real world and then generalized and formalized in a consistent fashion. The goal here is to understand the definition of a *spacetime*, where it comes from and what can we do with it. Some good references of these subjects are: for an introduction to General Topology [21], for Functional Analysis [7], for an introduction to Riemannian Geometry [66] and for Lorentzian Geometry [87].

To define a curved general spacetime we need to consider which properties of the Euclidean space we would like to maintain. A topological space is a generalization of a metric space, and a metric space is a generalization of the Euclidean space. Let's first take some properties of the real line¹: it is a topological manifold of dimension one, in particular it inherits a metric topology from its usual distance function and another topology from the fact that it is a totally ordered set. The real line is a locally compact space and a paracompact space, as well as second countable and normal, thus Hausdorff. The real line is path-connected and therefore connected. Also, it can be compactified in a circle by adding a point at infinity. Let's keep them in mind.

Let start with a set. Think of it as a collection of points that constitute our spacetime. We want to be able to say if one point is near another point, we need to understand how the points in this set connect with each other. This is done with the definition of *topology*. It is a generalization of the notion of *open sets* in the real line. The notion of “a point near another” is analyzed with the definition of *neighborhoods*. Well, with a topology we can study, in a way, how points connect with each other, how are they “near or far”. In fact, with a topology we can construct notions of *limits*, *continuity*, *compacity*, *convexity*, *etc*.

Now we have a set equipped with a topology (a certain collection of open sets). There are some minimum requirements we need regarding the fineness of the topology. Every open

¹If you don't understand the words in this paragraph, do not worry. We will see these definitions in the following.

set can be written as a union of elements of the topology. The Euclidean space has the nice second-countable property. This means that every open set can be written as a countable union of elements of the topology and we can look at it as a “well-behaviourness” imposition which we will ask out of our spacetime. On the other hand, if something is convergent, it is physically reasonable to require that the limit is unique. The Hausdorff separation property guarantees the latter. By Urysohn’s Metrizability Theorem, a second-countable Hausdorff topological space is metrizable. That is great because we definitely want to equip our spacetime with a distance notion.

We will consider a connected set. By that, we are saying that our spacetime is “whole”, in the sense that we could not write it as two disjoint subspacetimes. If there is a path connecting every two points of a set, we call it path-connected. Yet, remember that we can study how points connect using the topology, and indeed *connectedness* is a topological concept that is a generalization of the notion of path-connectedness².

So far, our spacetime is a set equipped with a topology (def B.1), satisfying the Hausdorff property (def B.2), second-countable (def B.3) and connected (def B.4). Formally, we have the following definitions.

Definition B.1. (Topological space) A set X equipped with a topology is said to be a *topological space*. A *topology on a set X* is a collection τ of subsets of X such that:

- (i) $\emptyset, X \in \tau$;
- (ii) if $A, B \in \tau \Rightarrow A \cup B \in \tau$ and $A \cap B \in \tau$.

We denote the topological space $(X, \tau) \equiv X$ and the elements of τ are called *open sets*. If U is open, we call its complement U^c a closed set. A *neighborhood* for $p \in X$ is an open set containing p .

Definition B.2. (Hausdorff topological space) A topological space X is said to be Hausdorff if for each pair of distinct points $p_1, p_2 \in X$ there are neighborhoods U_1, U_2 such that: $p_1 \in U_1, p_2 \in U_2$ and $U_1 \cap U_2 = \emptyset$.

Definition B.3. (Second-contable topological space) A topological space (X, τ) is said to be *second-countable* if its topology has a countable basis. A basis for τ is a collection $\mathcal{B} \subset \tau$ such that: for all $p \in X$ and for all open set $U \ni p, \exists B \in \mathcal{B}$ with $p \in B \subset U$. Every element in τ can be written as a union of elements of its basis \mathcal{B} .

Definition B.4. (Connected topological space) A topological space (X, τ) is said to be *connected* if the only subsets of X which are both open and closed are \emptyset and X . Equivalently, a topological space is connected if it cannot be divided into two disjoint nonempty open sets (or divided into two disjoint nonempty closed sets).

The inspiration for the definitions above is the Euclidean space, as said before. But now we are going to impose something a little stronger. We will say that our spacetime is *locally equivalent* to \mathbb{R}^n , topologically locally equivalent. This means we can continuously map a neighborhood of a point of the spacetime into an open set of \mathbb{R}^n , and continuously take it back. This map is called a *homeomorphism* (def B.5). A homeomorphism is a topological

²The idea of separation of our spacetime in components will come from General Relativity and the causality notion. It seems reasonable to start with a connected spacetime.

isomorphism, which means that it preserves topological concepts between the spaces. Two topological spaces that are homeomorphic, *i.e.* if there is a homeomorphism between them, are considered the same. Moreover, adding these homeomorphisms to our second-countable Hausdorff topological set, our spacetime is called an n -dimensional topological manifold (def B.6). Precisely, we have the following definitions.

Definition B.5. (Homeomorphism) A bijection f , between topological spaces X and Y , is called a *homeomorphism* if both f and f^{-1} are continuous. f is continuous if for every open set $U \subset Y$, the pre-image $f^{-1}(U) \subset X$ is an open set.

Definition B.6. (n -dimensional topological manifold) An *n -dimensional topological manifold* M is a second-countable Hausdorff topological space such that each point possesses a neighborhood homeomorphic to an open subset of \mathbb{R}^n .

Let M be an n -dimensional topological manifold, $U \subset M$ an open set and $\varphi : U \rightarrow \varphi(U) \subset \mathbb{R}^n$ a homeomorphism. Then, φ is called a *coordinate system* or *chart*, φ^{-1} is called a *parametrization* and the set $\varphi^{-1}(U)$ is called a *coordinate neighborhood*.

For every point in our manifold, we have at least one neighborhood and one homeomorphism from it onto an open set in \mathbb{R}^n . What happens when neighborhoods overlaps? We must be able to transit between charts: we get *transition maps*. If we further impose that these coordinate changes are differentiable maps, we get the idea of a *differentiable manifold*.

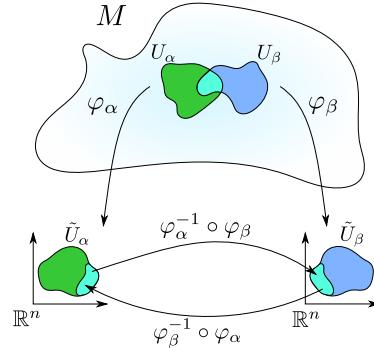


Figure B.1: Parametrizations and overlap maps.

Definition B.7. (n -dimensional smooth manifold) An *n -dimensional smooth manifold* M is an n -dimensional topological manifold equipped with a family of parametrizations $\varphi_\alpha : U_\alpha \rightarrow M$, where $U_\alpha \subset \mathbb{R}^n$ are open sets, such that:

- (i) $\bigcup_\alpha \varphi_\alpha(U_\alpha) = M$, *i.e.* the coordinate neighborhoods cover M .
- (ii) for each pair α, β with $W := \varphi_\alpha(U_\alpha) \cap \varphi_\beta(U_\beta) \neq \emptyset$, the transition maps $\varphi_\beta^{-1} \circ \varphi_\alpha : \varphi_\alpha^{-1}(W) \rightarrow \varphi_\beta^{-1}(W)$ and $\varphi_\alpha^{-1} \circ \varphi_\beta : \varphi_\beta^{-1}(W) \rightarrow \varphi_\alpha^{-1}(W)$ are smooth

(iii) $\mathcal{A} = \{(U_\alpha, \varphi_\alpha)\}$ is maximal, *i.e.* if $\tilde{\varphi} : \tilde{U} \rightarrow M$ is a parametrization such that $\tilde{\varphi}^{-1} \circ \varphi$ and $\varphi^{-1} \circ \tilde{\varphi}$ are smooth for all φ in \mathcal{A} , then $(\tilde{U}, \tilde{\varphi})$ is in \mathcal{A} . We call the family \mathcal{A} a *maximal Atlas* or a *differentiable structure*.

A *diffeomorphism* is an isomorphism for smooth manifolds. Two n -dimensional smooth manifolds M and N are considered the same if there is a diffeomorphism between them, then we say they are diffeomorphic.

Definition B.8. (Diffeomorphism) Let M and N be two n -dimensional smooth manifolds with parametrizations $(U_\alpha, \varphi_\alpha)$ and (V_β, Ψ_β) , respectively. A bijection $f : M \rightarrow N$ is called a diffeomorphism if f and f^{-1} are smooth, *i.e.* if f is smooth at every in every local chart $\Psi \circ f \circ \varphi^{-1}$ is smooth at $\varphi(x) \in \mathbb{R}^n$. Note that f is smooth if

With the global differentiable structure and the local Euclidean character, we can define differentiable properties of objects locally and independently of parametrizations. We do that using the definition of the tangent space $T_p(M)$ at a point $p \in M$. We can do approximations by locally replacing the manifold by its tangent space—this process is called *local linearization*. For us, in this appendix, the notable property of the tangent space is that it allows us to define vectors and take scalar products between them. There are three equivalent definitions for $T_p M$, using linear functions or the transformation law of coordinate changes or using the velocities of the curves of the manifold. The one I find most intuitive is the last one.

For a surface S in \mathbb{R}^3 , the tangent space at $p \in S$ is the tangent plane $T_p S$. For every vector $v \in \mathbb{R}$, tangent to S at p , there exists a differentiable curve c from an interval $I \subset \mathbb{R}$ into S such that $c(0) = p$ and $\dot{c}(0) = v$. This is the idea we use to define—intrinsically—the tangent space on manifolds. Let M be an n -dimensional smooth manifold, as before, and consider all curves c passing through $p \in M$, then $T_p M$ is the vector space generated by the *velocities* of c .

Definition B.9. (Parametrized curve) A *parametrized curve* is a mapping from $I \subset \mathbb{R}$ into M by $I \ni t \mapsto c(t) \in M$. If this mapping is differentiable, we say it is a *differentiable curve* (in M).

Definition B.10. (Velocity of a curve) Let c be a differentiable curve in M such that $c(0) = p$ and let $C^\infty(p)$ be the space of real functions on M that are smooth at p . For $f \in C^\infty(p)$, the composite mapping $f \circ c$ is a function on I differentiable at $t = 0$. The *velocity of the curve c at p* is the linear map

$$C^\infty(p) \ni f \mapsto \frac{d(f \circ c)}{dt}(t) \Big|_{t=0} \equiv v_{c,p}(f).$$

To see it makes sense to define a velocity as a linear map, imagine the following: consider you walk around describing a curve c and measuring some quantity—say, the temperature—which is given by a function f . What you obtain is the function $f \circ c$ that gives you how the temperature f changes along your movement c . Now, since you can do that with all quantities—for all $f \in C^\infty$ —and $\frac{d(f \circ c)}{dt}(t) \Big|_{t=0}$ is the directional derivative of f along c

at p , then you know the directional derivatives along c at p of all f . Recall from vector calculus that the directional derivative of a function f is the dot product of the velocity v by the gradient of the function ∇f , then the idea above is that: given that we know $f \mapsto v \nabla f, \forall f$, then we can recover v .

Definition B.11. (Tangent space) Let M be an n -dimensional smooth manifold, the *tangent space at p* , denoted $T_p M$, is the collection of all velocities at p :

$$T_p M := \{v_{c,p}(f) : c \text{ is a smooth curve passing through } p\}.$$

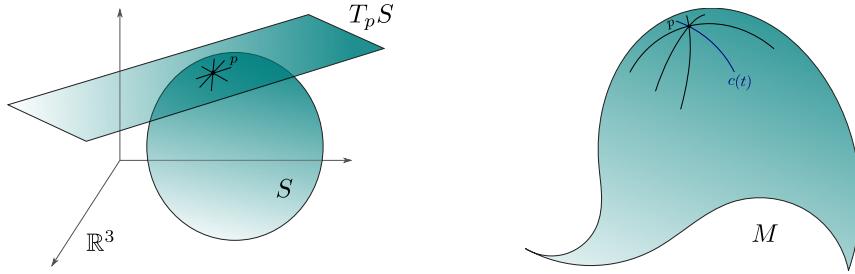


Figure B.2: On the left, a sphere $S \subset \mathbb{R}^3$ —easy to visualise $T_p M$, we can draw it as the tangent plane. On the right, a general manifold M and curves passing through p .

The tangent space $T_p M$ is an n -dimensional vector space. Chosing a parametrization (x^1, \dots, x^n) around p , we obtain that $T_p M = \text{span} \left\{ \left. \left(\frac{\partial}{\partial x^1} \right) \right|_p, \dots, \left. \left(\frac{\partial}{\partial x^n} \right) \right|_p \right\}$. The disjoint union of all tangent spaces is called the *tangent bundle*

$$TM := \bigcup_{p \in M} T_p M = \{v \in T_p M : p \in M\}.$$

Moreover, the *cotangent space at p* , denoted $T_p^* M$, is the dual space of $T_p M$; analogously, $T^* M := \bigcup_{p \in M} T_p^* M$ is the *cotangent bundle*.

A *vector field* on a smooth manifold M is the map that to each $p \in M$ associates a vector X_p in $T_p M$:

$$\begin{aligned} X : M &\rightarrow TM \\ p &\mapsto X(p) := X_p \in T_p M. \end{aligned}$$

Let V be a vector space, and V^* its dual space; a (k, m) -*tensor* is a real multi-linear function on the product space $V^* \times \dots \times V^* \times V \times \dots \times V$ that has k copies of V^* and m copies of V . The set of all (k, m) -tensors is denoted $\mathcal{T}^{k,m}(V^*, V)$.

Definition B.12. (Tensor field) A (k, m) -*tensor field* is a map that to each point $p \in M$ assigns a tensor $T \in \mathcal{T}^{k,m}(T_p^* M, T_p M)$.

As an example, note that a vector field is a $(0, 1)$ -tensor field. A metric tensor field—usually called just “metric”, in physics—is a $(0, 2)$ -tensor field.

Definition B.13. (Pseudo-Riemannian metric) A *pseudo-Riemannian metric* is smooth 2-tensor field $g \in \mathcal{T}^2(T^*M)$ on a connected n -dimensional smooth manifold M such that it holds:

$$\begin{aligned} g(v, w) &= g(w, v) \text{ (symmetry);} \\ g(v, w) &= 0 \forall w \in T_p M \Rightarrow v = 0 \text{ (non-degeneracy).} \end{aligned}$$

The signature of g is the pair $(p, -q)$, where p and q are the numbers of positive and negative, respectively, eigenvalues of the quadratic form associated to g .

Definition B.14. (n -dimensional Lorentzian manifold) An n -dimensional smooth manifold equipped with a pseudo-Riemannian metric g with signature $(1, 1 - n)$ is called an *n -dimensional Lorentzian manifold*, denoted by (M, g) —or just by M .

One could wonder why should the spacetime be smooth. We could define a spacetime using a k -times differentiable manifold, in spite of a smooth one. Indeed, we could have. Hawking discuss this in [72] and talks about how many degrees of differentiability we actually need. Yet, we could intuitively invoke Whitney embedding theorem to feel at ease with the smoothness imposed.

Given an n -dimensional Lorentzian manifold M and the other structures defined above, we can introduce *causality* notions. Let g be the Lorentzian metric and $p \in M$; a non-zero $v \in T_p M$ is:

$$\begin{aligned} &\text{timelike, if } g(v, v) < 0; \\ &\text{lightlike, if } g(v, v) = 0; \\ &\text{spacelike, if } g(v, v) > 0. \end{aligned}$$

Lighlike vectors and the zero vectors are called *null vectors*; timelike and lightlike vectors are called *causal vectors*. This characterization also applies to curves on M , they herd the causality notion of their tangent vectors and we use them to take these notions from TM to M . With this notion, we can define a *time-orientation* of our spacetime and then, introduce the notions of *causal future(past)* and *chronological future(past)*.

Let J be the set of all causal vectors and I the set of all timelike vectors in TM . For each $p \in M$, $J \cap T_p M$ and $I \cap T_p M$ have two connected components;

Definition B.15. (Time-orientability) A connected n -dimensional Lorentzian manifold M is *time-orientable* if J has exactly two connected components. This means we can choose a *time-orientation*, that is: choose one component as the *causal future* J^+ and one component as the *causal past* $J^- = -J^+$.

Time-orientability is equivalent to the existence of a nonvanishing vector field on M .

Definition B.16. (Spacetime) A (n -dimensional) *spacetime* is a connected time-orientable n -dimensional Lorentzian manifold.

We will restrain our study to globally hyperbolic spacetimes. The notion of globally hyperbolicity allow us to impose causality in the context of, not as the physical considerations of Special Relativity, but General Relativity—that is causality in the context of differential equations considering the particular case of Einstein equations—and to construct a well-posed Cauchy problem for the Klein-Gordon field, as showed in chapter 2. In fact, it is the largest class for which the Klein-Gordon Field is a well-posed Cauchy problem. The name was given due to the hyperbolic character of the solvable equations on spacetimes satisfying this condition.

Definition B.17. (Causality and strong causality conditions) A Lorentzian manifold is said to satisfy the *causality condition* if it does not contain closed causal curves—and we say M is causal. If it further does not contain almost closed causal curves, it is said to satisfy the *strong causality condition*.

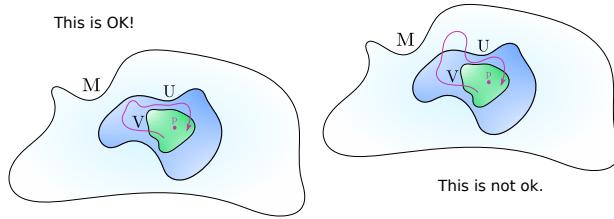


Figure B.3: Strong Causality Condition

If M is causal, it's guaranteed the *existence* of global solutions of linear differential operators for suitable initial values (on maximal achronal hypersurfaces). If M is *diamond-compact*, *i.e.* for all $p, q \in M$, $J_+^M(p) \cap J_-^M(q)$ is compact, then the *uniqueness* of those solutions is guaranteed. If M satisfies both these properties, M is said to be *globally hyperbolic*. To impose global hyperbolicity on the spacetime corresponds to impose *determinism* on nature—predictability and no time-machines. In 2006, Bernal e Sanchez proved a long-standing conjecture that allows us to state the following theorem with global hyperbolicity equivalences.

Theorem B.18. (Global Hyperbolicity equivalences) Let M be a connected time-oriented Lorentzian Manifold. Then the following are equivalent:

- (i) M is diamond-compact and satisfies the strong causality condition;
- (ii) There exists a Cauchy surface on M ;
- (iii) M is isometric to $\mathbb{R} \times S$ with metric $-\beta dt^2 + g_t$ where β is a smooth positive function, g_t is a Riemannian metric on S depending smoothly on $t \in \mathbb{R}$ and each $\{t\} \times S$ is a smooth spacelike Cauchy surface in M .

If M satisfies them, then it is said to be *globally hyperbolic*.

Proof. $[(iii) \Rightarrow (ii)]$ is trivial. $[(ii) \Rightarrow (i)]$ is well-known. $[(i) \Rightarrow (iii)]$ proved recently by Bernal and Sánchez[12]. \square

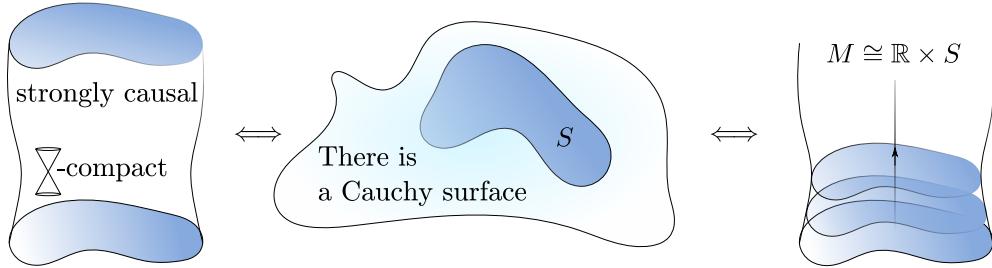


Figure B.4: Illustration of a global hyperbolic spacetime.

Global hyperbolicity is the Lorentzian analog to Riemannian completeness. We can equip any manifold with a Riemannian metric, we can associate any Riemannian manifold to a metric space and, due to minimizing properties of geodesics in Riemannian geometry, Hopf-Rinow theorem guarantees that a Riemannian manifold is metrically complete if and only if it is geodesically complete. Within Lorentzian geometry, the last sentence is completely changed. We can equip a non-compact manifold with a Lorentzian metric, but there is no metric space associated to it. The non-trivial character of it justifies definition 1.1 of a singular spacetime as a geodesically incomplete one. Due to causality notions—absent in Riemannian geometry—there are several types of completeness which are not logically equivalent: bounded-accelerated curves completeness, b -, timelike, lightlike and spacelike geodesic completeness. Yet, global hyperbolicity implies the following proposition.

Let $d : M \times M \rightarrow [0, \infty]$ be the Lorentzian distance function, that is: $d(p, q)$ gives the supremum of the lengths of the future-directed causal curves from p to q .

Definition B.19. (Avez-Seifert property) For any pair of distinct points p and q in M such that $q \in J^+(p)$, there is a causal geodesic from p to q with length equal to the Lorentzian distance function, *i.e* there is a maximal curve between p and q .

Proposition B.20. *In a globally hyperbolic spacetime M , the Lorentzian distance function is finite, continuous and satisfies the Avez-Seifert property.*

This is enough for now. If you want to continue studying this subject, a nice reference that talks about the transition from Riemannian Geometry to Lorentzian Geometry is [83]. Also, any free time can be filled with some article from Robert Geroch, for example, regarding global structures of spacetimes, [63].

C

A SHORT STORY OF THE VACUUM

Where we take a quick tour on the evolution of the vacuum concept, stopping at some curious experiments that verified the existence of the vacuum. Since this will not be historically precise, as so many episodes and subtleties will be left out, and since there will be no references to support it, we shall call it a short story; like a fabula, it will, hopefully, transmit an idea.

The word *vacuum* is naturally associated to *empty space*, to what is left after one removes all matter. Although, to use the word “naturally” in this first sentence is anachronical; throughout history, our conception of vacuum—of the reasonability of its existence—alternated. Could we talk about the ontology of the vacuum? Or even this question is contradictory? Let’s take a glance at the debate around the vacuum concept, by checking some of its many lives. A nice reference—for Portuguese readers—for reviewing “Greek Science” is [1].

The *vacuum* was born with the atomists answer to the “Problem of Change”: how can things change? Democritus¹(410b.C.) explained it terms of *atoms*; different things are due to different forms, positions and arrangements of these atoms. By postulating the existence of *things*—the atoms,—the idea of *not-things*—nothing, *emptiness*—arouse. For the atomists, reality consisted of atoms and emptiness.

The *vacuum*’s first life, as a brother of the *atom*, ended with Aristotle(384-322 a.C.). He approached the “Problem of Change” differently from the atomists, by introducing the notion of *potentiality* and *actuality*. The vacuum concept was dealt by Aristotle in the context of Dynamics and, for him, the empty space did not exist: there was a *medium* in touch with everything that it contained. With this filling medium and his law on the velocities of things², he introduced the *horror vacui* idea—*i.e* “nature abhors vacuum”³. In fact, this idea perpetuated until the seventeenth century, when it was used to explain the functioning of the suction pump, used since the Roman times.

The works of Torricelli—with the mercury barometer—and Otto von Guericke—with the

¹Let’s take Democritus as a representative of the atomists equivalence class.

²Check out: Aristotle Physics IV chapters 6 to 9.

³Curiosity: the stoics also denied the vacuum inside the world, but admitted it as infinite outside of the world; the world was filled, and things could move in the world just like a fish can move in water. Later on, the epicurists recovered the atomists conception of reality—Epicurus(341-241 a.C.) was, actually, also an atomist.

Magdeburg's hemispheres—gave the vacuum its second life. In 1630s, italians⁴ faced failures in using the suction pump. Either on wells or on coil mines, the pumps could not rise water from arbitrarily depths. This mistery was solved by Galileu's discipule Torricceli.

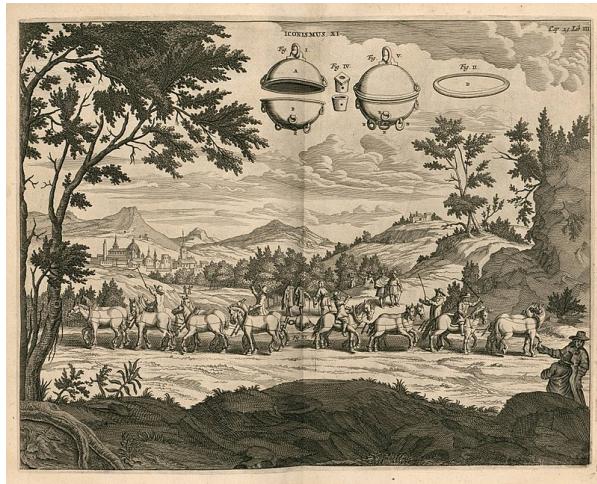


Figure C.1: Gaspar Schott's sketch of Otto von Guericke's experiment.

aside and made a vacuum inside—with the vacuum pump he invented—and he showed that not even 30 horses could separate them again. With this, he showed the power of the atmosphere and this experiment was recieved as a demonstration of the existence of the vacuum.

In the eighteenth and ninetheenth century, however, several background mediums—also called *aethers*—were proposed to mediate physical interactions, regarding, for example, electricity, magnetism, heat and gravity. They were all ruled out by experiments, or by the introduction of the concept of fields or by the development of the theories. The last aether, that was suppose to carry the propagation of electromagnetic waves, was showed to be unnecessary by Michelson-Morley experiment in 1887; with special relativity, the framework for the electromagnetism was set. Finally, in the beggining of the XX century, within Quantum Mechanics, the *vacuum* becomes the no-particle state, the ground energy state, which suprisingly has a non-zero energy—called the zero-point energy.

Let's connect this rambling on the vacuum concept with section 1.2.2. The goal was to illustrate how rich the debate on the vacuum concept is, in spite of more than two tousand years of discussion, there were only a handfull of experiments giving us information about it—the experimental validation of the Casimir effect is one them. Thus, the original work of Casimir [22] and the experimental validation [80] is an important piece on the history of the vacuum—we could even call it “the Quantum Physics Magdeburg's hemispheres”, as said in [101, Pg354]. The following poem summarizes the above.

In 1644, Torricceli repeated Berti's experiment, using mercury instead—this is referred to as “the invention of the mercury barometer”. This apparatus and the explanation of the phenomenon—that we live at the bottom of an ocean of air—had many consequences in science, but here, the relevant character is that it suggested that the vacuum exists. Not only the behaviour of fluids in tubes denied the *horror vacui* conception, in the mercury barometer one could see the vacuum rise. This idea was not absorbed so easily, but in 1657, Otto von Guericke made another interesting experiment: the “Magdeburg's hemispheres”. He took two heavy copper hemispheres, put them

⁴Leonardo Da Vinci and Galileo Galilei, seemingly.

Seven lifes

*The vacuum was born
because things transform,
to the problem of change,
atoms and vacuum arrange.*

*The vacuum fade out
because things move around,
a medium must be laid
for nature is afraid.*

*The vacuum rebirth
because things' moves are absurd,
nature is so brave
and atmosphere, it has weight.*

*With Torricceli's barometer
one sees vacuum rise,
after Magdeburg's hemispheres,
one creates vacuum as desires.*

*The vacuum was scrapped
because things interact,
several aethers were nominated
action at-a-distance, intermediated.*

*Not for planets to swing in⁵
Not for heat transfering
Not for body's sensations to convey
Not for carrying electromagnetic waves
one by one, they passed away.*

*The vacuum emanates
because things are both
particles and waves, they invoke
a non-empty no-particle state.*

*This curious energy
we believe that we can see,
by the work of Hendrik Casimir.*

⁵In Encyclopaedia Britannica, Maxwell wrote:

Aethers were invented for the planets to swing in, to constitute electric atmospheres and magnetic effluvia, to convey sensations from one part of our bodies to another, and so on, until all space had been filled three or four times over with aethers. (...) The only aether which has survived is that which was invented by Huygens to explain the propagation of light. [Maxwell, James Clerk (1878), "Ether", in Baynes, T.S., Encyclopædia Britannica, 8 (9th ed.), New York: Charles Scribner's Sons, pp. 568-572]

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