

Functional Methods in Quantum Fields and Disordered Systems

a Ph.D. thesis

by

Gustavo Olegário Heymans



Centro Brasileiro de Pesquisas Físicas | CBPF
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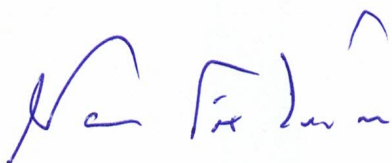
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"FUNCTIONAL METHODS IN QUANTUM FIELDS AND DISORDERED SYSTEMS"

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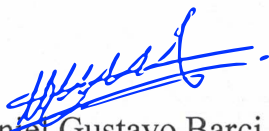
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Abstract

In this comprehensive study, we explore the theoretical frameworks of quantum field theory and statistical field theory, addressing both foundational principles and advanced methodologies across multiple chapters. The manuscript begins with a detailed exposition of the mathematical underpinnings of quantum theories, establishing the essential groundwork for introducing quantum mechanics and axiomatic quantum field theory. Within the context of axiomatic quantum field theory, we present novel results on the Casimir effect in dielectric materials and on the detection of zero-point fluctuations. We then introduce the functional integral formalism, encompassing both constructive field theory and statistical field theory. A dedicated section presents the distributional zeta function method, which is employed to investigate disordered systems. Furthermore, a wide array of applications, several of which are novel, of the distributional zeta function are discussed, expanding the formalism's utility and deepening our physical understanding of disordered systems.

Keywords: Functional methods, Quantum field theory, Disordered systems.

Resumo

Neste estudo abrangente, exploramos os fundamentos teóricos da teoria quântica de campos e da teoria estatística de campos, abordando tanto os princípios fundamentais quanto metodologias avançadas ao longo de múltiplos capítulos. O manuscrito começa com uma exposição detalhada das bases matemáticas das teorias quânticas, estabelecendo o alicerce essencial para a introdução da mecânica quântica e da teoria quântica de campos axiomática. No contexto da teoria quântica de campos axiomática, apresentamos resultados inéditos sobre o efeito Casimir em materiais dielétricos e sobre a detecção de flutuações do ponto zero. Em seguida, introduzimos o formalismo do integral funcional, abrangendo tanto a teoria construtiva de campos quanto a teoria estatística de campos. Uma seção dedicada apresenta o método da função zeta distribucional, que é empregado para investigar sistemas desordenados. Além disso, é discutida uma ampla gama de aplicações, várias delas inéditas, da função zeta distribucional, ampliando a utilidade do formalismo e aprofundando nossa compreensão física de sistemas desordenados.

Palavras-chave: Métodos funcionais, Teoria quântica de campos, Sistemas desordenados.

List of Publications

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- G. O. Heymans, N. F. Svaiter, B. F. Svaiter, and G. Krein. “Critical Casimir effect in a disordered $O(2)$ –symmetric model”. *Phys. Rev. E* **109**, 054108 (2024).
- E. Arias, G. O. Heymans, and N. F. Svaiter. “Casimir-Lifshitz formula for rectangular dielectric waveguide”. *Phys. Rev. A* **110**, 042813 (2024).
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Chapter 1

Introduction

The study of quantum and statistical field theory has long been central to our understanding of the fundamental interactions of nature and the collective behavior of matter. From the early developments of quantum mechanics to modern formulations of quantum field theory, the central goal has been to provide a consistent and predictive framework for describing particles and fields across microscopic and macroscopic scales. Over the past century, this pursuit has not only shaped high-energy physics, culminating in the Standard Model, but has also permeated condensed matter physics, statistical mechanics, and even interdisciplinary domains such as information theory and complex systems.

One of the milestones in this development was the formulation of quantum electrodynamics, the first successful quantum field theory combining quantum mechanics and special relativity. Its principles were later extended to the electroweak and strong interactions, leading to the construction of the Standard Model. Despite its success, the Standard Model leaves many open questions, such as the incorporation of gravity, the origin of dark matter and dark energy, and the mechanisms underlying neutrino and Higgs masses. These open problems continue to motivate the development of new field-theoretic approaches that go beyond perturbation theory and that extend into regimes of strong coupling, critical phenomena, and disordered systems.

In parallel, statistical field theory has emerged as a unifying framework for the study of collective phenomena in condensed matter physics. The functional integral formalism provides a natural bridge between quantum fields and statistical mechanics, allowing one to describe partition functions, correlation functions, and fluctuation-driven effects within a common language. This connection has been particularly fruitful in the study of phase transitions and critical phenomena, where renormalization group methods have revealed the deep concept of universality: the insensitivity of large-scale behavior to microscopic details. Such insights, initially motivated by equilibrium statistical mechanics, have

since been extended to systems ranging from turbulent fluids to early-universe cosmology.

Disorder is ubiquitous in real materials and manifests in many forms: random impurities in solids, spatially varying couplings, quenched external fields, and inhomogeneous boundary conditions. Physically, disorder can profoundly alter transport properties, shift critical points, generate glassy dynamics and induce localization of excitations. Seminal examples include Anderson localization of electronic waves [1] and glassy phases in spin systems; in the latter context the Edwards–Anderson model and the associated replica methods set the paradigm for theoretical investigations [2, 3]. Beyond condensed matter, disorder-like effects appear in classical and quantum models of fluids, soft condensed matter, and can be used to construct analog models related to cosmology and black-hole physics. The ubiquity and diversity of disorder make it a central topic for any comprehensive understanding of many-body physics.

From a theoretical viewpoint, quenched disorder presents two main technical challenges. First, physical observables generally require averaging nonlinear functionals of the partition function (for example the quenched free energy involves $\mathbb{E}[\ln Z]$), which complicates analytic treatment. Second, disorder often enhances the role of rare configurations and non-perturbative effects; consequently, methods that rely solely on naive perturbation theory can fail or be misleading. Traditional analytic approaches include the replica trick and supersymmetric formulations that trade disorder averages for integrals over commuting and anti-commuting fields [4]. While successful in many contexts, these techniques have mathematical subtleties (notably analytic continuation in the replica limit) and may obscure the spectral character of certain problems.

This thesis advocates and develops an alternative perspective based on the *distributional zeta-function* (DZF), a method which expresses disorder averages through zeta-like integrals over partition functions. The DZF offers several complementary advantages: (i) it emphasizes the statistical distribution of the partition function across disorder realizations, (ii) it bypasses the need for a replica analytic continuation in many cases, and (iii) it admits natural connections to spectral zeta functions and random-matrix techniques. In Chapters 4 and 5 we develop the mathematical foundations of this approach and apply it to paradigmatic models of quenched disorder (random-mass and random-field models), obtaining both new bounds and concrete computations of thermodynamic and Casimir-like observables.

The primary aims of the thesis are to review and unify functional approaches to quantum and statistical field theory with careful attention to mathematical foundations, and to develop and apply the distributional zeta-function method to physically relevant disordered models.

The remainder of this thesis is organized as follows: Chapter 2 we discuss the

similarities and differences between Classical and Quantum mechanics, fixing the notation and language that we use in this thesis. The Chapter 3 is dedicated to Axiomatic Quantum Field Theory, with a lengthy discussion about zero-point energies, finishing with a brief discussion of the interaction theory. In Chapter 4, we introduce Constructive Quantum Field Theory in the formulation of functional integrals. Chapter 5 introduces statistical field theory and presents disordered systems. The distributional zeta-function method, with applications, is also presented in this chapter. Finally, in Chapter 6, we present the general conclusions of this thesis. The Appendix A, present the fundamental mathematical background that guides us through this thesis.

Chapter 2

Quantum Mechanics

The goal of this chapter is to explore physical applications of the basic ideas of functional analysis (see Appendix A), establishing a connection between the formal mathematical theory and well-known physical results. For this, we assume that the reader has some familiarity with basic results in quantum mechanics. We begin our construction with very simple aspects that are widely known in the physics community. However, we do not intend to cover all aspects that fall under the “Quantum Mechanics” umbrella. For those without prior knowledge of the subject, we recommend any good book from the vast literature, particularly [5, 6]. For those eager for a formal collection of results and an in-depth discussion, Reference [7] is a great option. Here, we present a qualitative discussion emphasizing the construction and mathematical results. For the sake of brevity, we choose to begin directly with the canonical quantization procedure and omit the Heisenberg-Born-Jordan matrix approach. In what follows, we assume that the reader is familiar with the Lagrangian and Hamiltonian approaches to classical mechanics [8, 9]. However, to introduce the necessary formalism, we start with a brief review of the fundamental ideas of classical mechanics. Moreover, we would like to clarify that the same set of mathematical ideas used to obtain results in quantum mechanics can, with suitable modifications, be applied to treat a non-commutative algebra instead of a commutative one. Many of the results presented here can be found scattered in the mathematical literature; a useful collection that covers many of these results is Reference [10].

2.1 Classical Mechanics: Observables and States

As usual, a physical system can be defined in terms of generalized coordinates and their time derivative $(q, \dot{q})$. In such a coordinate system, the physical system is characterized by its number of degrees of freedom. The time derivative of the generalized coordinates defines the generalized velocities. For example, a system consisting of a free point particle moving along a line has only one degree of freedom, and its combination with the generalized velocity forms a two-dimensional space (a plane), it is usual to refer to such a space as *configuration space*. Given the generalized coordinates and velocities of a system, one can construct its “Lagrangian.” In general, the Lagrangian is a function of the generalized coordinates, let's assume N of them, the respective generalized velocities, and time, $L : \mathbb{R}^{2N+1} \rightarrow \mathbb{R}$, and can be expressed in terms of the kinetic energy (K) and the potential energy (V) as

$$L(q(t), \dot{q}(t), t) \equiv K(q(t), \dot{q}(t), t) - V(q(t), \dot{q}(t), t). \quad (2.1)$$

In the simplest case, a free point particle of mass m moving on a line, the Lagrangian consists only of the kinetic energy expressed in terms of the generalized velocity:

$$L(\dot{q}) = K(\dot{q}) = \frac{1}{2}m^2\dot{q}^2. \quad (2.2)$$

If we consider a free particle in three-dimensional space, we obtain a six-dimensional space, and the Lagrangian must account for $\dot{q}^2 \equiv \dot{q}_1^2 + \dot{q}_2^2 + \dot{q}_3^2$. Although the free point particle scenario is trivial, adding a non-trivial potential reveals the advantages of the Lagrangian formulation.

At first glance, the Lagrangian formulation may appear to be just another coordinate-based approach to Newtonian mechanics. However, its computational advantages become evident when one introduces the concept of the *action* functional,

$$S[L; t_i, t_f] \equiv \int_{t_i}^{t_f} L(q(t), \dot{q}(t), t) dt. \quad (2.3)$$

As its name suggests, the action functional is a linear functional of the Lagrangian and a function of the parameters t_i (initial time) and t_f (final time). This functional plays a central role in the development of Quantum Field Theory, as will become explicit in the next chapter. For now, the introduction of the action is useful for obtaining the equations of motion used to describe physical systems. Applying Hamilton's principle, which states that *between the times t_i and t_f , a physical*

system follows the path from q_1 to q_2 for which the action is stationary, i. e.

$$\delta S[L; t_i, t_f] = 0. \quad (2.4)$$

From that, one can take the variation of the action (2.3) with respect to each generalized coordinate to obtain the so-called **Euler-Lagrange Equations**

$$\frac{\partial L}{\partial q_n} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_n} = 0, \quad (2.5)$$

where, for the sake of clarity, we have specified that this equation must be applied to each degree of freedom of the system, i.e., $n = 1, 2, \dots, N$. Returning to our simple example, we find that our Euler-Lagrange equation results in the following second-order ordinary differential equation; for the free particle

$$m^2 \ddot{q} = 0, \quad (2.6)$$

In such a simple situation, one can solve the equation of motion directly to obtain a function for the generalized velocity of the system:

$$\dot{q}(t) = \dot{q}_0 + \frac{c}{m^2}(t - t_i), \quad (2.7)$$

where $\dot{q}_0$ is a constant determined by the initial conditions at t_i , and c is an arbitrary integration constant. Further integration results in a function of the generalized coordinate in terms of time and initial parameters. It is interesting to note that solving the equation of motion at a given time allows us to determine the system at any time in the past or future. This deterministic behavior is not merely a feature of the free particle but holds for any case in classical mechanics. Moreover, systems in which the total energy is conserved are those in which the Lagrangian has no explicit dependence on time, that is,

$$\frac{\partial L}{\partial t} = 0. \quad (2.8)$$

Before proceeding further, let us examine the instructive case of a harmonic oscillator. First, we consider the usual harmonic oscillator by adding the potential $V(q) = \frac{1}{2}kq^2$ to the free particle, where k is a system-dependent constant (for example, the stiffness of a spring). In this case, the Lagrangian and the equation of motion of the system are given by

$$\begin{aligned} L(q, \dot{q}) &= \frac{1}{2}m^2\dot{q}^2 - \frac{1}{2}kq^2, \\ m^2\ddot{q} + kq &= 0. \end{aligned} \quad (2.9)$$

Before solving the equation, we observe that this is a system with conserved energy and that we have an elliptic second-order ordinary differential equation. There are many ways to solve such an equation, and the solution is given by

$$q(t) = A \sin \left(\sqrt{\frac{k}{m^2}} t + \theta \right), \quad (2.10)$$

where the amplitude, A , and the phase, θ , are determined by the initial conditions.

Now, we introduce another formalism in classical mechanics that is useful for quantum systems. The **Hamiltonian** is a function of the generalized coordinates, conjugate momenta, and time, $H : \mathbb{R}^{2N+1} \rightarrow \mathbb{R}$, given by the Legendre transform in the generalized velocities of the Lagrangian. By definition, it can be written as

$$H(q, p, t) \equiv \sup_{\dot{q} \in \mathbb{R}^N} [(\dot{q}, p) - L(q, \dot{q}, t)], \quad (2.11)$$

where $(\dot{q}, p) = \sum_{n=1}^N \dot{q}_n p_n$, and the conjugate momentum is given by

$$p_n \equiv \frac{\partial L}{\partial \dot{q}_n}. \quad (2.12)$$

In particular, if the Lagrangian has no explicit time dependence, the Hamiltonian will also share this property. Unless explicitly stated otherwise, we assume that we are dealing only with conservative systems. The $2N$ -dimensional space generated by the generalized coordinates and conjugate momenta is called **phase space**. By analyzing the trajectories of a physical system in phase space, one can obtain many insights. For the harmonic oscillator, we obtain the following Hamiltonian:

$$H(q, p) = \frac{p^2}{2m^2} + \frac{1}{2}kq^2, \quad (2.13)$$

which represents an ellipse in phase space, due its energy conservation. The graph of the Hamiltonian in the phase space of a periodic system is characterized by closed curves. Taking the differential of the definition of the Hamiltonian and using the definition of conjugate momenta, one obtains

$$\frac{dq_n}{dt} = \frac{\partial H}{\partial p_n}, \quad \frac{dp_n}{dt} = -\frac{\partial H}{\partial q_n}, \quad \text{and} \quad \frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}. \quad (2.14)$$

This system of equations is known as **Hamilton's Equations**, which are the equations of motion in this formalism. Returning to the harmonic oscillator, we get

$$\dot{q} = \frac{p}{m^2}, \quad \text{and} \quad \dot{p} = -kq, \quad (2.15)$$

which are two first-order differential equations. For linear systems, the usual behavior is as follows: while the Lagrangian formalism yields N differential equations of order 2, the Hamiltonian formalism results in a system of $2N$ first-order differential equations.

Definition 2.1. For two dynamical functions, $u = u(q, p, t)$ and $v = v(q, p, t)$, the **Poisson bracket** is defined by the bilinear, skew-symmetric relation (over the usual product and sum)

$$[u, v]_P \equiv \sum_{n=1}^N \left(\frac{\partial u}{\partial q_n} \frac{\partial v}{\partial p_n} - \frac{\partial u}{\partial p_n} \frac{\partial v}{\partial q_n} \right). \quad (2.16)$$

Straight from the previous definition¹, one can find the *fundamental Poisson brackets*, which are given by:

$$[p_n, q_m]_P = [p_n, p_m]_P = 0, \text{ and } [q_i, p_j]_P = \delta_{ij}. \quad (2.17)$$

With the fundamental relations and some algebraic manipulations, one finds directly for any dynamical function u that

$$[u, p_i]_P = \frac{\partial u}{\partial q_i}. \quad (2.18)$$

Setting $u = H$ and analyzing Hamilton's equations (2.14), one can see directly that

$$[q_n, H]_P = \frac{\partial H}{\partial p_n} = \dot{q}_n, \text{ and } [p_n, H]_P = -\frac{\partial H}{\partial q_n} = \dot{p}_n. \quad (2.19)$$

Such relations confirm that our definition of the Poisson bracket in Eq. (2.16) is dynamically consistent.

Moreover, if $u = u(q(t), p(t), t)$, we can use the Poisson bracket and the previous relations to write the usual total derivative of u with respect to time as

$$\frac{du}{dt} = [u, H]_P + \frac{\partial u}{\partial t}, \quad (2.20)$$

if u does not have any explicit time dependence, the total derivative is simply the Poisson bracket with H . Thus, one can say that the Hamiltonian of a system generates time translations. If the Poisson bracket of a dynamical function with the Hamiltonian vanishes, we say that the function is a *constant of motion*.

¹One can also define the Poisson bracket for any set of canonical variables (variables that relate to each other via Hamilton's equations (2.14)). Here we only use the set (q, p) , choosing not to discuss canonical transformations. However, it can be easily shown that the Poisson bracket is invariant under canonical transformations. For those interested, see Refs. [8, 9].

It is interesting to notice that the Poisson bracket can be regarded as a first-order linear operator. Take the dynamical functions u and v , and define the following first-order linear operator

$$P_u \equiv \sum_{n=1}^N \left(\frac{\partial u}{\partial q_n} \frac{\partial}{\partial p_n} - \frac{\partial u}{\partial p_n} \frac{\partial}{\partial q_n} \right), \quad (2.21)$$

it is straightforward to see that

$$[u, v]_P = P_u v. \quad (2.22)$$

From this point of view, it is clear that

$$P_u(vh) = (P_u v)h + vP_u h \Rightarrow [u, vh]_P = [u, v]_P h + v[u, h]_P, \quad (2.23)$$

for any dynamical functions u , v , and h . Applying the Poisson bracket recursively and using the skew-symmetric property, one can write that

$$[u, [v, h]_P]_P + [v, [h, u]_P]_P = (P_u P_v - P_v P_u)h, \quad (2.24)$$

which contains second-order derivatives in the phase space coordinates. Thus, the only second derivatives that can appear are due to the application of the Poisson bracket. But a linear combination of first-order differential operators is itself a first-order differential operator, so there are no second-order derivatives of h in the previous equation. This means that the second-order derivatives that appear must vanish identically, leading to the following expression:

$$(P_u P_v - P_v P_u)h = \sum_{n=1}^N \left(A_n \frac{\partial}{\partial p_k} - B_n \frac{\partial}{\partial q_n} \right) h. \quad (2.25)$$

The coefficients A_n and B_n cannot depend on h , since they are determined by differential equations. So we can choose h for convenience. First, take $h = p_i$ and use Eq. (2.18) to write

$$\begin{aligned} (P_u P_v - P_v P_u)p_i &= P_u \frac{\partial v}{\partial q_i} - P_v \frac{\partial u}{\partial q_i} = P_u \frac{\partial v}{\partial q_i} + P_{\frac{\partial u}{\partial q_i}} v = A_i \\ &\Rightarrow A_i = \frac{\partial}{\partial q_i} P_u v, \end{aligned} \quad (2.26)$$

now, taking $h = q_i$ and proceeding with the same manipulations, one finds

$$B_i = -\frac{\partial}{\partial p_i} P_u v. \quad (2.27)$$

Returning to Eq. (2.25), we can write

$$(P_u P_v - P_v P_u)h = [u, [v, h]_P]_P + [v, [u, h]_P]_P = [[u, v]_P, h]_P, \quad (2.28)$$

or, in a more enlightening form,

$$[u, [v, h]_P]_P + [v, [u, h]_P]_P + [h, [u, v]_P]_P = 0, \quad (2.29)$$

which is the **Jacobi identity**. Now, it is interesting to remember that our definition of the Poisson bracket in Eq. (2.16) is skew-symmetric and bilinear under the usual multiplication by a scalar and under the usual addition by a function. With this definition and the fact that the Poisson bracket satisfies the Jacobi identity, we can affirm that the operation

$$[\bullet, \bullet]_P \quad (2.30)$$

defines a **Lie algebra** over the phase space. This Lie algebra is known as the **algebra of observables**, $\mathcal{O}$, in classical mechanics. If, in the phase space $\mathcal{P}$, we define a one-parameter commutative group $T_t : \mathcal{P} \rightarrow \mathcal{P}$, the family of transformations generated by T_t , denoted by U_t , preserves the algebra of observables, i.e., $U_t : \mathcal{O} \rightarrow \mathcal{O}$. In other words, if the evolution in phase space is governed by a single parameter (e.g., time), then time evolution preserves the properties of the Poisson brackets. In particular, if we define any function in the phase space in terms of initial coordinates q_0 and p_0 , such as $f(q_0, p_0)$, its time evolution is given by²

$$U_t f(p_0, q_0) = f_t(p_0, q_0) = f(q(q_0, p_0, t), p(q_0, p_0, t)) \equiv f_t(q, p), \quad (2.31)$$

and it follows directly that $f_t(q, p)$ satisfies the differential equation

$$\frac{df_t}{dt} = [H, f_t]_P, \quad (2.32)$$

which is not only another way of expressing Eq. (2.20) but also highlights why the Hamiltonian is the time evolution generator of the algebra of observables. From this, we see that time evolution is an automorphism of the algebra of operators. With these clarifications, we can now formally define what an observable in classical mechanics is: *An observable is a real-valued smooth function defined on the phase space.*

To fully describe a physical system, we must define not only observables but also **states**. Loosely speaking (and we will formalize this shortly), a state is what

²One can also consider functions with explicit time dependence. However, this leads to longer expressions, which we do not consider in this text.

is measured in an experiment. Thus, one could say that a state corresponds to the numerical outcome displayed by laboratory equipment. In this view, when the same physical experiment is performed multiple times, there are two possibilities:

1. If the experiments are *exactly* replicated, the measured states remain the same in every repetition. This means that if we collect all possible experimental outcomes into a set, that set contains only a single element, and the experiment always selects that element. In other words, the experiment uniquely determines the state of the system.

2. Even if the experiments are precisely replicated, they yield different results. That is, the non-uniqueness of the state is an intrinsic property of the system, independent of the experiment. In this case, collecting all possible states into a set results in a set with multiple elements, meaning that different experimental runs may select different elements from this set. In other words, a series of experiments determines the set of **possible** states of a system, and each experiment may yield a different state.

Next, we will formalize these two types of physical systems.

Regardless of the preceding scenario, the state of the system is the element selected from the set of possible states. The probability of selecting a particular state is not necessarily fixed and depends on the system. However, for any observable f in the algebra of observables $\mathcal{O}$, the probability of measuring a state μ follows a probability distribution. To formalize this concept, we assert:

A **state**, μ , defined over the algebra of observables, determines the probability distribution (measure) for each observable. Since we are dealing only with classical quantities, this measure must be defined on the real line, *i.e.*, as a Borel measure (see the discussion after Theorem A.23), as defined in Section A.1.

We are now ready to define a state:

Definition 2.2. A **state** μ is a linear map, $\mu : \mathcal{O} \rightarrow \mathbb{R}$, acting on an observable $f \in \mathcal{O}$ and a Borel set $B \subset \mathbb{R}$, thereby defining a measure $\mu(f)|_B \equiv \mu_f(B)$.

From this definition, it follows directly that $\mu_f(B)$ defines a probability measure (see the discussion after Eq. (A.67)). Since the algebra of observables consists of continuous functions, the state over ϕ can be intuitively expressed as

$$\mu_{\phi(f)}(B) = \mu_f(\phi^{-1}(B)), \quad (2.33)$$

where ϕ^{-1} is the inverse map and $\phi^{-1}(B)$ is an open set, given that ϕ is continuous and B is a Borel set. As discussed in the Appendix (see Definition A.15), a measure can be expressed as a linear combination of measures. In particular, a convex combination of states,

$$\mu = \alpha\mu_1 + (1 - \alpha)\mu_2, \quad 0 < \alpha < 1, \quad (2.34)$$

may yield a corresponding convex combination of measures. If a state cannot be represented as in Eq. (2.34), i.e., if $\mu_1 = \mu_2 = \mu$, we say it is a **pure state**; otherwise, it is called a **mixed state**.

It is common to determine the probability that an observable f does not exceed a certain value λ when measured in state μ . We define this as $\mu_f((-\infty, \lambda]) \equiv \mu_f(\lambda)$ ³. With the state, the observable, and the associated probability measure defined, we ask: what is the probability of the observable f taking values less than λ in state μ ?

The answer is given by the **mean value** with respect to the appropriate probability measure:

$$\langle f \rangle_\mu \equiv \int_{-\infty}^{+\infty} \lambda d\mu_f(\lambda), \quad (2.35)$$

which must be interpreted as a Riemann-Stieltjes integral, Eq. (A.67). The three key properties of the mean value are:

Proposition 2.3. For any arbitrary constant $c \in \mathbb{R}$ and any functions $f, g \in \mathcal{O}$, the mean values satisfy:

- (i) $\langle c \rangle_\mu = c$,
- (ii) $\langle f + cg \rangle_\mu = \langle f \rangle_\mu + c\langle g \rangle_\mu$,
- (iii) $\langle f^2 \rangle_\mu \geq 0$.

Proof. (i) follows from the fact that $\mu_f(\mathbb{R}) = 1$. (ii) follows from the linearity of the integral. For the proof of (iii), we can first decompose f into measurable functions and use Lemma A.14 to show that f^2 is integrable. To get the non-negative values of the mean value of f^2 , we observe that $f^2 \geq |f|$, so

$$\langle f^2 \rangle_\mu \geq \langle |f| \rangle_\mu \geq 0. \quad (2.36)$$

■

Now, in order to grasp more properties, we can use the properties of the mean value to interpret such a quantity as a positive linear functional acting over $\mathcal{O}$. We can represent such a functional in the phase space as follows:

$$\langle f \rangle_\mu = \int_{\mathcal{P}} f(p, q) dv_\mu(p, q), \quad (2.37)$$

with $dv_\mu(p, q)$ being the differential of the measure on the phase space. Straight from our definitions and using (i), we can check that

$$\langle 1 \rangle_\mu = \int_{\mathcal{P}} dv_\mu(p, q) = v_\mu(\mathcal{P}) = 1, \quad (2.38)$$

³Of course, we have $\mu_f(-\infty) = 0$ and $\mu_f(+\infty) = \mu_f(\mathbb{R}) = 1$.

that is, the mean value of the identity is normalized. From the last integral, we can infer also that the “volume” of the phase space is unity. Soon we will return to the analysis of the volume of the phase space.

Using the fact that the measure $dv_\mu(p, q)$ is σ -finite, we can make use of the Radon-Nikodým theorem (Theorem A.35) to rewrite the mean value of an observable f as

$$\langle f \rangle_\mu = \int_{\mathcal{O}} f(p, q) \rho_\mu(p, q) dq dp, \quad (2.39)$$

where dq and dp are properly Lebesgue measures and $\rho_\mu(p, q)$ is a distribution function (the Radon-Nikodým derivatives of $v_\mu(p, q)$). Worth noting that, in general, $\rho_\mu(p, q)$ is a positive definite generalized function, as the ones analyzed in Section A.4. With that in mind, now we can use the same notation as before and see the mean value of an observable as the linear functional generated by the distribution function’s action over them in the phase space, that is, as a map $\rho_\mu : \mathcal{O} \rightarrow \mathbb{R}^+$, defined by

$$(\rho_\mu, f) = \langle f \rangle_\mu. \quad (2.40)$$

Physically, the last discussion can be translated as saying that a state in **classical** mechanics is described by the corresponding **probability** distribution on the phase space. Because of that, we drop the subscript μ whenever there is no risk of confusion. Now we can go back to the previous discussion about pure and mixed states. For pure states, the element of the phase space is fixed uniquely, *i.e.*, the probability distribution is entirely concentrated at one point. In our meaningless notation of Section A.4, we get that

$$\rho(p, q) = \delta(q - q_0) \delta(p - p_0), \quad (2.41)$$

which receives its meaning acting over an observable:

$$\langle f \rangle = (\rho, f) = f(q_0, p_0). \quad (2.42)$$

Usually, in classical mechanics, only pure states are investigated. The mixed states are objects of statistical mechanics, which one possible formulation is reviewed in Section 5.1. For now, we are only to show that the variance of a pure state is zero. The variance is defined by

$$\text{Var}_\mu(f) = \langle (f - \langle f \rangle_\mu)^2 \rangle_\mu = \langle f^2 \rangle_\mu - \langle f \rangle_\mu^2. \quad (2.43)$$

Using the previous notation and the fact that we are in a pure state, we get

$$\text{Var}(f) = (\rho, f^2) - (\rho, f)^2 = f^2(q_0, p_0) - (f(q_0, p_0))^2 = 0. \quad (2.44)$$

It is easy to see, and we show later, that the variance is greater than zero if we are in a mixed state. Finally, we will state and prove an important theorem of classical mechanics and discuss some of its implications.

Theorem 2.4 (Liouville's theorem). Let Ω be a domain in the phase space $\mathcal{P}$. Set $\Omega(t)$ as the image under the one-parameter transformations T_t , that is $T_t\mu \in \Omega(t)$, for $\mu \in \Omega$. Denote by $V(t)$ the volume of the domain $\Omega(t)$, then

$$\frac{dV(t)}{dt} = 0. \quad (2.45)$$

Proof. Let us denote by $d\nu$ the product of the Lebesgue measures dq and dp . The volume of $\Omega(t)$ can be written as

$$V(t) = \int_{\Omega(t)} d\nu = \int_{\Omega} |J_\nu(T_t\nu)| d\nu, \quad (2.46)$$

with $J_\nu(T_t\nu)$ denoting the Jacobian of the transformation with respect to the original set of coordinates ν . From that, it is direct to see that to prove the theorem, it is enough to show that the time derivative of the Jacobian determinant vanishes identically. Of course, if $t = 0$, we get that $J_\nu(T_0\nu) = 1$, and the theorem holds. Now, let us suppose $t \neq 0$. An arbitrary one-parameter transformation can be written as the application of two consecutive transformations, that is $T_{t+s}\nu = T_s T_t\nu$, so the Jacobian determinant can be written as

$$J_\nu(T_{t+s}\nu) = J_{T_t\nu}(T_{t+s}\nu) J_\nu(T_t\nu). \quad (2.47)$$

Taking the derivative with respect to s , one can write

$$\frac{d}{ds} J_{T_t\nu}(T_{t+s}\nu) = \frac{\partial(\dot{q}(t+s), p(t+s))}{\partial(q(t), p(t))} + \frac{\partial(q(t+s), \dot{p}(t+s))}{\partial(q(t), p(t))} = \frac{\partial\dot{q}(t+s)}{\partial q(t)} + \frac{\partial\dot{p}(t+s)}{\partial p(t)}, \quad (2.48)$$

setting $s = 0$ and using Hamilton's Equations (2.14), we get that

$$\frac{\partial\dot{q}(t)}{\partial q(t)} + \frac{\partial\dot{p}(t)}{\partial p(t)} = \frac{\partial^2 H}{\partial q \partial p} - \frac{\partial^2 H}{\partial p \partial q} = 0, \quad (2.49)$$

which implies that

$$\frac{d}{dt} J_\nu(T_{t+s}\nu) = 0. \quad (2.50)$$

■

As we had seen, the time evolution of an observable can be obtained by equation (2.20). From such a point of view, we have that the mean value will be given by

$$\langle f_t \rangle = \int_{\mathcal{P}} f_t(\nu) \rho_\mu(\nu) d\nu = \int_{\mathcal{P}} f(T_t\nu) \rho_\mu(\nu) d\nu. \quad (2.51)$$

One should notice that it is equivalent to say that the states, determined by the probability distribution, do not depend on time, so we have that

$$\frac{df_t}{dt} = [H, f_t]_P \quad \text{and} \quad \frac{d\rho_\mu}{dt} = 0, \quad (2.52)$$

which is called the *Hamiltonian picture*. However, alternatively, one can write

$$\begin{aligned} \int_{\mathcal{P}} f_t(v) \rho_\mu(v) dv &= \int_{\mathcal{P}} f(T_t v) \rho_\mu(v) dv = \int_{\mathcal{P}} f(v) \rho_\mu(T_{-t} v) |J_v(T_{-t} v)| dv \\ &= \int_{\mathcal{P}} f(v) \rho_{\mu_t}(v) dv = \langle f \rangle_{\mu_t}. \end{aligned} \quad (2.53)$$

where the coordinates transformations $T_t v \rightarrow v$ were performed, $\rho_\mu(T_{-t} v) = \rho_{\mu_t}(v)$ was defined, and Theorem 2.4 was used. From that, it is straightforward to obtain that

$$\frac{df}{dt} = 0 \quad \text{and} \quad \frac{d\rho_{\mu_t}}{dt} = -[H, \rho_{\mu_t}]_P, \quad (2.54)$$

which means that the observables are constants in time while the states evolve. Such a point of view is called the *Liouville's picture*. Of course, we have that

$$\langle f_t \rangle_\mu = \langle f \rangle_{\mu_t}, \quad (2.55)$$

the equivalence between the two pictures of motion.

2.2 Canonical Quantization: Observables and States

Once we have seen that classical mechanics can be formulated in terms of probabilities and mean values, it is completely natural to ask yourselves what the differences are when we change from a macroscopic “deterministic” (at least, for pure states) physics to a microscopic inherently probabilistic physics. We hope that we are able to make clear the differences and similarities along this section. Once it is assumed that the reader has a background in some Quantum Mechanics courses, we do not take a long time with much physical reasoning or justifying some foundations of quantum theory, such as black body radiation and the Stern-Gerlach experiment. Unless stated otherwise, we assume that $\hbar = 1$, the natural system of units.

First, just like before, we need to define what the quantum observables and the quantum states are. It is important to point out that the previous construction of the Lagrangian and Hamiltonian formalisms remains valid with some suitable changes that we are going to clarify in a while.

Definition 2.5. A **quantum pure state** is a vector in a complex Hilbert space $\mathcal{H}$. Such a quantum pure state can also have components in different Hilbert spaces, if its linear combination preserves the algebraic separability of the total Hilbert space, i.e., $\mathcal{H} = \bigoplus_{i=1}^n \mathcal{H}_i$. A **quantum mixed state**, or **entangled state**, defines an algebraically non-separable Hilbert space.

Usually, for some regularity properties of the Schrödinger equation, the Hilbert space taken to accommodate the quantum states is the space of complex-valued square integrable functions over $\mathbb{R}^d$, that is, $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^d)$. So, any pure quantum state is just a vector. A composite vector of pure states can be constructed by copies of the complex-valued square integrable functions space. For example, for a non-relativistic spin-1/2 system, the Hilbert space is given by $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^d) \oplus \mathcal{L}^2(\mathbb{R}^d)$, which preserves the algebraic separability. The most used example for an entangled state is the Bell state for a system of two spin-1/2 particles. The Hilbert space of such a system cannot be expressed as an analogous form to the ones before. Here we are not interested in entangled states, but such a subject will emerge later. For notation clarity, we will work with $\mathcal{L}^2(\mathbb{R})$ instead of $\mathcal{L}^2(\mathbb{R}^d)$, but all the results can be carried out trivially.

Definition 2.6. An **quantum observable** is a *essentially* self-adjoint operator over $\mathcal{H}$.

Such operators are often unbounded. Due to the unboundedness and the Hellinger-Toeplitz theorem (Theorem A.66), such operators cannot be defined everywhere, only in a dense domain in $\mathcal{H}$. This leads us into some difficulties in dealing with algebraic operations in the context of those operators. Later, we will return to this subject.

Just like in the previous section, we can assume that a measurement is the mean value of a observable in a given state, or expectation value of an observable. This means that the measurable value of the observable A is going to be the application of the linear functional defined on the dual Hilbert space, $\mathcal{H}^*$, by ψ over the state $A\psi$,

$$\langle A \rangle = \Psi(A\psi), \quad (2.56)$$

where $\Psi : \mathcal{H}^* \rightarrow \mathbb{R}$ is the linear functional associated with ψ . Of course, the weak-* (or vague) topology is taken in order for any functional Ψ on $\mathcal{H}^*$ to be continuous. The properties of Proposition 2.3 are naturally extended to the complex case.

Using the result from Theorem A.60, we can write the mean value of the observable A as

$$\langle A \rangle = \Psi(A\psi) = (\psi, A\psi), \quad (2.57)$$

as is usually used. One should remember that we are, in general, in a complex Hilbert space, so the inner product is a sesquilinear form⁴. Two important observables in quantum mechanics are the *position operator*, Q , and the *momentum operator*, P .

In the coordinates representation, the position operator, $Q(x)$, is the multiplication by the coordinates x , i.e.,

$$Q(x)\psi(x) = x\psi(x), \quad x \in \mathbb{R}. \quad (2.58)$$

If we take the **domain**, $D_x(Q)$, of such an operator in the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R})$ given by

$$D_x(Q) = \left\{ \psi \in \mathcal{H} \mid \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx < \infty \right\}, \quad (2.59)$$

we clearly see that we get an unbounded operator. Such a class of operators can present some issues. The main one is due to the Hellinger-Toeplitz theorem, which ensures that an everywhere-defined operator A that satisfies $(A\phi, \psi) = (\phi, A\psi)$ is bounded. This implies that an unbounded operator, such as $Q(x)$, is defined only in a dense linear subset of the Hilbert space $\mathcal{H}$. Such a subset is called a **domain**, D . Of course, $x\psi(x)$ for any $\psi(x) \in \mathcal{L}^2(\mathbb{R})$ is meaningful as a function, but it is not in $\mathcal{L}^2(\mathbb{R})$. To ensure the definiteness of such operators, we must choose the domain D carefully. In particular, if we define the subspace K as

$$K = \left\{ \psi(x) \mid |x^n \psi^{(\alpha)}(x)| \leq C_{n\alpha}, \quad \forall n \in \mathbb{R} \right\}, \quad (2.60)$$

then K is the space of all infinitely differentiable functions that decay faster than any power of x . It is clear that K is dense in $\mathcal{L}^2(\mathbb{R})$. So, if we take $D_x(Q) = K$, it is possible to ensure that $x\psi(x) \in \mathcal{L}^2(\mathbb{R})$.

Now that we are in the appropriate domain, we can observe that $K \subset \mathcal{L}^1 \cap \mathcal{L}^2 \subset \mathcal{L}^2$, which means that the usual Fourier transform and its inverse are well defined⁵, allowing us to write

$$\psi(x) = \mathcal{F}^{-1}(\psi)(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ipx} \psi(p) dp, \quad (2.61)$$

now, using the coordinates representation of $Q(x)$, Eq. (2.58), and the Fourier representation of $\psi \in K$, we obtain

$$\mathcal{F}^{-1}(Q(x)\psi)(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} x e^{-ipx} \psi(p) dp = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(i \frac{\partial}{\partial p} \right) e^{-ipx} \psi(p) dp. \quad (2.62)$$

⁴The rule for multiplication by numbers $\alpha, \beta \in \mathbb{C}$ is: $(\alpha\phi, \beta\psi) = \alpha^* \beta (\phi, \psi)$.

⁵The Fourier transform on $\mathcal{L}^2$ can also be obtained directly (Carleson's theorem [11]) or using density and some regularity arguments. But it is a more sensitive subject, and we do not need to touch it here. Fourier transform on $\mathcal{L}^p$ spaces can also be obtained, this is known as the Carleson-Hunt theorem [12].

The previous equation allows us to identify the so-called *momentum representation* of the position operator, $Q(p)$, namely

$$Q(p)\psi(p) = i\frac{\partial}{\partial p}\psi(p). \quad (2.63)$$

In the momentum representation, the momentum operator, P , is given by

$$P(p)\psi(p) = p\psi(p), \quad p \in \mathbb{R}. \quad (2.64)$$

Using the same procedure, but now with the Fourier transform, $\mathcal{F}$, one can find the coordinates representation of the momentum operator, $P(x)$, which is

$$P(x)\psi(x) = -i\frac{\partial}{\partial x}\psi(x). \quad (2.65)$$

The unitarity equivalence of those representations can be checked in different ways. We will return to this question at the end of this section.

With the coordinate and momentum representation of both operators, we are able to obtain their commutator. If now we assume that $x \in \mathbb{R}^d$, that is, $Q(x)$ and $P(x)$ are vector-valued operators, we can obtain the so-called **canonical commutation relations**, which are given by

$$[Q(x), Q(x)]\psi(x) = [P(x), P(x)]\psi(x) = 0, \text{ and } [Q_i(x), P_j(x)]\psi(x) = i\delta_{ij}\psi(x), \quad (2.66)$$

which encapsulates the non-commutative characteristic of quantum systems. One should remember that we are in the natural system of units. A direct comparison with the fundamental Poisson brackets, Eq. (2.17), allows us to establish a direct link between the two quantities. While in classical systems we use the Poisson bracket, see definition 2.1, which is a differential operator to define the algebra of observables, in quantum mechanics the algebra of observables, $\mathcal{O}$, is defined by the usual commutator⁶

$$[\bullet, \bullet]. \quad (2.67)$$

Clearly, the commutator defines the Lie Algebra of the quantum observables.

Using the definition of the mean-value from Eq. (2.57), one can verify that $\langle Q \rangle = \langle P \rangle = 0$. Using the definition of variance, Eq. (2.43), we can write that

$$\text{Var}(Q)\text{Var}(P) = \langle Q^2 \rangle \langle P^2 \rangle \geq |\langle QP \rangle|^2, \quad (2.68)$$

where the last inequality follows from the Schwarz inequality. Using the fact that, for any $z \in \mathbb{C}$, we have

$$|z|^2 \geq (\text{Im}(z))^2 = \left(\frac{z - \bar{z}}{2i} \right)^2, \quad (2.69)$$

⁶We denote the algebra of operators of classical and quantum mechanics by the same letter $\mathcal{O}$. Hopefully, the context will clarify any doubts that this may raise.

we can set $z = QP$ and use the linearity of the inner product to write

$$|\langle QP \rangle|^2 \geq \left(\frac{\langle [Q, P] \rangle}{2i} \right)^2 = \frac{1}{4}. \quad (2.70)$$

In the last equality, the canonical commutation relation, Eq. (2.66), was used. Then we get that the product of the variances has a natural bound given by

$$\text{Var}(Q)\text{Var}(P) \geq \frac{1}{4}, \quad (2.71)$$

which is known in the literature as the **Heisenberg uncertainty relation**. As one can see from its direct derivation, such a result is a direct manifestation of the canonical commutation relation. If one goes back and performs a similar calculation in the classical case, the information that will be extracted from the product of the variances is that it must be greater than or equal to zero, which is a triviality. In other words, the main difference between classical and quantum physics is that a quantum pure state can, at best, be characterized by the values of a complete set of commuting observables, and not *all* observables. So, the canonical commutation relations (2.66) determine a minimum value for the states in the phase space. The non-commutative aspect of such a theory is intrinsically related to its probabilistic interpretation, since measures on the phase space can be interpreted as a probability measure. Such a lower bound can be improved and it is known as the *Robertson-Schrödinger uncertainty relation* [13, 14].

Given a classical Hamiltonian, see Eq. (2.11), it is straightforward to obtain its quantum mechanical counterpart. The quantum mechanical Hamiltonian can be obtained by making a simple substitution in the representation of the variables. For concreteness, let us use the free particle Hamiltonian. If we take the coordinates representation, the quantum mechanical one-dimensional free particle is obtained by the substitutions: $q \rightarrow x$ and $p \rightarrow -i\partial/\partial x$, which gives us the following Hamiltonian:

$$H = -\frac{1}{2m} \frac{\partial^2}{\partial x^2}. \quad (2.72)$$

To verify that such a Hamiltonian is a quantum observable, one needs to prove that there exists a domain where such an operator is self-adjoint. Depending on the Hamiltonian, this can be very hard. In our case, one can verify that such a Hamiltonian is essentially self-adjoint on the domain K defined in Eq. (2.60). So, in order to obtain a measurable quantity from the Hamiltonian, we need to compute $\langle H \rangle$, for some $\psi \in D(H) = K$. Such a calculation can be simplified if we use the Spectral Theorem for unbounded operators. There are many different formulations of this theorem, however, here we present the that we are going to use more frequently in this thesis.

Theorem 2.7. (Spectral theorem – multiplication operator form). Let A be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ with domain $D(A)$. Then there is a measure space $\langle M, \mu \rangle$, with μ a finite measure, a unitary operator $U : \mathcal{H} \rightarrow \mathcal{L}^2(M, d\mu)$, and a real-valued function f on M which is finite almost everywhere so that

$$(a) \quad \psi \in D(A) \text{ if and only if } f(\cdot)(U\psi)(\cdot) \in \mathcal{L}^2(M, d\mu)$$

$$(b) \quad \text{If } \phi \in U[D(A)], \text{ then } (UAU^{-1}\phi)(m) = f(m)\phi(m)$$

Proof. First, we will show that $\text{Ran}(A \pm iI) = \mathcal{H}$ and that $(A + iI)$ and $(A - iI)$ are one-to-one. This follows if we can prove that $\text{Ran}(A \pm iI)$ is dense and closed.

A is a self-adjoint operator, so take $\phi \in D(A) = D(A^*)$ such that $A^*\phi = i\phi$. Thus, $A\phi = i\phi$, and therefore

$$-i(\phi, \phi) = (i\phi, \phi) = (A\phi, \phi) = (\phi, A^*\phi) = (\phi, i\phi) = i(\phi, \phi), \quad (2.73)$$

such an equation is satisfied only if $\phi = 0$. Similarly, $A^*\phi = -i\phi$ will have only the trivial solution. This implies that $\text{Ker}(A^* \pm iI) = \{0\}$. From this result, we can show that $\text{Ran}(A \pm iI)$ is dense. Now, take $\psi \in \text{Ran}(A - iI)^\perp$, so from orthogonality, we have that $((A - iI)\phi, \psi) = 0 \quad \forall \phi \in D(A)$. Thus, $\psi \in D(A^*)$, and then $(A - iI)^*\psi = (A^* + i)\psi = 0$, but since $A^*\psi = -i\psi$ has no solution, this equality is impossible. Therefore, $\text{Ran}(A - iI)$ is dense. One should note that the condition $\text{Ker}(A \pm iI) = \{0\}$ can be used to verify if an operator is self-adjoint. In some cases, this is called the *basic criterion of self-adjointness*.

To prove that $\text{Ran}(A \pm iI)$ is closed, we note that $\forall \phi \in D(A)$; $\|(A - iI)\phi\|^2 = \|A\phi\|^2 + \|\phi\|^2$. Now, take the sequence $\phi_n \in D(A)$ such that $(A - iI)\phi_n \rightarrow \psi_0$. Thus, ϕ_n converges to some vector ϕ_0 , and $A\phi_n$ also converges. Since A is a closed operator, we have that $\phi_0 \in D(A)$ and $(A - iI)\phi_0 = \psi_0$, which proves that $\text{Ran}(A - iI)$ is closed. The fact that $\text{Ran}(A + iI)$ is also closed follows similarly. Thus, $\text{Ran}(A \pm iI)$ are closed, and $\text{Ran}(A \pm iI) = \mathcal{H}$.

Once $(A \pm iI)$ are closed, the closed graph theorem (Theorem A.51) can be used to conclude that $(A \pm iI)^{-1}$ are closed and *bounded*. Using the first resolvent formula (Theorem A.73), we conclude that $(A - iI)^{-1}$ and $(A + iI)^{-1}$ commute.

Now, we note that

$$\begin{aligned} ((A - iI)\psi, (A + iI)^{-1}(A + iI)\phi) &= ((A - iI)^{-1}(A - iI)\psi, (A + iI)\phi) \\ &\Rightarrow ((A + iI)^{-1})^* = (A - iI)^{-1}, \end{aligned} \quad (2.74)$$

which shows that $(A + iI)^{-1}$ is a normal operator. Similarly, one proves that $(A - iI)^{-1}$ is also normal.

In possession of the spectral theorem for self-adjoint bounded operators (Theorem A.83), we can extend it to bounded normal operators. For such, take any

bounded normal operator T , we can construct the operators $S_1 = \frac{1}{2}(T + T^*)$ and $S_2 = \frac{1}{2i}(T - T^*)$ such that $S_{1,2}$ are self-adjoint and $T = S_1 + iS_2$. Using the fact that T is normal, it follows that S_1 and S_2 are spectral measures. Therefore, the spectral theorem for bounded normal operators follows by applying the spectral theorem for bounded self-adjoint operators on S_1 and S_2 .

Now, we can start the proof of (a). By the last reasoning, we can conclude that there is a measure space $\langle M, \mu \rangle$, where μ is a finite measure, a unitary operator $U : \mathcal{H} \rightarrow \mathcal{L}^2(M, d\mu)$, and a measurable, bounded, complex-valued function $g(m)$ such that

$$U(A + iI)^{-1}U^{-1}\phi(m) = g(m)\phi(m) \quad \forall \phi \in \mathcal{L}^2(M, d\mu). \quad (2.75)$$

Once that $\text{Ker}(A + iI)^{-1}$ is empty, we have that $g(m) \neq 0$ a.e. μ , which implies that $g(m)^{-1}$ is finite a.e. μ .

Now, take $f(m) = g(m)^{-1} - i$ and suppose that $\psi \in D(A)$. This implies that $\psi = (A + iI)^{-1}\phi$ for some $\phi \in \mathcal{H}$, and by Eq.(2.75), we have that $U\psi = gU\phi$. Notice that the product fg is bounded, so, by the last equality, $f(U\psi) \in \mathcal{L}^2(M, d\mu)$.

Conversely, assume that $f(U\psi) \in \mathcal{L}^2(M, d\mu)$. Then there is a $\phi \in \mathcal{H}$ such that $U\phi = (f + i)U\psi$. Thus, we have that $gU\phi = g(f + i)U\psi = U\psi$, and comparing with Eq. (2.75), we conclude that $\psi = (A + iI)^{-1}\phi \Rightarrow \psi \in D(A)$.

To prove (b), we take $\psi \in D(A)$. By (a), we have that $\psi = (A + iI)^{-1}\phi$ for some $\phi \in \mathcal{H}$. This implies that $A\psi = \phi - i\psi$, and then

$$\begin{aligned} (UA\psi)(m) &= (U\phi)(m) - i(U\psi)(m) \\ &= (g(m)^{-1} - iI)(U\psi)(m) \\ &= f(m)(U\psi)(m). \end{aligned} \quad (2.76)$$

If f is a complex-valued function in a set of non-zero measure, there is a bounded set B on the upper half-complex plane so that $S = \{x | f(x) \in B\}$ has non-zero measure. Take χ_S as the indicator function of S , then $f\chi_S \in \mathcal{L}^2(M, d\mu)$, and $\text{Im}(f\chi_S, f\chi_S) > 0$. However, this contradicts the self-adjointness of multiplication by f . Thus, f is a real-valued function. ■

Why such a theorem is important for quantum mechanics follows almost directly. Suppose that we have a physical system described by a self-adjoint Hamiltonian acting over a state ψ . We can use the spectral theorem to write

$$H\psi(x) = E(x)\psi(x), \quad (2.77)$$

which is directly identified as the *time-independent Schrödinger equation*. Plugging the Hamiltonian of one-dimensional free particle, Eq. (2.72), we get

$$-\frac{1}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E(x)\psi(x). \quad (2.78)$$

There are many ways to solve the last equation if we impose boundary conditions over $\psi(x)$. If we consider that we have Dirichlet boundary conditions, $\psi(0) = \psi(L) = 0$, or, equivalently, that we restricted the problem to a compact domain of length L . The solution is directly obtained as a linear combination of sine and cosine. Using the boundary conditions we get that

$$\psi(x) = \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \quad \text{and} \quad E(x) = E_n = \frac{n^2\pi^2}{2mL^2}, \quad (2.79)$$

where $n \in \{0, 1, \dots\}$. Now we can in fact compute $\langle H \rangle$ using Eq. (2.57) and the time-independent Schrödinger equation

$$\begin{aligned} \sum_{n,n'=0}^{\infty} \int_{-\infty}^{\infty} \psi_{n'}(x) H \psi_n(x) dx &= (\psi_{n'}, H \psi_n) = (\psi_{n'}, E_n \psi_n) = E_n (\psi_{n'}, \psi_n) \\ \Rightarrow \langle H \rangle &= E_n = \frac{n^2\pi^2}{2mL^2}. \end{aligned} \quad (2.80)$$

So, by using the spectral theorem, it is enough to find the spectrum of an operator in order to find the mean-value of an observable.

Before we introduce another formulation of the spectral theorem let us prove the following

Lemma 2.8. Let $\mathcal{H}_1, \mathcal{H}_2, \mathcal{H}_3, \dots, \mathcal{H}_i, \dots$ be a sequence of subspaces of the Hilbert space $\mathcal{H}$ which are pairwise orthogonal and span the entire space $\mathcal{H}$. If ψ is an arbitrary element of $\mathcal{H}$, we denote its projection on $\mathcal{H}_i$ by ψ_i . Let $A_1, A_2, \dots, A_i, \dots$ be a given sequence of linear transformations with the property that A_i reduces in $\mathcal{H}_i$ to a bounded self-adjoint transformation of $\mathcal{H}_i$ into itself. Then there is a *unique* self-adjoint transformation A of $\mathcal{H}$, in general not bounded, which reduces in each $\mathcal{H}_i$ to A_i . Its domain consists of the elements ψ for which the series

$$\sum_{i=1}^{\infty} \|A_i \psi_i\|^2 \quad (2.81)$$

converges, and for these ψ

$$A\psi = \sum_{i=1}^{\infty} A_i \psi_i. \quad (2.82)$$

Proof. First we notice that the domain of A , $D(A)$, is dense, since it contains all elements of the form $\sum_i f_i$. Also, we have that

$$(A\psi, \phi) = \sum_i (A_i \psi_i, \phi_i) = \sum_i (\psi_i, A_i \phi_i) = (\psi, A\phi), \quad (2.83)$$

which implies that A is symmetric for all $\psi, \phi \in D(A)$. Now we are able to prove that A is self-adjoint. For that, take $\phi \in D(A^*)$ and $\psi \in D(A)$; then

$$\begin{aligned} (A\psi, g) &= (f, A^*g) \\ \Rightarrow \sum_{i=1}^{\infty} (A_i\psi_i, \phi_i) &= \sum_{i=1}^{\infty} (\psi_i, (A^*\phi)_i), \end{aligned} \quad (2.84)$$

once each $\mathcal{H}_j$ is orthogonal to an arbitrary element ψ of $\mathcal{H}_j$ must have $\psi_i = 0$ if $i \neq j$, using the assumption that each A_j is self-adjoint in $\mathcal{H}_j$, we get that

$$\begin{aligned} (A_j\psi_j, \phi_j) &= (\psi_j, (A^*\phi)_j) \\ \Rightarrow (A^*\phi)_j &= A_j\phi_j. \end{aligned} \quad (2.85)$$

From the last equation follows that

$$\sum_{i=1}^{\infty} \|A_i\phi_i\|^2 = \sum_{i=1}^{\infty} \|(A^*\phi)_i\|^2 = \|A^*\phi\|^2, \quad (2.86)$$

so ϕ also belongs to $D(A)$ and we also have that $A\phi = A^*\phi$ which, with the fact that A is symmetric, proves that $A = A^*$, that is A is self-adjoint.

To prove uniqueness let A' be an arbitrary self-adjoint transformation which reduces to A_i in each $\mathcal{H}_i$. A' is closed and defined for all elements ψ such that the series

$$\sum_{i=1}^{\infty} A'_i\psi_i \quad (2.87)$$

converges. The sum of this series is equal to $A'\psi$. We have that $A'_i\psi_i = A_i\psi_i$, and since we are summing orthogonal elements, this implies that the elements ψ also belong to $D(A)$. For such elements we can define $A'\psi - A\psi$. But A is self-adjoint, hence A is maximal symmetric, so $A' = A$. ■

The previous lemma ensures that we can decompose unbounded operators and vectors in the Hilbert space into orthogonal components. A useful and practical result.

Theorem 2.9. (Spectral theorem – spectral family form) Every self-adjoint operator A has the representation

$$A = \int_{-\infty}^{\infty} \lambda dE_{\lambda}, \quad (2.88)$$

where $\{E_{\lambda}\}$ is a spectral family which is uniquely determined by the operator A ; E_{λ} commutes with A , as well as with all the bounded operators which commute with A .

Proof. To start, let us define the following operator

$$R_z = (A - zI)^{-1}, \quad (2.89)$$

from the first part of the proof of the spectral theorem in its multiplication form (theorem 2.7), we know that $R_{\pm i}$ exists and is closed. We also know that its inverse exists, and that $D(R_{\pm i}) = \text{Ran}(A \pm iI) = \mathcal{H}$. From the same proof we obtained that

$$\|(A \pm iI)\psi\| \geq \|\psi\| \quad (2.90)$$

$$\Rightarrow \|\phi\| \geq \|R_{\pm i}\phi\|, \quad \forall \phi \in D(R_{\pm i}). \quad (2.91)$$

The same properties are true for $R_z = R_{x+iy}$, for $y \neq 0$, since

$$(A - (x + iy)I)^{-1} = \frac{1}{y} \left(\frac{A - xI}{y} - iI \right)^{-1}. \quad (2.92)$$

From Eq. (2.90), we obtain that

$$\begin{aligned} \|(A - iI)\psi\| &= \|(A + iI)\psi\| \\ \Rightarrow \|(A - iI)(A + iI)^{-1}\phi\| &= \|V\phi\| = \|\phi\|, \end{aligned} \quad (2.93)$$

where the operator $V = (A - iI)(A + iI)^{-1}$ is called the *Cayley transformation* of A . This transformation is isometric and is defined for elements in the form $\phi = (A + iI)\psi$ by $V\phi = (A - iI)\psi$ such that $\psi \in D(A)$. One should notice that both ϕ and $V\phi$ are elements of $\mathcal{H}$, which implies that V is an isomorphism and, therefore, a *unitary* transformation.

It is direct to see that

$$(I + V)\phi = 2A\psi, \quad \text{and}, \quad (I - V)\phi = 2i\psi, \quad (2.94)$$

if $(I - V)\phi = 0$, then $\psi = 0$, and $\phi = 0$, so $(I - V)^{-1}$ exists and

$$\begin{aligned} 2A\psi &= (I + V)(I - V)^{-1}2i\psi \\ \Rightarrow A &= i(I + V)(I - V)^{-1}. \end{aligned} \quad (2.95)$$

The last expression shows us how to recover A from V .

Once V is unitary, we can represent it in terms of its spectral decomposition (Theorem A.84)

$$V = \int_0^{2\pi} e^{i\theta} dF_\theta, \quad (2.96)$$

where $F_0 = 0$ and $F_{2\pi} = 1$. So, by the relation between V and A , we expect to be able to obtain the spectral decomposition of A . For that, we notice that F_θ

is a continuous function of θ . In particular, F_θ is continuous at $\theta = 0$ and also at $\theta = 2\pi$. Now we decompose the interval $[0, 2\pi]$ into infinite pieces using θ_m , where the two endpoints are limit points. For such, we take

$$-\cot \frac{\theta_m}{2} = m, \quad m \in \mathbb{Z}. \quad (2.97)$$

Now construct the pairwise orthogonal projections as

$$P_m = F_{\theta_m} - F_{\theta_{m-1}}, \quad (2.98)$$

note that

$$\sum_{m=-\infty}^{\infty} P_m = \lim_{\theta \rightarrow 2\pi} F_\theta - \lim_{\theta \rightarrow 0} F_\theta = I - 0 = I. \quad (2.99)$$

Note that P_m commutes with both V and A . So, the space $\mathcal{H}_m$ corresponding to P_m reduces the operators A and V . For a $\psi \in \mathcal{H}_m$, we have that

$$\begin{aligned} A\psi &= AP_m\psi = i(I+V)(I-V)^{-1}P_m\psi \\ &= \int_{\theta_{m-1}}^{\theta_m} i(1+e^{i\phi})(1-e^{i\phi})^{-1} dF_\theta \psi \\ &= \int_{\theta_{m-1}}^{\theta_m} \left(-\cot \frac{\theta}{2}\right) dF_\theta \psi, \end{aligned} \quad (2.100)$$

or

$$A\psi = \int_{m-1}^m \lambda dE_\lambda \psi, \quad (2.101)$$

where we set $E_\lambda = F_{-2\cot^{-1}\lambda}$, with $\{E_\lambda\}$ being the spectral family of A over $(-\infty, \infty)$. To recover the spectral representation of the operator, we sum over all the projections, recovering

$$A = \int_{-\infty}^{\infty} \lambda dE_\lambda, \quad (2.102)$$

■

It is worth noting that, in the same way we present here, von Neumann first proved the spectral theorem for unbounded operators [15, 16]. An obvious, but necessary, disclaimer about the last result is that our integral in the spectral theorem must be understood as the Riemann-Stieltjes integral.

Now let us go back to the free particle. In light of this version of the spectral theorem, we can use the spectrum given in Eq. (2.79) to write

$$H = \int_{-\infty}^{\infty} \lambda dE_\lambda = \sum_{n=-\infty}^{\infty} \frac{\pi^2 n^2}{2mL^2}, \quad (2.103)$$

obviously, such a result is divergent, but we must remember that the Hamiltonian is an operator and the measurable quantities are the mean value of the operators. Once we compute $\langle H \rangle$, only a finite number of contributions will remain in the sum (depending of the stucture of the state, see Definition 2.5), and the final result is finite (for finite n), which agrees with Eq. (2.80). This last theorem makes clear that our measurables are the averages of the operator's spectrum, where the probability measure is given by the inner product between the state and the probability family.

Evidently, all the previous discussion was general and holds for any operator. However, in physics, we have some operators that are more interesting than others. In particular, we would like to have an operator that can evolve the system in time. From the *time-dependent* Schrödinger equation,

$$H\psi(x, t) = i\frac{\partial}{\partial t}\psi(x, t), \quad (2.104)$$

we can formally obtain that

$$\psi(x, t) = U(t)\psi(x, 0), \quad U(t) = e^{-itH}. \quad (2.105)$$

In this picture, $U(t)$ is the operator responsible for the time evolution. However, we should remember that, in general, the Hamiltonian is an unbounded operator and, therefore, we must take care to ensure that our formal expressions have a practical meaning. Another possible question is whether this is the only possible way to evolve our system in time.

In order to answer the previous questions, we must be able to define functions of self-adjoint operators. Before investigating the general case, let us prove two results for polynomials.

Lemma 2.10. Let $P(x) = \sum_{n=0}^N a_n x^n$. Let $P(A) = \sum_{n=0}^N a_n A^n$. Then

$$\sigma(P(A)) = \{P(\lambda) \mid \lambda \in \sigma(A)\} \quad (2.106)$$

Proof. Take $\lambda \in \sigma(A)$. So, $x = \lambda$ is a root of $P(x) - P(\lambda)$. From that, it follows that $P(x) - P(\lambda) = (x - \lambda)Q(x)$. Using our hypothesis, we can write

$$P(A) - P(\lambda) = (A - \lambda)Q(A), \quad (2.107)$$

once $\lambda \in \sigma(A)$, $(A - \lambda)$ does not have an inverse. Thus, $P(A) - P(\lambda)$ cannot have an inverse, so $P(\lambda) \in \sigma(P(A))$.

Now, let $\mu \in \sigma(P(A))$ and $\lambda_1, \dots, \lambda_n$ be the roots of $P(x) - \mu$. Then $P(x) - \mu = a(x - \lambda_1) \dots (x - \lambda_n)$. If $\lambda_1, \dots, \lambda_n \notin \sigma(A)$, we have that

$$(P(A) - \mu)^{-1} = a^{-1}(A - \lambda_1)^{-1} \dots (A - \lambda_n)^{-1}, \quad (2.108)$$

which is a contradiction with the fact that $\mu \in \sigma(P(A))$. So, some $\lambda_i \in \sigma(A)$, that is, $\mu = P(\lambda)$ for some $\lambda \in \sigma(A)$. ■

Lemma 2.11. Let A be a bounded self-adjoint operator. Then

$$\|P(A)\| = \sup_{\lambda \in \sigma(A)} |P(\lambda)| \quad (2.109)$$

Proof. First, we note that

$$\|P(A)\|^2 = \|P(A)^* P(A)\| = \|(\bar{P}P)(A)\|. \quad (2.110)$$

Now, using Theorem (Theorem A.80) and Lemma 2.10, we can write

$$\|(\bar{P}P)(A)\| = \sup_{\lambda \in \sigma(\bar{P}P(A))} |\lambda| = \sup_{\lambda \in \sigma(A)} |(\bar{P}P)(A)| = \left(\sup_{\lambda \in \sigma(A)} |P(A)| \right)^2 \quad (2.111)$$

■

With these two results, we can construct the functional calculus for continuous functions, that is, we can prove that continuous functions of operators have the following properties:

Theorem 2.12. (Properties of the continuous functional calculus) Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Then, there exists a *unique* map $f : C(\sigma(A)) \rightarrow \mathcal{L}(\mathcal{H})$ with the following properties:

(i) f is an algebraic $*$ -homomorphism, that is:

$$f(ab) = f(a)f(b), \quad f(\lambda a) = \lambda f(a),$$

$$f(1) = I, \quad f(\bar{a}) = f(a)^*$$

for any $a, b \in C(\sigma(A))$ and any $\lambda \in \mathbb{C}$;

(ii) f is continuous, that is, $\|f(a)\|_{\mathcal{L}(\mathcal{H})} \leq C\|a\|_{\infty}$;

(iii) Let a be the function $a(x) = x$, then $f(a) = A$;

(iv) If $A\psi = \lambda\psi$, then $f(a)\psi = a(\lambda)\psi$, for any $\psi \in \mathcal{H}$ and any $\lambda \in \sigma(A)$;

(v) $\sigma[f(a)] = \{a(\lambda) | \lambda \in \sigma(A)\}$;

(vi) If $a \geq 0$, then, $f(a) \geq 0$;

(vii) $\|f(a)\| = \|a\|_{\infty}$.

Proof. First, take $f(P) = P(A)$, where P stands for a polynomial. Thus, $\|f(P)\|_{\mathcal{H}} = \|P\|_{C(\sigma(A))}$, by the B.L.T. theorem (theorem A.38). This implies that f has a unique linear extension to the closure of the polynomial in $C(\sigma(A))$. The polynomials form an algebra containing 1, containing complex conjugates, and separating points, so its closure is all of $C(\sigma(A))$.

Denote the extension of f by $\tilde{f}$. $\tilde{f}$ satisfies (i), (ii), (iii), and (vii). Additionally, it agrees with f on the polynomials, which are dense in $C(\sigma(A))$ (Stone-Weierstrass theorem). By continuity, it agrees on all of $C(\sigma(A))$. Hence, (i), (ii), (iii), and (vii) follow.

To prove (iv), we first note that, if $f(P)\psi = P(\lambda)\psi$, then by continuity, we have that $f(a)\psi = a(\lambda)\psi$.

(v). Set $f(a) = f(P)$, where P is a polynomial. By lemma 2.10, we have that $\sigma[f(P)] = \{P(\lambda) | \lambda \in \sigma(A)\}$. By the Stone-Weierstrass theorem and continuity, we have that $\sigma[f(a)] = \{a(\lambda) | \lambda \in \sigma(A)\}$.

We can prove (vi) by setting $a = b^2 \geq 0$, where b is real and $b \in C(\sigma(A))$. Thus, $f(a) = f(b)^2$, which implies that $f(b)$ is self-adjoint. Therefore, $f(b) \geq 0$. ■

The last properties establish the fundamental building blocks to work with functions of self-adjoint operators. Worth noting that the functional calculus provides almost immediately another formulation of the spectral theorem.

Theorem 2.13. Let A be a self-adjoint operator and define $U(t) = e^{itA}$. Then:

- (i) For each $t \in \mathbb{R}$, $U(t)$ is a unitary operator and $U(t+s) = U(t)U(s)$ for all $s, t \in \mathbb{R}$;
- (ii) If $\psi \in \mathcal{H}$ and $t \rightarrow t_0$, then $U(t)\psi \rightarrow U(t_0)\psi$;
- (iii) For $\phi \in D(A)$,

$$\frac{U(t)\phi - \phi}{t} \rightarrow iA\phi, \quad \text{as } t \rightarrow 0; \quad (2.112)$$

- (iv) If $\lim_{t \rightarrow 0} \frac{U(t)\phi - \phi}{t}$ exists, then $\phi \in D(A)$.

Proof. To prove (i), it is sufficient to use property (i) of theorem 2.12. Since f is a $*$ -homomorphism, we have that $f(ab) = f(a)f(b)$. Take $f_t = e^{it}$, so $f_t(A) = e^{itA}$, then

$$f_t(A)f_s(A) = e^{itA}e^{isA} = e^{i(t+s)A} = U(t+s). \quad (2.113)$$

Unitarity follows from the same expression.

(ii) follows from the spectral theorem and some arguments of convergence. Observe that, for $\psi \in D(A)$

$$\|e^{itA}\psi - \psi\|^2 = \int_{\mathbb{R}} |e^{it\lambda} - 1|^2 d(\psi, P_\lambda\psi), \quad (2.114)$$

but we know that $|e^{it\lambda} - 1|^2 < g(\lambda) = 2$ and $|e^{it\lambda} - 1|^2 \rightarrow 0$ as $t \rightarrow 0, \forall \lambda \in \mathbb{R}$. So, by the Lebesgue dominated convergence theorem (Theorem A.32), we get that $\|U(t)\psi - \psi\|^2 \rightarrow 0$. Thus, $t \rightarrow U(t)$ is strongly continuous at $t = 0$, and by item (i), it is continuous everywhere.

(iii) follows similarly. First, we note that

$$\left\| \frac{U(t)\phi - \phi}{t} \right\|^2 = \int_{\mathbb{R}} \left| \frac{e^{it\lambda} - 1}{t} \right|^2 d(\phi, P_\lambda \phi) \quad (2.115)$$

but $|e^{it\lambda} - 1| \leq |t\lambda|$, so $\left| \frac{e^{it\lambda} - 1}{t} \right| \leq |\lambda|$, which is integrable. Also, we have that

$$\lim_{t \rightarrow 0} \left| \frac{e^{it\lambda} - 1}{t} \right| \leq |\lambda| = |i\lambda| = |\lambda| \quad (2.116)$$

This implies that

$$\lim_{t \rightarrow 0} \left\| \frac{U(t)\phi - \phi}{t} \right\|^2 = \int_{\mathbb{R}} |\lambda|^2 d(\phi, P_\lambda \phi) = \|iA\phi\|^2. \quad (2.117)$$

To prove (iv), we define $D(B) = \{\phi \mid \lim_{t \rightarrow 0} \frac{U(t)\phi - \phi}{t} \text{ exists}\}$, and let

$$iB\phi = \lim_{t \rightarrow 0} \frac{U(t)\phi - \phi}{t}. \quad (2.118)$$

Since B is symmetric, $B = A$, and $\phi \in D(A)$. ■

Definition 2.14. An operator-valued function $U(t)$ satisfying (i) and (ii) of theorem 2.13 is called a **strongly continuous one-parameter unitary group**.

Theorem 2.15. (Stone's theorem) Let $U(t)$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then there is a *unique* self-adjoint operator A on $\mathcal{H}$ such that $U(t) = e^{itA}$.

Proof. Take $f \in C_0^\infty(\mathbb{R})$, and for each $\phi \in \mathcal{H}$, define

$$\phi_f = \int_{-\infty}^{\infty} f(t)U(t)\phi dt, \quad (2.119)$$

where, since $U(t)$ is strongly continuous, this integral can be taken as a Riemann integral. Define D as the set of all linear combinations of such ϕ_f . Now define the approximate identity as

$$j_\varepsilon(x) = \varepsilon^{-1} j\left(\frac{x}{\varepsilon}\right), \quad (2.120)$$

where $j \in C_0^\infty(-1, 1) \subset C_0^\infty(\mathbb{R})$ and $\int_{-\infty}^{\infty} j(x) dx = 1$. Then

$$\|\phi_{j_\varepsilon} - \phi\| = \left\| \int_{-\infty}^{\infty} j_\varepsilon(t)[U(t)\phi - \phi] dt \right\| \leq \left(\int_{-\infty}^{\infty} j_\varepsilon(t) dt \right) \sup_{t \in [-\varepsilon, \varepsilon]} \|U(t)\phi - \phi\|, \quad (2.121)$$

Since $U(t)$ is strongly continuous, we get that D is dense in $\mathcal{H}$.

Take $\phi_f \in D$, so

$$\left(\frac{U(s) - I}{s} \right) \phi_f = \int_{-\infty}^{\infty} f(t) \left(\frac{U(s+t) - U(t)}{s} \right) \phi dt = \int_{-\infty}^{\infty} \left(\frac{f(\tau-s) - f(\tau)}{s} \right) U(\tau)\phi d\tau, \quad (2.122)$$

We know that $\left(\frac{f(\tau-s) - f(\tau)}{s} \right)$ converges uniformly to the derivative of f as $s \rightarrow 0$, so

$$\int_{-\infty}^{\infty} \left(\frac{f(\tau-s) - f(\tau)}{s} \right) U(\tau)\phi d\tau \rightarrow - \int_{-\infty}^{\infty} f'(\tau) U(\tau)\phi d\tau = \phi_{-f'}, \quad (2.123)$$

as $s \rightarrow 0$.

Now, for any $\phi_f \in D$, define $A\phi_f = i^{-1}\phi_{-f'}$. Thus, we have that $U : D \rightarrow D$, $A : D \rightarrow D$, such that $U(t)A\phi_f = AU(t)\phi_f$. If $\phi_f, \phi_g \in D$, then

$$\begin{aligned} (A\phi_f, \phi_g) &= \lim_{s \rightarrow 0} \left(\left(\frac{U(s) - I}{is} \right) \phi_f, \phi_g \right) = \lim_{s \rightarrow 0} \left(\phi_f, \left(\frac{I - U(-s)}{is} \right) \phi_g \right) \\ &= \left(\phi_f, \frac{1}{i} \phi_{-g'} \right) = (\phi_f, A\phi_g), \end{aligned} \quad (2.124)$$

which implies that A is a symmetric operator.

Now suppose there is a $u \in D(A^*)$ such that $A^*u = iu$. Then, for each $\phi \in D = D(A)$, we have that

$$\begin{aligned} \frac{d}{dt} (U(t)\phi, u) &= (iAU(t)\phi, u) = -i(U(t)\phi, A^*u) \\ &= -i(U(t)\phi, iu) = (U(t)\phi, u) = g(t). \end{aligned} \quad (2.125)$$

So we have a complex-valued function $g(t)$, which satisfies the equation $g' = g$, so $g(t) = g(0)e^t$. But since $U(t)$ has norm one, $|g(t)|$ is bounded, and this can only happen if $g(0) = (\phi, u) = 0$. This is only satisfied if $u = 0$. Similarly, defining $A^*u = -iu$, one can verify that the only solution is $u = 0$. Therefore, we have that $\text{Ker}(A^* \pm iI) = \{0\}$, so by the first part of the proof of theorem 2.7, we have that A is essentially self-adjoint on D .

To prove uniqueness, let $V(t) = e^{itB}$. Take $\phi \in D$ and also $\phi \in D(B)$. Then, $V(t)\phi \in D(B)$ and, by (iii) of theorem 2.13, $V'(t)\phi = iAV(t)\phi$. Since $U(t)\phi \in D \subset$

$D(B) \forall t$, we can let $w(t) = U(t)\phi - V(t)\phi$, so

$$\begin{aligned} w'(t) &= iAU(t)\phi - iBV(t)\phi = iBw(t) \\ \Rightarrow \frac{d}{dt} \|w(t)\|^2 &= -i(Bw(t), w(t)) + i(w(t), Bw(t)) = 0, \end{aligned} \quad (2.126)$$

since $w(0) = 0$, then $w(t) = 0, \forall t$. This implies that $U(t)\phi = V(t)\phi, \forall t \in \mathbb{R}$ and $\phi \in D$. But D is dense, so $U(t) = V(t) \Rightarrow A = B$. ■

So, by the functional calculus and by Stone's theorem, we can ensure that our time evolution given by $U(t) = e^{-itH}$ is not only well-defined but also unique for each self-adjoint Hamiltonian. With a further definition, we can explore more applications of Stone's theorem in quantum mechanics.

Definition 2.16. If $U(t)$ is a strongly continuous one-parameter unitary group, then the self-adjoint operator A with $U(t) = e^{itA}$ is called the **infinitesimal generator** of $U(t)$.

In other words, we can say that the *Hamiltonian is the time-evolution infinitesimal generator* in quantum systems. This is a scenario very similar to classical mechanics, as discussed previously. The case where the Hamiltonian is time-dependent can be easily obtained. However, we ask ourselves whether we can evolve the observable in time instead of the state ψ , as in Eq. (2.105). Using the fact that our measurables are expected values of observables, consider that we have an observable A and the **time evolution operator** $U(t) = e^{-itH}$, so we can write

$$\begin{aligned} \langle A \rangle &= (A\psi(x, t), \psi(x, t)) = (U(t)\psi(x), AU(t)\psi(x)) = (\psi(x), U(-t)AU(t)\psi(x)) \\ &= \langle A(t) \rangle, \end{aligned} \quad (2.127)$$

where we have defined $A(t) = U(-t)AU(t)$. Taking the derivative of $A(t)$ and using the properties of $U(t)$, we can obtain

$$\frac{d}{dt} A(t) = i[H, A]. \quad (2.128)$$

This is called the **Heisenberg equation**. Such an equation has an astonishing similarity with the time evolution in classical mechanics; see Eq. (2.32). In our system of units, the difference is just that instead of working with the Poisson bracket (see definition 2.1), we work with the complex unity times the commutator. These two different time evolutions define the so-called pictures of motion in quantum mechanics. When we consider the evolution of the state (Eq. (2.105)), we say that we are in the **Schrödinger picture**, while the time evolution of the operators (Eq. (2.128)) is referred to as the **Heisenberg picture**. The two pictures are completely equivalent.

As we believe that it is clear at this point, dealing with unbounded operators, like P and Q , is, in general, difficult. However, Stone's theorem allows us to deal with bounded and unitary operators instead of the self-adjoint unbounded operators. Defining $U(a) = e^{iaP}$ and $V(s) = e^{isQ}$. In order to find how these operators act over a function we formally write

$$\begin{aligned} U(a)\phi(x) &= e^{iaP}\phi(x) = \sum_{n=0}^{\infty} \frac{(iaP)^n}{n!}\phi(x), \\ V(s)\phi(x) &= e^{isQ}\phi(x) = \sum_{n=0}^{\infty} \frac{(isQ)^n}{n!}\phi(x), \end{aligned} \quad (2.129)$$

now, using the coordinate representation, we get

$$\begin{aligned} U(a)\phi(x) &= \sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{d^n}{dx^n} \phi(x) = \phi(x+a), \\ V(s)\phi(x) &= \sum_{n=0}^{\infty} \frac{(isx)^n}{n!} \phi(x) = e^{isx} \phi(x). \end{aligned} \quad (2.130)$$

Such a relation allows us to identify the momentum as the infinitesimal generator of space translations. An analogous computation, but using the momentum representation, shows that the position operator is the infinitesimal generator of the momentum translation.

Our realization of the canonical commutation relations given at Eq. (2.66) is called **Schrödinger representation**. Once that we are dealing with functions of the operators P and Q , it is interesting to ask how the canonical commutation relation behaves under such a map. For that, we first notice that

$$\begin{aligned} U(a)V(s)\phi(x) &= e^{ias}e^{isx}\phi(x+a) \\ V(s)U(a)\phi(x) &= e^{isx}\phi(x+a) \\ \Rightarrow U(a)V(s) &= e^{ias}V(s)U(a), \end{aligned} \quad (2.131)$$

The last equation is called **Weyl relation**. We are going to show that any realization of the Weyl relation is also a realization of the canonical commutation relation. Before that, let us construct some auxiliary machinery.

Proposition 2.17. (i) All operators defined by

$$W(s, t) = e^{-\frac{i}{2}st} U(s) V(t), \quad (2.132)$$

are unitary, and, for all $s_1, s_2, t_1, t_2 \in \mathbb{R}$ we have

$$W(s_1, t_1)W(s_2, t_2) = e^{\frac{i}{2}(s_1 t_2 - s_2 t_1)} W(s_1 + s_2, t_1 + t_2). \quad (2.133)$$

In particular, $W(0, 0) = 1$ and $W^*(s, t) = W(-s, -t)$;

(ii) for any $h \in \mathcal{L}(\mathbb{R}^2)$ we define

$$W_h = \int h(s, t) W(s, t) ds dt, \quad (2.134)$$

if $h \neq 0$ then $W_h \neq 0$;

(iii) take $h_1, h_2 \in \mathcal{L}(\mathbb{R}^2)$ and define $h \in \mathcal{L}(\mathbb{R}^2)$ by

$$h(s, t) = \int e^{i(st' - s't)} h_1(s - s', t - t') h_2(s', t') ds' dt', \quad (2.135)$$

then $W_{h_1} W_{h_2} = W_h$.

Proof. Parts (i) and (iii) follow from direct computation.

To prove (ii), first assume that $W_h = 0$. Then, for any $x, y \in \mathbb{R}$ we have that $W(-x, -y) W_h W(x, y) = 0$. Using the definitions, one obtains that

$$0 = \int h(s, t) e^{i(sy - tx)} W(s, t) ds dt, \quad (2.136)$$

but this needs to be true for any $\psi \in \mathcal{H}$, that is, $(\psi, W(s, t)\psi) = 0$. However, $W(s, t)$ is unitary, so $\|W\psi\| = \|\psi\| \neq 0$ if $\psi \neq 0$. Thus, $W_h \neq 0$ if $h \neq 0$. ■

Theorem 2.18. (Stone-von Neumann theorem) Any representation of the Weyl relations is unitarily equivalent to an at most countable direct sum of Schrödinger representations. In particular, any irreducible representation of the Weyl relation is unitarily equivalent to the Schrödinger representation.

Proof. First, we set $h(s, t) = \frac{1}{2\pi} e^{-\frac{1}{4}(s^2 + t^2)}$ to construct the following object:

$$P = W_h = \frac{1}{2\pi} \int W(s, t) e^{-\frac{1}{4}(s^2 + t^2)} ds dt. \quad (2.137)$$

Now we will prove that P is an orthogonal projection, that is, $P = P^*$ and $P^2 = P$. The self-adjointness follows from

$$\begin{aligned} P^* &= \frac{1}{2\pi} \int W^*(s, t) e^{-\frac{1}{4}(s^2 + t^2)} ds dt = \frac{1}{2\pi} \int W(-s, -t) e^{-\frac{1}{4}(s^2 + t^2)} ds dt \\ &= \frac{1}{2\pi} \int W(s, t) e^{-\frac{1}{4}(s^2 + t^2)} ds dt = P. \end{aligned} \quad (2.138)$$

Using the definitions, proposition 2.17, and with some algebraic manipulations, one can recover that $PW(x, y)P = e^{\frac{1}{4}(x^2 + y^2)} P$, which is $P^2 = P$ when $x = y = 0$. Thus, P is indeed an orthogonal projection operator.

From (ii) of proposition 2.17, we know that P is not the zero operator, so $P\mathcal{H} \neq 0$. In the subspace $P\mathcal{H}$, take an orthonormal basis $\{\Omega_n\}_{n=1}^N$, where $N = \{1, 2, \dots\}$. For $1 \leq n \leq N$, take $\mathcal{H}_n = \overline{\text{span}}\{W(s, t)\Omega_n | s, t \in \mathbb{R}\}$.

Using (i) of proposition 2.17, we obtain that $W(s_1, t_1)W(s_2, t_2)\Omega_n = e^{i(s_1 t_2 - s_2 t_1)} \times W(s_1 + s_2, t_1 + t_2)\Omega_n$, so each $\mathcal{H}_n$ is invariant under $W(s, t)$. Also, using the fact that each subspace is invariant under projection into itself, and the properties of proposition 2.17, we can compute the following property:

$$\begin{aligned} (W(x, y)\Omega_n, W(s, t)\Omega_m) &= (W(x, y)P\Omega_n, W(s, t)P\Omega_m) \\ &= (\Omega_n, PW(-x, -y)W(s, t)P\Omega_m) = e^{\frac{i}{2}(-xt+ys)} e^{\frac{1}{4}[(s-x)^2 - (t-y)^2]} (\Omega_n, \Omega_m) \\ &= e^{\frac{i}{2}(-xt+ys)} e^{\frac{1}{4}[(s-x)^2 - (t-y)^2]} \delta_{nm} \end{aligned} \quad (2.139)$$

The last equality follows from the fact that we chose an orthonormal basis system. This last result shows us that the spaces $\mathcal{H}_n$ and $\mathcal{H}_m$ are orthogonal for $n \neq m$.

To finish the first part of the proof, we need to show that the direct sum of our projections reconstructs the whole Hilbert space. For that, take $D = \bigoplus_{n=1}^N \mathcal{H}_n$ and assume that $D \subset \mathcal{H}$. Then $\{W(s, t)\}_{|D^\perp}$ is a representation of the Weyl relations, and the respective projection is given by $P|_{D^\perp}$, which is not the zero operator. Now take $f \neq 0 \in D^\perp$ such that $Pf = f$, but $\text{Ran}(Pf) = D$, so $D^\perp = \{0\}$. This means that $D = \mathcal{H}$.

To prove that all representations are unitarily equivalent, we fix some Ω_n and define $f(s, t) = W(s, t)\Omega_n \in \mathcal{H}_n$ for some $s, t \in \mathbb{R}$. We have that

$$W(x, y)f(s, t) = e^{\frac{i}{2}(xt-ys)} W(x+s, y+t)\Omega_n = e^{\frac{i}{2}(xt-ys)} f(x+s, y+t), \quad (2.140)$$

and

$$\begin{aligned} (f(x, y), f(s, t)) &= (W(x, y)\Omega_n, W(s, t)\Omega_n) = (W(x, y)P\Omega_n, W(s, t)P\Omega_n) \\ &= (\Omega_n, PW(-x, -y)W(s, t)P\Omega_n) = e^{\frac{i}{2}(-xt+ys)} e^{\frac{1}{4}[(s-x)^2 - (t-y)^2]} (\Omega_n, P\Omega_n) \\ &= e^{\frac{i}{2}(-xt+ys)} e^{\frac{1}{4}[(s-x)^2 - (t-y)^2]}. \end{aligned} \quad (2.141)$$

The important fact about the last two equations is that the action of the operator W and the inner product in $\mathcal{H}_n$ are entirely determined by the properties of W . This means that, if we have a second representation, say $\mathcal{H}_m$, and define $f'(s, t) = W'(s, t)\Omega_m$, we get the same action of the operator and the same inner product in the Hilbert space $\mathcal{H}_m$. Thus, the map between the two representations must be given by a unitary operator, in order to preserve the inner product. Once we know that the Schrödinger representation satisfies the Weyl relations, we can affirm that all representations are unitarily equivalent to the Schrödinger representation. $\blacksquare$

It is important to notice that the last theorem and its proof can be directly extended to any finite number of degrees of freedom. In the case of an infinite number of degrees of freedom, not only the proof but the theorem is not true anymore. As we are going to explore in the next section and chapters, the non-unique representations of the canonical commutation relations will be responsible for many interesting mechanisms in quantum field theory.

Let us use the liberty of representation choice to discuss the last example that will be useful throughout this thesis: The Harmonic Oscillator. Its classical Hamiltonian in one dimension has been presented in Eq. (2.13), and in order to obtain its quantum version, we use the maps $p \rightarrow P$ and $q \rightarrow Q$. For convenience, we set $m = 1$ and $k = \omega^2$,

$$H = \frac{1}{2}P^2 + \frac{1}{2}\omega^2Q^2. \quad (2.142)$$

We wish to verify how these operators evolve in time, so using the Heisenberg equation (Eq. (2.128)), we easily get that

$$\frac{dQ}{dt} = P, \quad \frac{dP}{dt} = -\omega^2Q. \quad (2.143)$$

Instead of working in the coordinate or momentum representation, we are going to use the liberty that the Stone-von Neumann theorem gives to us to choose a more convenient representation⁷. Let us define

$$a = \frac{1}{\sqrt{2\omega}}(\omega Q + iP), \quad a^\dagger = \frac{1}{\sqrt{2\omega}}(\omega Q - iP), \quad (2.144)$$

$$Q = \sqrt{\frac{2}{\omega}}(a + a^\dagger), \quad P = -i\sqrt{2\omega}(a - a^\dagger). \quad (2.145)$$

Using the canonical commutation relation, one finds that

$$[a, a^\dagger] = 1. \quad (2.146)$$

It is worth noting that $a, a^\dagger$ are not self-adjoint, so, by our definition 2.6, they are not observables. From the equations of motion for Q and P and the previous definitions, we obtain that

$$\frac{da}{dt} = -i\omega a, \quad \frac{da^\dagger}{dt} = -i\omega a^\dagger, \quad (2.147)$$

⁷Some care must be taken here. The Stone-von Neumann theorem ensures that any representation of the Weyl relation obeys the canonical commutation relation, however, its converse may not be true. That is, not all representations that obey the canonical commutation relation obey the Weyl relation. We are going to use a well-known representation, and for this reason, we ignore such a technical feature.

The solution can be obtained easily and reads

$$a(t) = e^{-i\omega t} a(0), \quad a^\dagger(t) = e^{i\omega t} a^\dagger(0), \quad (2.148)$$

$$Q(t) = \frac{1}{\omega} \left[a(0)e^{-i\omega t} + a^\dagger(0)e^{i\omega t} \right], \quad (2.149)$$

$$P(t) = -i\omega \left[a(0)e^{-i\omega t} - a^\dagger(0)e^{i\omega t} \right]. \quad (2.150)$$

We can investigate what we can get from this representation further. First, let us consider only the static case, that is, $t = 0$, fix $a = a(0)$, $a^\dagger = a^\dagger(0)$ and denote $N = a^\dagger a$. In this representation we can use the definitions and the commutation relations to write the harmonic oscillator Hamiltonian as follows

$$H = \omega \left(a^\dagger a + \frac{1}{2} I \right) = \omega \left(N + \frac{1}{2} I \right), \quad (2.151)$$

from the spectral theorem 2.7, we get that

$$H\psi_n = E_n\psi_n = \omega \left(N + \frac{1}{2} I \right) \psi_n, \quad (2.152)$$

so

$$E_n = \omega \sigma \left(N + \frac{1}{2} I \right), \quad N\psi_n = F_n\psi_n. \quad (2.153)$$

So, to find the expectation value of H we only need to find the spectrum of the operator N . For that let us define the ground state of our system. The ground state will be the vector of a , such that,

$$a\psi_0 = 0 = \frac{1}{\sqrt{2}\omega} (\omega^2 Q + iP)\psi_0 = \frac{1}{\sqrt{2}\omega} \left(\omega^2 x + \frac{d}{dx} \right) \psi_0(x) = 0, \quad (2.154)$$

the solution of this differential equation gives to us

$$\psi_0(x) = Ce^{-\omega^2 x^2}, \quad (2.155)$$

where C is a normalization constant that can be fixed by imposing $(\psi_0, \psi_0) = 1$. Now we can verify successive actions of $a^\dagger$ over the ground state

$$\begin{aligned} a^\dagger \psi_0 &= \frac{1}{\sqrt{2}\omega} (\omega^2 Q - iP)\psi_0 = \frac{1}{\sqrt{2}\omega} \left(\omega^2 x - \frac{d}{dx} \right) Ce^{-\omega^2 x^2} \\ &= \frac{3}{\sqrt{2}} \omega x \psi_0(x) = C_1 \text{He}_1(\omega x) \psi_0(x) = C_1 \psi_1(x) \\ a^\dagger \psi_1 &= \frac{3}{2} (3\omega^2 x^2 - 1) \psi_0 = C_2 \text{He}_2(\omega x) \psi_0(x) = C_2 \psi_2(x) \\ &\vdots \\ a^\dagger \psi_{n-1} &= C_n \text{He}_n(\omega x) \psi_0(x) = C_n \psi_n(x), \end{aligned} \quad (2.156)$$

where $C_1, \dots, C_n$ are normalizations and He_n is the n -th Hermite polynomial. In the last equation we can note that ψ_0 is always an eigenfunction of the operator $(a^\dagger)^n$, $n = 1, 2, \dots$. Therefore, we could define the ground state as the cyclic vector of $a^\dagger$ ⁸. Also, with the appropriate normalization of the Hermite polynomials, we can choose to have the normalization constants C_n as

$$a^\dagger \psi_n = \sqrt{n+1} \psi_{n+1}(x), \quad (2.157)$$

in this normalization we get that

$$a \psi_n = \sqrt{n} \psi_{n-1}(x). \quad (2.158)$$

Once that we know how the operators act, we can analyse the action of N over these vectors,

$$N \psi_n = a^\dagger a \psi_n = a^\dagger \sqrt{n} \psi_{n-1} = n \psi_n. \quad (2.159)$$

We have found that the complete set of eigenfunctions of N is $\{\psi_n\}_{n=0}^\infty$, this allows to identify that $\sigma(N) = \{0, 1, 2, \dots\}$. The action of these operators justifies the respective name: $a^\dagger$ is the **creation operator**, a the **annihilation operator**, and N the **number operator**. One possible interpretation for each of those is that one creates a particle in a state, another annihilates a particle, and the last one counts the total number of particles in a given state.

Back to the Hamiltonian, Eq. (2.152), we can fix a vector ψ_n to get

$$E_n = \omega \left(n + \frac{1}{2} \right), \quad (2.160)$$

it is interesting to notice that

$$E_0 = \frac{\omega}{2}, \quad (2.161)$$

which means that the ground state has a non-zero energy. Later, this fact will emerge again in a quantum field theory scenario.

It is worth mentioning that this solution can be obtained more rigorously using the idea of generalized functions and a family of seminorms, see [17]. Due to the number of concepts that need to be fully developed to obtain this solution, we choose not to present such a beautiful construction.

As we have noticed, the Stone-von Neumann theorem allows us to use those operators to solve the problem, and it also guarantees that the solution is well posed, once we could solve it, for example, in the coordinate representation and obtain the same result. In the next section we see that the situation where this theorem does not hold is even more interesting.

⁸An operator A on a Hilbert space is said to have a **cyclic** vector ϕ , if $\text{span}\{\phi, A\phi, A^2\phi, \dots, A^n\phi, \dots\} = \mathcal{H}$

Chapter 3

Axiomatic Quantum Field Theory

In this chapter, we introduce Quantum Field Theory in its first stage of development. First, we would like to establish that the physical justification for the mathematical objects we call “Quantum Fields” arises naturally once we use two basic concepts of quantum theory and relativity. These concepts are that quantum systems are described by a space of functions belonging to a Hilbert space (particularly square-integrable functions) and that relativistic systems should conserve their total momentum. A well-structured but not entirely clear, physically oriented exposition of how these two ideas can be combined to conclude that Quantum Fields are inevitable can be found in Reference [18].

While the necessary mathematics for fully understanding both concepts is not particularly complicated, the physics literature has primarily focused on group theory, which suffices to treat classical relativistic systems. To gain a deeper understanding of a quantum relativistic system, such as Quantum Fields, it is necessary to delve further into the mathematical aspects of measure theory, Hilbert spaces, and Banach spaces. Since there is a substantial amount of literature presenting group theory for physicists, *e.g.*, References [19, 20], the literature on measure theory, Hilbert spaces, and Banach spaces for physicists exists but is relatively limited [17]. For this reason, the reader which is unfamiliar with some basic notions of functional analysis can be vastly favored reading Appendix A.

In Section 3.1, we justify the title of this chapter by introducing the concept of quantum fields and the well-known Wightman axioms. Following this development, we present Section 3.2 with the simplest, yet one of the most elegant, applications of Quantum Field Theory: the zero-point energy and the Casimir effect. In particular, we discuss cases involving perfect conductors and dielectrics. In the dielectric case, we present two novel contributions of this thesis: how to obtain finite corrections to the Casimir energy using approximate functional equations for slab and rectangular geometries, and how to apply the surface wave

approach in a rectangular waveguide. Still within the context of zero-point fluctuations, we also propose that a charge in the vicinity of a dielectric can act as a sensor for zero-point fluctuations, with the velocity induced by the zero-point fluctuations exceeding that due to thermal motion.

For the remainder of this chapter, Section 3.3, we dedicate ourselves to discussing interacting fields.

3.1 Quantum Fields and Wightman Axioms

As we stressed out previously, the quantum fields represent the culmination of the ideas of special relativity and quantum mechanics. Since the construction that generalizes quantum systems to systems with an uncountable number of degrees of freedom, resulting in relativistic wave mechanics, is well presented in the literature (see, e.g., [18]), we do not devote further pages and time to it.

The mathematical principles of any quantum field theory are derived from those of nonrelativistic quantum mechanics of particles. That is, quantum field theory also relies on Hilbert spaces and operators acting on such spaces. However, some fundamental changes in previously presented formalism are needed to deal with states with a non-fixed number of particles, as imposed by the energy conservation of the relativity. A more formal construction of the fields from the particle point of view can be found in Reference [21].

Just like in the last chapter, we are not interested in constructing our theory from first principles. Rather, we aim only to present and justify some known results and constructions. Many other approaches to achieve the same results can be found in the literature [22–24].

Unless stated otherwise, in this section we use the metric with signature $(+, -, -, -)$, the natural system of units ($c = \hbar = k_B = 1$), and the Einstein summation convention. In general, Greek letters refer to space-time indices. Space-time functions are denoted solely by $f(x)$; we distinguish between space and time only when necessary.

3.1.1 Free Scalar Field

To start our construction, we choose the simplest case of a field theory: the neutral scalar field. The quantity that we generically refer to as a “field” is an operator-valued generalized function; we hope to clarify this throughout the section. Such a field is governed by the following Lagrangian density

$$L = \frac{1}{2} \partial^\mu \phi(x) \partial_\mu \phi(x) - \frac{1}{2} m^2 \phi(x)^2, \quad (3.1)$$

where m^2 is a spectral (mass) parameter. From this Lagrangian, we can apply the same steps as in Sec. 2 to derive both the equation of motion, known as the **Klein-Gordon equation**

$$\square\phi(x) + m^2\phi(x) = 0, \quad (3.2)$$

where $\square = \partial^\mu\partial_\mu$ is the d'Alembertian operator, and the Hamiltonian

$$H = \frac{1}{2}\pi^2(x) + \frac{1}{2}(\nabla\phi(x))^2 + \frac{1}{2}m^2\phi^2(x), \quad (3.3)$$

with $\pi(x) = \partial L/\partial\dot{\phi}(x)$, the conjugate momentum of the field variable $\phi(x)$. As can be directly verified, the Lagrangian, and therefore the equation of motion and the Hamiltonian, are all Poincaré invariant. That is, they are scalars under Poincaré transformations. It also follows that the Hamiltonian is an unbounded self-adjoint operator.

We can now proceed in two ways. We can analyze the equation of motion directly and then impose commutation relations on a more fundamental operator from which the fields can be constructed, or we can impose commutation relations directly on $\phi(x)$ and $\pi(x)$. The second approach is more natural, given the development in the previous chapter.

Let us assume now that $m^2 = 0$. Then the Hamiltonian of the neutral scalar field resembles the Hamiltonian of the harmonic oscillator of Eq. (2.142). For that reason, let us *impose* the following commutation relations in the same simultaneity surface ($t = t'$)

$$[\phi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = i\delta(\mathbf{x} - \mathbf{x}'), \quad [\phi(\mathbf{x}, t), \phi(\mathbf{x}', t)] = [\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = 0, \quad (3.4)$$

which, in analogy to Eq. (2.66), are referred to as the **canonical commutation relations**. The process of imposing commutation relations to fields is sometimes referred to as *second quantization*.

As we prove in Sec. A.2.2, every Hilbert space has an orthonormal basis (see theorem A.62). Therefore, we can expand each $\phi(x)$ and $\pi(x)$ in terms of the components of the orthonormal basis. Let us assume that

$$\phi(x) = \sum_n a_n \varphi_n(x), \quad \pi(x) = \sum_l a_l^\dagger \varphi_l(x), \quad (3.5)$$

By a direct computation using the fact that an orthonormal basis forms a complete set, we obtain

$$[a_n, a_l^\dagger] = \delta_{n,l}, \quad [a_n, a_l] = [a_n^\dagger, a_l^\dagger] = 0. \quad (3.6)$$

From here, we can define the number operator and analyze the spectrum of the Hamiltonian. However, before proceeding further, let us return to the equation of motion, Eq. (3.2). Inspired by the discussion on coordinate and momentum representations in the previous section, let us use the following Fourier representation of the field

$$\phi(x) = \frac{1}{(2\pi)^4} \int e^{ipx} \tilde{\phi}(p) d^4 p \quad (3.7)$$

where $px = p_0 t - \mathbf{x} \cdot \mathbf{p}$ is the Lorentzian product. Back to Eq. (3.2), we obtain that

$$p^2 + m^2 = 0 \Rightarrow p_0^2 = \sqrt{\mathbf{p}^2 + m^2} \quad (3.8)$$

which is the relativistic condition of energy conservation. Now if we perform only a spatial Fourier representation,

$$\phi(\mathbf{x}, t) = \frac{1}{(2\pi)^3} \int e^{i\mathbf{p} \cdot \mathbf{x}} \tilde{\phi}(\mathbf{p}, t) d^3 p, \quad (3.9)$$

we obtain the following equation of motion

$$\left(\frac{\partial^2}{\partial t^2} + (\mathbf{p}^2 + m^2) \right) \tilde{\phi}(\mathbf{p}, t) = 0, \quad (3.10)$$

which is a harmonic oscillator for each $\mathbf{p}$, with frequency $\omega_{\mathbf{p}}^2 = \mathbf{p}^2 + m^2$. We have already solved the case of a harmonic oscillator in the last section; therefore, we can identify that

$$\phi(\mathbf{x}, t) = \frac{1}{(2\pi)^3} \int \frac{1}{\sqrt{2\omega_{\mathbf{p}}}} \left[a(\mathbf{p}) e^{-ipx} + a^\dagger(\mathbf{p}) e^{ipx} \right] d^3 p = \phi_+(x) + \phi_-(x). \quad (3.11)$$

Where the integral arises from the fact that there are infinitely many momenta over which we sum. The contribution of ϕ_+ is called the *positive frequencies modes*, while ϕ_- is called *negative frequencies modes*. Now we turn to the conjugate momentum, $\pi(x)$, to write

$$\pi(\mathbf{x}, t) = -i \frac{1}{(2\pi)^3} \int \sqrt{\frac{\omega_{\mathbf{p}}}{2}} \left(a(\mathbf{p}) e^{ipx} - a^\dagger(\mathbf{p}) e^{-ipx} \right) d^3 p. \quad (3.12)$$

By imposing the canonical commutation relation of Eq. (3.4), we can verify that

$$[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = (2\pi)^3 \delta(\mathbf{p} - \mathbf{p}'), \quad [a(\mathbf{p}), a(\mathbf{p}')] = [a^\dagger(\mathbf{p}), a^\dagger(\mathbf{p}')] = 0. \quad (3.13)$$

Thus, the $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$ are the continuum limit of the a_n and $a_n^\dagger$ that we used as coefficients in the orthonormal basis expansion of our field, where the basis is

given by the exponential. Instead of investigating the action of the field operator itself, we can turn our attention to $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$.

If we wish to express the Hamiltonian operator in terms of the operators $a(\mathbf{p})$, $a^\dagger(\mathbf{p})$ we can substitute the expansions of $\phi(x)$ and $\pi(x)$ into Eq. (3.3) to obtain

$$H = \frac{1}{2} \int \frac{\omega_{\mathbf{p}}}{(2\pi)^3} [a(\mathbf{p})a^\dagger(\mathbf{p}) + a^\dagger(\mathbf{p})a(\mathbf{p})] d^3p = \frac{1}{2} \int \frac{\omega_{\mathbf{p}}}{(2\pi)^3} [a(\mathbf{p})a^\dagger(\mathbf{p}) + N_{\mathbf{p}}] d^3p, \quad (3.14)$$

where we have defined $N_{\mathbf{p}} = a^\dagger(\mathbf{p})a(\mathbf{p})$. Like in the quantum harmonic oscillator, we can define a vector Ω , which we call the vacuum, for which the operator $a(\mathbf{p})$ vanishes

$$a(\mathbf{p})\Omega = 0. \quad (3.15)$$

This might tempt us to proceed as in the harmonic oscillator; however, the scenario differs significantly. Note that, in the quantum harmonic oscillator, we describe a one-dimensional particle with distinct excitation states, labeled by n , and we interpret a and $a^\dagger$ as operators that, respectively, annihilate and create an excitation of the particle. In the quantum harmonic oscillator, we have constructed the Hilbert space $\mathcal{H} = \mathcal{L}^2$ for *one particle* using its excited states.

In the present description of fields, so far, we have no particles. Furthermore, because we require the number of particles to be not fixed, we cannot restrict the Hilbert space to that of one, two, or n particles. We must allow the number of particles to be indefinite and, for that, choose the Hilbert space wisely. To do that, let us take a few steps back. By construction, quantum fields are intrinsically noncommutative and probabilistic. Let us say that $\tilde{\phi}_1(j_1) \in \mathcal{L}^2$ represents one particle in the state j_1 , and $|\tilde{\phi}_1(j_1)|$ is the probability density for finding the particle in that state. Now, if we have a state of two particles, which we represent by $\tilde{\phi}_2(j_1, j_2)$, then by analogy, $\tilde{\phi}_2(j_1, j_2) \in \mathcal{L}^2 \otimes \mathcal{L}^2$ represents the probability of finding the *first* particle in the state j_1 and the *second* particle in the state j_2 . However, we know from quantum mechanics that particles of the same type (bosons or fermions) are indistinguishable; thus, we must have $|\tilde{\phi}_2(j_1, j_2)| = |\tilde{\phi}_2(j_2, j_1)|$ ¹, so the correct space for the two-particle system is not $\mathcal{L}^2 \otimes \mathcal{L}^2$, but the *symmetrized tensor product* $\mathcal{L}^2 \odot \mathcal{L}^2 = [\mathcal{L}^2]^{\odot 2}$. For fields that represent spinors (half-integer spins), we must have the *antisymmetrized tensor product* $\mathcal{L}^2 \wedge \mathcal{L}^2 = [\mathcal{L}^2]^{\wedge 2}$.

Since we expect our field operator to be able to generate states with any number of particles, and to be consistent with relativity, such an operator must act on a space that is a linear combination of states with varying particle numbers. Let us define $[\mathcal{L}^2]^{\odot 0} = \mathbb{C}$; then we write the **symmetric Fock space** as the

¹Here we use the fact that the scalar field behaves as a scalar under the Poincaré group, and therefore represents states of spin 0, which are bosons and have symmetric wave functions in quantum mechanics.

following

$$\mathcal{F} = \mathbb{C} \bigoplus_{n=1}^{\infty} [\mathcal{L}^2]^{\odot n} = \bigoplus_{n=0}^{\infty} [\mathcal{L}^2]^{\odot n}. \quad (3.16)$$

Analogously, one can define the **antisymmetric Fock space**. In this thesis, we are only interested in the symmetric case; therefore, we call it the Fock space. One should notice that the Fock space is a Hilbert space.

An element of the Fock space, Φ , is given by

$$\Phi = \{\tilde{\phi}_0, \tilde{\phi}_1(j_1), \dots, \tilde{\phi}_n(j_1, \dots, j_n), \dots\}, \quad (3.17)$$

where, for each $n = 1, 2, \dots$, we have $\tilde{\phi}_n \in [\mathcal{L}^2]^{\odot n}$. We remark that the quantity $\tilde{\phi}_n$ is not the field operator. Let us take the element Ω that we defined in Eq. (3.15). This element represents the state of no particles and, as an element of the Fock space, is represented by

$$\Omega = \{1, 0, 0, \dots\}, \quad (3.18)$$

and is called the **vacuum state**.

Since each $[\mathcal{L}^2]^{\odot n}$ is a Hilbert space, we can choose a basis for each of them and construct the basis of the Fock space. With this particle-oriented construction, we see that, in addition to the similarity with the harmonic oscillator, the operators $a(\mathbf{p})$ and $a^\dagger(\mathbf{p})$ serve as the operators of **annihilation** and **creation** of particles. Therefore, the action of $a^\dagger(\mathbf{p})$ is to create a particle in the state $\mathbf{p}^2$. As one can directly show, the state Ω is Poincaré invariant. Therefore, we have shown that the scalar field satisfies the following axioms

Axiom 3.1. (0th Wightman axiom – Relativistic quantum mechanics) The field's equations of motion are invariant under the Poincaré group. The energy-momentum spectrum is contained within the forward cone, and there is a unique state, called the vacuum state, which is invariant under the Poincaré group.

Axiom 3.2. (1th Wightman axiom – The domain of fields) There is a set of operators which, together with their adjoints, are defined on the Hilbert space containing the vacuum. The Hilbert space can be reconstructed by successive actions of these operators.

The set of operators is, evidently, $a(\mathbf{p}), a^\dagger(\mathbf{p})$.

Axiom 3.3. (2th Wightman axiom – Transformation law of the field) The fields are covariant under the Poincaré group and transform according to some representation of the Lorentz group.

Note that in our case, the field is a scalar under Lorentz transformations.

²We use the label $\mathbf{p}$ to represent any number that distinguishes one state from another.

Axiom 3.4. (3th Wightman axiom – Microscopic causality or microcausality) If the supports of two fields are space-like separated, then the fields either commute or anticommute.

The third Wightman axiom is the only one that we need to check. To do that, let us choose the normalization constant such that $a(\mathbf{p})\tilde{\phi}_n = \sqrt{n}\tilde{\phi}_{n-1}$ and $a^\dagger(\mathbf{p})\tilde{\phi}_n = \sqrt{n+1}\tilde{\phi}_{n+1}$, so $a^\dagger(\mathbf{p})\Omega = \tilde{\phi}_1$. Now we fix some simultaneity surface at t , then we have

$$\begin{aligned}\phi(x)\Omega &= \frac{1}{(2\pi)^3} \int \frac{1}{\sqrt{2\omega_{\mathbf{p}}}} [a(\mathbf{p})\Omega e^{-ipx} + a^\dagger(\mathbf{p})\Omega e^{ipx}] d^3 p \\ &= \frac{1}{(2\pi)^3} \int \frac{1}{\sqrt{2\omega_{\mathbf{p}}}} [a^\dagger(\mathbf{p})\Omega e^{ipx}] d^3 p\end{aligned}\quad (3.19)$$

$$\begin{aligned}(\phi(y))^*\Omega &= \frac{1}{(2\pi)^3} \int \frac{1}{\sqrt{2\omega_{\mathbf{p}}}} [a(\mathbf{p}')e^{-ip'y} + a^\dagger(\mathbf{p}')e^{ip'y}]^* \Omega d^3 p' \\ &= \frac{1}{(2\pi)^3} \int \frac{1}{\sqrt{2\omega_{\mathbf{p}}'}} [a^\dagger(\mathbf{p}')\Omega e^{-ip'y}] d^3 p'.\end{aligned}\quad (3.20)$$

Therefore, we can use the last two equations in conjunction with the commutation relation of Eq. (3.13)

$$\begin{aligned}(\phi(y)\phi(x)\Omega, \Omega) &= (\phi(x)\Omega, (\phi(y))^*\Omega) \equiv \langle \phi(y)\phi(x) \rangle \\ &= \frac{1}{(2\pi)^6} \int \frac{1}{\sqrt{4\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} [(a^\dagger(\mathbf{p})\Omega, a^\dagger(\mathbf{p}')\Omega)] e^{ipx-ip'y} d^3 p d^3 p' \\ &= \frac{1}{(2\pi)^6} \int \frac{1}{\sqrt{4\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} [(a(\mathbf{p}')a^\dagger(\mathbf{p})\Omega, \Omega)] e^{ipx-ip'y} d^3 p d^3 p' \\ &= \frac{1}{(2\pi)^3} \int \frac{1}{\sqrt{4\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} [(a(\mathbf{p}')a^\dagger(\mathbf{p})\Omega, \Omega) - (a^\dagger(\mathbf{p})a(\mathbf{p}')\Omega, \Omega)] e^{ipx-ip'y} d^3 p d^3 p' \\ &= \frac{1}{(2\pi)^6} \int \frac{1}{\sqrt{4\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} [([a(\mathbf{p}'), a^\dagger(\mathbf{p})]\Omega, \Omega)] e^{ipx-ip'y} d^3 p d^3 p' \\ &= \frac{(2\pi)^3}{(2\pi)^6} \int \frac{1}{\sqrt{4\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}} \delta(\mathbf{p} - \mathbf{p}') (\Omega, \Omega) e^{ipx-ip'y} d^3 p d^3 p' \\ &= \frac{1}{(2\pi)^3} \int \frac{1}{2\omega_{\mathbf{p}}} e^{ip(x-y)} d^3 p = \Delta_+(x, y)\end{aligned}\quad (3.21)$$

This expectation value is the correlation function of the field at two separated points; such a function is called the **Wightman positive frequency two-point function**. Using the analogous calculation, one shows that

$$\Delta_-(x, y) = \Delta_+(y, x) = \frac{1}{(2\pi)^3} \int \frac{1}{2\omega_{\mathbf{p}}} e^{-ip(x-y)} d^3 p, \quad (3.22)$$

which is called the **Wightman negative frequency two-point function**. As expected, such a function is Lorentz invariant. If we take a spacelike case, $(x - y)^2 < 0$, and fix $t = t'$, a direct calculation shows that

$$\Delta_+(x, y) = \frac{1}{(2\pi)^3} \int \frac{1}{2\omega_{\mathbf{p}}} e^{ip(x-y)} d^3 p = \frac{m}{4\pi^2 r} K_1(m, r) \rightarrow \sqrt{\frac{\pi m r}{2}} \frac{e^{-mr}}{4\pi^2 r^2} \quad \text{as } rm \gg 1, \quad (3.23)$$

where we have defined $r = |\mathbf{x} - \mathbf{y}|$, so the Wightman function goes to zero.

Now we can directly obtain the so-called **Pauli-Jordan function**

$$\begin{aligned} ([\phi(x), \phi(y)]\Omega, \Omega) &= \Delta_+(x, y) - \Delta_+(y, x) \\ &= -\frac{1}{(2\pi)^3} \int \frac{1}{\omega_{\mathbf{p}}} \sin[p(x - y)] d^3 p. \end{aligned} \quad (3.24)$$

It is straightforward to observe that for $x_0 = y_0$, the last integral vanishes. However, if we fix $(x - y)^2 < 0$, this quantity also vanishes. Therefore, we have found the **microcausality** condition of axiom 3.4. This is the basis of the free scalar field in axiomatic quantum field theory.

Before finishing our general discussion about the scalar field, let us connect the idea of the Green's function with the Wightman function. We know that the Green's function, $G(x, y)$, of an operator is the integral kernel of the inverse operator; therefore, for the Klein-Gordon equation (Eq. (3.2))

$$(\square + m^2)G(x, y) = \delta(x - y), \quad (3.25)$$

performing a Fourier transform³ over x we get

$$\begin{aligned} (p^2 + m^2)\tilde{G}(\omega, \mathbf{p}; y) &= e^{ipy} \\ G(x, y) = G(x - y) &= \frac{1}{(2\pi)^4} \int \frac{e^{-ip(x-y)}}{\omega^2 - p^2 + m^2} d\omega d^3 p, \end{aligned} \quad (3.26)$$

Thus, the Green's function has poles at $\omega = \pm\sqrt{p^2 + m^2} = \pm M$. Hence, we can choose how to contour the poles. This possibility leads to an ambiguity in defining the Green's function. Some of these choices are more common than others. Here we present some of them.

For $x_0 < y_0$ we can contour over the poles and close the curve on the lower-half plane; see Fig. 3.1a. In this case we have the *Retarded Green's function*, given by

$$G_{\text{ret}}(x, y) = \int \frac{1}{\omega_{\mathbf{p}}} \sin[\omega_{\mathbf{p}}(x_0 - y_0)] \theta(x_0 - y_0) d^3 \mathbf{p}. \quad (3.27)$$

³Some care must be taken here. As we discuss in Sec. A.4, the δ -function is not a function, it is an irregular generalized function. The same may be true for $G(x, y)$, depending on the operator. Therefore, the Fourier transform must be taken in the sense of generalized functions.

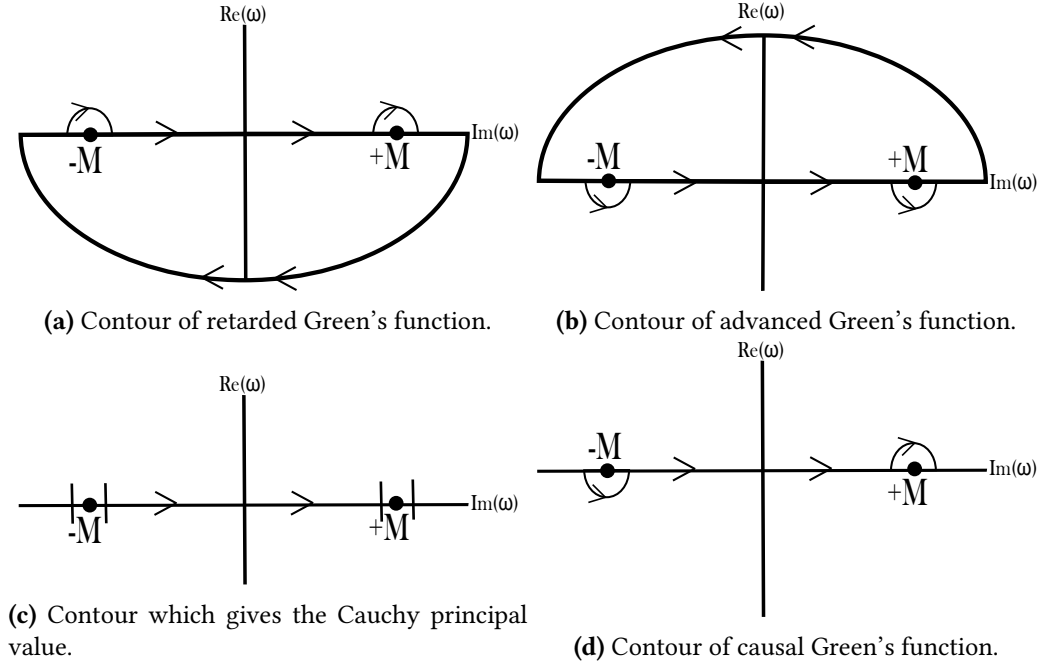


Figure 3.1: Different complex plane contours.

If $y_0 < x_0$ we can contour the poles from below and close the curve on the upper-half plane; see Fig. 3.1b. Thus, we have the *Advanced Green's function*, given by

$$G_{\text{adv}}(x, y) = - \int \frac{1}{\omega_{\mathbf{p}}} \sin [\omega_{\mathbf{p}}(x_0 - y_0)] \theta(y_0 - x_0) d^3 \mathbf{p}. \quad (3.28)$$

If we go right through the poles, see Fig. 3.1c, we must take the Cauchy principal values of each divergent integral; this gives us

$$\bar{G}(x, y) = \frac{1}{2} (G_{\text{ret}}(x, y) + G_{\text{adv}}). \quad (3.29)$$

Passing under the left pole but over the right one (see Fig. 3.1d), we obtain the *Causal (or Feynman) Green's function* given by

$$G_{\text{F}}(x, y) = i \int \frac{1}{2\omega_{\mathbf{p}}} e^{-ip(x-y)} d^4 p. \quad (3.30)$$

If we choose a contour that encloses only the right pole, we obtain the Wightman positive two-point function (see Eq. (3.21) and Fig. 3.2a). In contrast, a contour that encloses only the left pole yields the Wightman negative frequency two-point function (see Eq. (3.22) and Fig. 3.2b). We note that

$$G_{\text{F}}(x, y) = \theta(x^0 - y^0) \Delta_+(x, y) + \theta(y^0 - x^0) \Delta_-(x, y). \quad (3.31)$$

If we take the contour around both poles counterclockwise (see Fig. 3.2c), we obtain the commutator, that is, the Pauli-Jordan function given in Eq. (3.24).

Taking a clockwise contour around the left pole and a counterclockwise contour around the right pole (see Fig. 3.2d), we obtain the *Hadamard function*, given by

$$G^{(1)}(x, y) = -2i(G_F - \bar{G}) \quad (3.32)$$

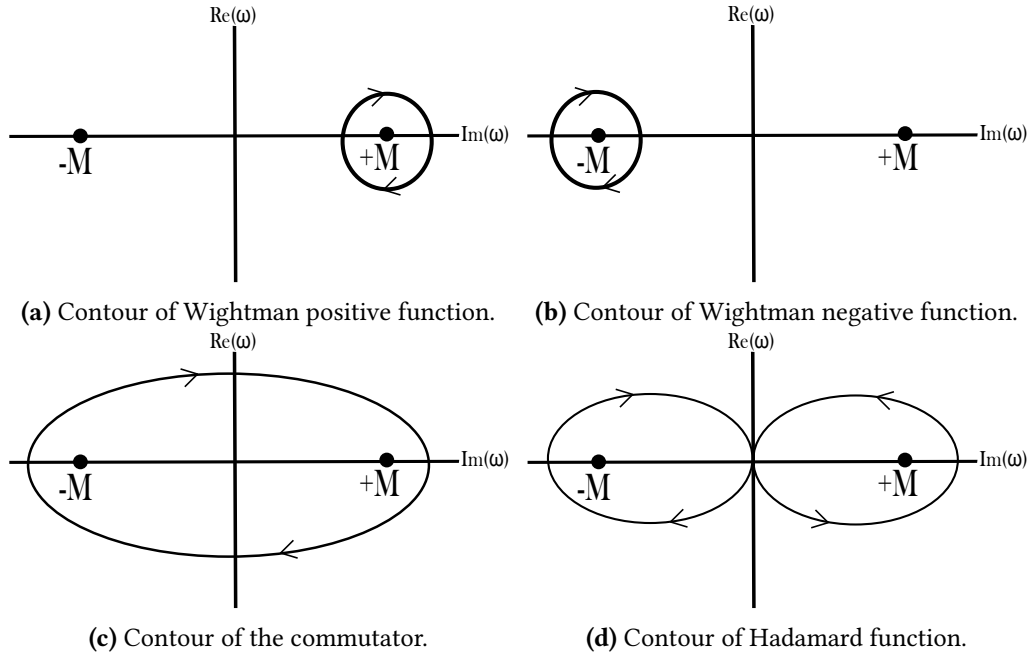


Figure 3.2: Different complex plane contours.

Naturally, all these Green's functions are solutions of the Klein-Gordon Equation (for $x \neq y$). To finish the discussion about the scalar field, we note that the support of the commutator is inside the light cone, while the support of the causal Green's function is the entire Minkowski spacetime.

3.1.2 Electromagnetic field

Vector fields are very similar to scalar fields, since both of them represent bosons. However, when we follow the quantization procedure described in the last section for vector fields, some peculiarities must be handled. Here we follow Ref. [25].

The Lagrangian density of classical electrodynamics is given by

$$L = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}, \quad (3.33)$$

where $F_{\mu\nu}$ is the electromagnetic field tensor given in terms of the four-potential A_μ by

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \quad (3.34)$$

If one tries to quantize the electromagnetic field using the procedure of the last section with this Lagrangian, one finds that the conjugate momentum of A_4 vanishes identically; thus, the method does not work.

So, instead of working with the original Lagrangian, we adopt the following Lagrangian density

$$L = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2}\partial^\mu A_\mu \partial^\nu A_\nu, \quad (3.35)$$

and impose the additional initial condition that, for some fixed time $x_0 = t$, we have

$$\partial^\mu A_\mu = \partial^0 (\partial^\nu A_\nu) = 0, \quad (3.36)$$

for all $\mathbf{x}$. Using this Lagrangian, we obtain the following equation of motion

$$\square (\partial^\nu A_\nu) = 0. \quad (3.37)$$

From the initial condition, we obtain that $\partial^\nu A_\nu$ must vanish for all times, which reflects the invariance under gauge transformations that arises when imposing Lorentz invariance on the equation of motion derived from Eq. (3.33); thus, the usual electromagnetism is recovered. Therefore, the equation of motion is the usual one, given by

$$\square A_\nu = 0. \quad (3.38)$$

We return to the problem of gauge invariance at the end of this section.

Proceeding with the Lagrangian of Eq. (3.35), we can construct the conjugate momenta

$$\pi_i(x) = iF_{0i} = \partial_0 A_i(x) - \partial_i A_0(x), \quad \pi_0 = i\partial_\nu A^\nu. \quad (3.39)$$

Now we impose the commutation relation at *equal times*

$$\begin{aligned} [\partial_0 A_\mu(\mathbf{x}, t), A_\nu(\mathbf{x}', t)] &= \delta_{\mu\nu} \delta(\mathbf{x} - \mathbf{x}'), \\ [A_\mu(\mathbf{x}, t), A_\nu(\mathbf{x}', t)] &= [\pi_\mu(\mathbf{x}, t), \pi_\nu(\mathbf{x}', t)] = 0. \end{aligned} \quad (3.40)$$

We wish to decompose the vector field A_μ on a basis in the Hilbert space, similarly to the procedure that led us to Eq. (3.11). We notice from the equation of motion (3.38) that each component behaves like a massless harmonic oscillator⁴. However, for each p we have four possible directions; therefore, it is convenient

⁴Recall that we require the equation of motion to be Lorentz invariant (axiom 3.1). Therefore, the vector A_μ transforms as a vector, and its components do not necessarily transform as scalars by themselves.

to introduce an orthonormal basis for each possible direction of the vector p . Let us denote this basis by $e_\mu^{(\lambda)}$, where $\lambda = 0, 1, 2, 3$, and refer to $e_\mu^{(\lambda)}$ as *polarization vectors*. The vector $e_\mu^{(\lambda)}$ satisfies the following conditions

$$\begin{cases} e_0^{(\lambda)} = e_i^{(0)} = e_\mu^{(0)} = 0, \\ e_i^{(1)} k^i = e_i^{(2)} k^i = 0, \\ e_i^{(3)} = \frac{k_i}{\omega}, \\ e_0^{(0)} = 1, \end{cases} \quad (3.41)$$

$$e_\mu^{(\lambda)} e_\mu^{(\lambda')} = \delta_{\lambda\lambda'}. \quad (3.42)$$

This choice justifies calling the polarizations associated with $\lambda = 1, 2$ the **transverse polarizations**, the polarization corresponding to $\lambda = 3$ the **longitudinal polarization**, and that corresponding to $\lambda = 0$ the **scalar polarization**. It also follows directly that $\sum_\lambda e_\mu^{(\lambda)} e_\nu^{(\lambda')} = \delta_{\mu\nu}$. Within such a picture, the most general solution of the equation of motion is given by

$$A_\mu(x) = \frac{1}{(2\pi)^3} \int \sum_{\lambda=0}^3 \frac{e_\mu^{(\lambda)}}{\sqrt{2\omega}} \left[a^{(\lambda)}(\mathbf{p}) e^{-ipx} + a^{(\lambda)\dagger}(\mathbf{p}) e^{ipx} \right] d^3 p = A_\mu^+(x) + A_\mu^-(x). \quad (3.43)$$

Directly from this expansion and the commutation relation given in Eq. (3.40) (at equal times), it follows that

$$[a^{(\lambda)}(\mathbf{p}), a^{(\lambda')\dagger}(\mathbf{p}')] = \delta_{\lambda\lambda'} \delta_{\mathbf{p}\mathbf{p}'}. \quad (3.44)$$

From this, we can assume the second part of axiom 3.1 to define the vacuum Ω and, by an analysis similar to that for the scalar field and the quantum harmonic oscillator, we can define the Fock space of the system and interpret the action of $a^{(l)}(\mathbf{p})$ and $a^{(l)\dagger}(\mathbf{p})$ as the **annihilation** and **creation** of a photon with polarization $l = 1, 2, 3$ and momentum $\mathbf{p}$. It also follows that the vacuum state is a cyclic vector for $a^\dagger$. However, now the scalar polarization introduces some differences. For example, the creation operator is $a^{(0)}(\mathbf{p})$ while the annihilation operator is $a^{(0)\dagger}(\mathbf{p})$. This occurs because the operators of the scalar polarization are anti-self-adjoint⁵.

Now, if we compute the Hamiltonian density associated with the Lagrangian in Eq. (3.35) and use the expansion of A_μ , we obtain

$$H = \frac{1}{2} \int \omega \sum_{\lambda=0}^3 \left[a^{(\lambda)}(\mathbf{p}) a^{(\lambda)\dagger}(\mathbf{p}) + a^{(\lambda)\dagger}(\mathbf{p}) a^{(\lambda)}(\mathbf{p}) \right] d^3 p. \quad (3.45)$$

⁵ A is anti-self-adjoint if $A^* = -A$.

Also, we can now compute the commutation relation for arbitrary times. Straight from the expansion of A_μ , we get

$$[A_\mu(x), A_\nu(x')] = \frac{\delta_{\mu\nu}}{(2\pi)^3} \int \frac{1}{\omega} \sin[p(x - y)] d^3 p, \quad (3.46)$$

which is just the Pauli-Jordan function with an additional Kronecker δ . Therefore, the microcausality condition is satisfied. Actually, to be historically precise, the first quantization of a field is the quantization of the electromagnetic field by M. Born, W. Heisenberg, and P. Jordan in Ref. [26], which follows the ideas developed some months earlier by M. Born and P. Jordan in Ref. [27]. This last equation was first obtained in the electromagnetic case, and Wightman used it to propose the third axiom (axiom 3.4).

As in the scalar case, the commutator is a solution of the equation of motion and also serves as a Green's function. In fact, all the previous contours of the complex plane that we presented in Fig. 3.1 and Fig. 3.2 can be discussed here by setting $m^2 = 0$.

Let us suppose that we have a system with only scalar polarization. Considering that the respective creation and annihilation operators are anti-self-adjoint, we have that for a system with n “scalar” photons the relation

$$a^{(0)\dagger} a^{(0)} \tilde{\phi}^{(n)} = -n \tilde{\phi}^{(n)}, \quad (3.47)$$

holds, and the Hamiltonian of such a system will have negative energy contributions (see Eq. (3.45)); therefore, we must eliminate such scalar-polarized photons.

Up to now, we have ignored the condition that ensures the theory is gauge invariant; that is, we have ignored that the correct equations of motion (Maxwell's equations) follow from the Lagrangian given in Eq. (3.35) only if we ensure that $\partial_\mu A^\mu = 0$. In order to do that, we first change the representation of the creation and annihilation operators for the scalar polarization to ensure that they are self-adjoint and behave as the other operators,⁶

$$\left(a^{(0)\dagger} \tilde{\phi}_n^{(0)}, \tilde{\phi}_n^{(0)} \right) = \left(\tilde{\phi}_n^{(0)}, a^{(0)} \tilde{\phi}_n^{(0)} \right) = \sqrt{n+1}, \quad (3.48)$$

This ensures that A_μ is a self-adjoint operator; however, it contradicts the reality requirements for the classical electromagnetic potentials. Through direct calculation, one can check that it leads to states with negative norm, which is not a desirable property in any mathematical or physical theory. But this leads us to a clue about what is happening. If we have some undesirable states, it may happen

⁶Remember that $\tilde{\phi}_n^{(0)}$ stands for an element of the respective Fock space, which can be interpreted as “ n photons with scalar polarization”.

that the induced norm is not appropriate. Let us take any ψ in the Fock space; now we define the norm of ψ by

$$\|\psi\|_\eta = (\eta\psi, \psi), \quad (3.49)$$

where η is some unitary self-adjoint operator. Now the expectation value of any operator will be given by

$$\langle F \rangle_\eta = (\eta F \psi, \psi). \quad (3.50)$$

Within this definition, a self-adjoint operator may have a non-real expectation value. Of course, even within this norm, we impose that any physical state has a positive norm.

Computing the expectation value of A_μ , one immediately finds that

$$[A_i(x), \eta] = 0, \quad (3.51)$$

$$\{A_0(x), \eta\} = 0. \quad (3.52)$$

Alternatively, using the expansion of A_μ given in Eq. (3.43), we obtain

$$[a^{(i)}(\mathbf{p}), \eta] = 0, \quad (3.53)$$

$$\{a^{(0)}(\mathbf{p}), \eta\} = 0. \quad (3.54)$$

Now we notice that the condition $\partial^\nu A_\nu$ does not need to be satisfied as an operator equation; we require only that its expectation value vanishes, that is $\langle \partial^\nu A_\nu \rangle_\eta = 0$. Therefore, we can rewrite this condition as

$$\partial^\nu A_\nu^-(x)\psi = 0, \quad \text{and} \quad (\partial^\nu A_\nu^+(x)\eta)\psi = 0, \quad (3.55)$$

$$\text{or} \quad [a^{(3)}(\mathbf{p}) + ia^{(0)}(\mathbf{p})]\psi = 0 \quad (3.56)$$

and it follows that

$$(\eta \partial^\nu A_\nu(x)\psi, \psi) = (\psi, (\partial^\nu A_\nu^+(x)\eta)\psi) + (\eta \partial^\nu A_\nu^-(x)\psi, \psi) = 0. \quad (3.57)$$

Thus, our connection with the classical theory is ensured by any state that satisfies Eq. (3.56). Let us construct a general state given by

$$\psi = \psi_T \prod_{\mathbf{p}} \Phi_{\mathbf{p}}, \quad (3.58)$$

such that on ψ_T only the operators related to the transverse polarization act, and on $\Phi_{\mathbf{p}} = \Phi^{(0)} + \sum_r c_r(\mathbf{p}) \Phi^{(r)}(\mathbf{p})$ the operators of the longitudinal and scalar polarizations act. On each $\Phi^{(n)}$, $a^{(3)}$ and $a^{(0)}$ act as usual; that is,

$$a^{(3)}\Phi^{(n)} = \sqrt{n} \Phi^{(n-1)} \quad \text{and} \quad a^{(0)}\Phi^{(n)} = i\sqrt{n} \Phi^{(n-1)}. \quad (3.59)$$

Let us choose the quantities $\Phi^{(n)}$ to be orthogonal in the inner product induced by η and with norm

$$\|\Phi^{(n)}\|_\eta = \delta_{n0}. \quad (3.60)$$

If we assume that there are no transverse photons, we obtain

$$\begin{aligned} \langle A_\mu \rangle_\eta = \frac{1}{(2\pi)^3} \int \frac{1}{2\omega} \left\{ e^{ipx} \left[e_\mu^{(3)}(\eta a^{(3)}(\mathbf{p})\Phi_{\mathbf{p}}, \Phi_{\mathbf{p}}) + e_\mu^{(0)}(\eta a^{(0)}(\mathbf{p})\Phi_{\mathbf{p}}, \Phi_{\mathbf{p}}) \right] \right. \\ \left. + e^{-ipx} \left[e_\mu^{(3)}(\eta a^{(0)\dagger}(\mathbf{p})\Phi_{\mathbf{p}}, \Phi_{\mathbf{p}}) + e_\mu^{(4)}(\eta a^{(0)\dagger}(\mathbf{p})\Phi_{\mathbf{p}}, \Phi_{\mathbf{p}}) \right] \right\} d^3 p, \end{aligned} \quad (3.61)$$

and using the action of the annihilation operators, we get

$$\langle A_\mu \rangle_\eta = \partial_\mu \Lambda(\mathbf{x}), \quad (3.62)$$

where

$$\Lambda(\mathbf{x}) = \frac{1}{(2\pi)^3} \int \frac{1}{2\omega^3} \left[c^{*(1)}(\mathbf{p})e^{ipx} - c^{(1)}(\mathbf{p})e^{-ipx} \right] d^3 p. \quad (3.63)$$

Therefore, the gauge condition $\partial_\mu \Lambda(\mathbf{x}) = 0$ ensures the connection with the classical equation of motion.

Within this scenario, we can compute the expectation value of the Hamiltonian in a state with only scalar and transverse photons; it will be given by

$$\langle H \rangle_\eta = \int \omega \left[a^{(1)}(\mathbf{p})a^{(1)\dagger}(\mathbf{p}) + N^{(1)}(\mathbf{p}) + a^{(2)}(\mathbf{p})a^{(2)\dagger}(\mathbf{p}) + N^{(2)}(\mathbf{p}) \right] d^3 p, \quad (3.64)$$

where $N^{(1)}(\mathbf{p})$ and $N^{(2)}(\mathbf{p})$ are the number operators of the transverse polarizations. Therefore, in practice, the last procedure uses the longitudinal polarization to cancel out the scalar polarization. Thus, such polarizations do not contribute. This procedure is known in the literature as the Gupta-Bleuler approach [28, 29].

As we have seen, the scalar and the electromagnetic fields have many similarities. Most of the applications in this thesis are developed in terms of the scalar field, but some of them can be extended to the electromagnetic case. The next section is one of these cases; we are going to explore the simplest observable feature of quantum fields in both the scalar and electromagnetic cases.

3.2 Zero-Point Energy

Let's compute the expectation value of the Hamiltonian of Eq. (3.14) in the vacuum state

$$\begin{aligned} \langle H \rangle = (H\Omega, \Omega) &= \frac{1}{2} \int \frac{\omega_{\mathbf{p}}}{(2\pi)^3} \left[(a(\mathbf{p})a^\dagger(\mathbf{p})\Omega, \Omega) + (N_{\mathbf{p}}\Omega, \Omega) \right] d^3 p \\ &= \frac{1}{2} \int \frac{\omega_{\mathbf{p}}}{(2\pi)^3} d^3 p = \frac{1}{2} \int \frac{p^2}{(2\pi)^3} d^3 p, \end{aligned} \quad (3.65)$$

Performing a change of variables to a spherical coordinate system, we have that $d^3p = 4\pi r^2 dr$, where $r = \|\mathbf{p}\| = \sqrt{\mathbf{p} \cdot \mathbf{p}}$, so it follows that

$$\langle H \rangle = \frac{1}{(2\pi)^2} \int_0^\infty r^3 dr \rightarrow \infty. \quad (3.66)$$

Of course, the physical interpretation of a divergent quantity must be taken with some care. We can see directly from the previous equations that such a problem arises from the contribution of $a(\mathbf{p})a^\dagger$ in the Hamiltonian. A simple way to solve that is to consider that only differences of energy are measurable and then subtract $a(\mathbf{p})a^\dagger$ from the Hamiltonian so that the expected value of the energy in the vacuum becomes zero. However, one may also suspect that such a divergence appears because we have not used any boundary condition to obtain the field expansion Eq. (3.11), and therefore, the differential equation is ill-posed.

As we have seen from the application of the spectral theorem (see theorem 2.9), the energy of the system can be obtained from its eigenvalues. Since the Hamiltonian (3.14) and the Klein-Gordon equation (Eq. (3.2)) describe the same system, let us analyze the massless Klein-Gordon equation

$$\square\phi(x) = 0, \quad (3.67)$$

and in order for the differential equation to be well-posed, we need to impose some boundary conditions on the fields. Let's say that we have the field between two plates, one located at $x = 0$ and another at $x = L$; for simplicity, let's take the system in one spatial dimension with Dirichlet boundary conditions, that is, $\phi(0) = \phi(L) = 0$. With these boundary conditions, the momentum is now a discrete variable given by

$$\mathbf{p} = \frac{n\pi}{L} \hat{x}, \quad n = 1, 2, \dots \quad (3.68)$$

With this new set of momenta, the energy of the system per unit area between the plates is given by

$$E(L) = \frac{1}{2} \sum_{n=1}^{\infty} \frac{n\pi}{L}, \quad (3.69)$$

which remains a divergent quantity. But, as we prove in Sec. A.4, this kind of divergence can be regularized in the context of generalized functions. Let us

choose the test function as $e^{-\lambda n\pi/L}$ where $n \in \mathbb{N} \setminus \{0\}$, so we have

$$\begin{aligned}
 \left(\frac{n\pi}{2L}, e^{-\lambda n\pi/L}\right) &= \int \frac{n\pi}{2L} e^{-\lambda n\pi/L} dn = \frac{\pi}{2L} \sum_{n=1}^{\infty} n e^{-\lambda n\pi/L} \\
 &= -\frac{1}{2} \frac{\partial}{\partial \lambda} \sum_{n=1}^{\infty} e^{-\lambda n\pi/L} \\
 &= -\frac{1}{2} \frac{\partial}{\partial \lambda} \frac{1}{1 - e^{-\lambda\pi/L}} \\
 &= \frac{\pi}{2L} \frac{e^{-\lambda\pi/L}}{(e^{-\lambda\pi/L} - 1)^2} = E(L, \lambda),
 \end{aligned} \tag{3.70}$$

Expanding it into a power series, we can write the first two terms as

$$E(L, \lambda) = \frac{L}{2\pi\lambda^2} - \frac{\pi}{24L}. \tag{3.71}$$

Now, if we compute in a similar way the vacuum energy outside the two plates, we get

$$E(x - L, \lambda) = \frac{x - L}{2\pi\lambda^2} - \frac{\pi}{24(x - L)}, \tag{3.72}$$

Then, the total energy is given by

$$E_C = E(L, \lambda) + E(x - L, \lambda) = \frac{x}{2\pi\lambda^2} - \frac{\pi}{24} \left(\frac{1}{L} + \frac{1}{x - L} \right), \tag{3.73}$$

and the force between the plates is given by

$$F_C = -\frac{d}{dL} E_C = -\frac{\pi}{24L^2} + O(\lambda, x^{-1}), \tag{3.74}$$

Therefore, in the limit $\lambda \rightarrow 0$ and $x \rightarrow \infty$, the force between the plates is finite. With a similar calculation, in 1948 Casimir in Ref. [30] showed that there is a measurable quantum field effect associated solely with the vacuum. In fact, the existence of this force has been experimentally verified in many ways over the years; see Refs. [31–33]. This effect has been called the **Casimir effect**.

3.2.1 Casimir effect

As we have explicitly shown, the last procedure is able to recover a finite force, but not a finite energy. Can we use some mathematical method to obtain the

energy as a finite quantity? To do that, let us take Eq. (3.69) and introduce a parameter s as follows

$$E(L; s) = \frac{\pi}{2L} \sum_{n=1}^{\infty} \frac{1}{n^s}, \quad (3.75)$$

noting that we recover the previous equation if $s = -1$; however, the series converges only if $\Re(s) > 0$. Now, we notice that using a Mellin transform, $\frac{1}{n^s}$ can be represented as

$$\frac{1}{n^s} = \frac{\pi^{s/2}}{\Gamma\left(\frac{s}{2}\right)} \int_0^{\infty} x^{\frac{s}{2}-1} e^{-n^2 \pi x} dx, \quad (3.76)$$

where $\Gamma(z)$ is the Gamma function. Therefore, we have that

$$E(L; s) = \frac{\pi^{\frac{s}{2}+1}}{2L\Gamma\left(\frac{s}{2}\right)} \int_0^{\infty} x^{\frac{s}{2}-1} \sum_{n=1}^{\infty} e^{-n^2 \pi x} dx. \quad (3.77)$$

Let us analyze the last series by denoting

$$\psi(x) = \sum_{n=1}^{\infty} e^{-n^2 \pi x}. \quad (3.78)$$

Using the Poisson summation formula (see Ref. [34]), one can prove that

$$\Theta(x) = \sum_{n=-\infty}^{\infty} e^{-\pi n^2 x} = \frac{1}{\sqrt{x}} \sum_{n=-\infty}^{\infty} e^{-\pi n^2 / x} = \frac{1}{\sqrt{x}} \Theta\left(\frac{1}{x}\right), \quad (3.79)$$

so the Θ function is a modular function of weight $1/2$. It follows directly that

$$\Theta(x) = 2\psi(x) + 1 = \frac{1}{\sqrt{x}} \left(2\psi\left(\frac{1}{x}\right) + 1 \right). \quad (3.80)$$

If we use this in Eq. (3.77), we obtain

$$\begin{aligned}
E(L; s) &= \frac{\pi^{\frac{s}{2}+1}}{2L\Gamma\left(\frac{s}{2}\right)} \int_0^\infty x^{\frac{s}{2}-1} \psi(x) dx \\
&= \frac{\pi^{\frac{s}{2}+1}}{2L\Gamma\left(\frac{s}{2}\right)} \left[\int_0^1 x^{\frac{s}{2}-1} \psi(x) dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x) dx \right] \\
&= \frac{\pi^{\frac{s}{2}+1}}{2L\Gamma\left(\frac{s}{2}\right)} \left\{ \int_0^1 x^{\frac{s}{2}-1} \left[\frac{1}{\sqrt{x}} \psi\left(\frac{1}{x}\right) + \frac{1}{2\sqrt{x}} - \frac{1}{2} \right] dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x) dx \right\} \\
&= \frac{\pi^{\frac{s}{2}+1}}{2L\Gamma\left(\frac{s}{2}\right)} \left[\frac{1}{s-1} - \frac{1}{s} + \int_0^1 x^{\frac{s}{2}-\frac{3}{2}} \psi\left(\frac{1}{x}\right) dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x) dx \right] \\
&= \frac{\pi^{\frac{s}{2}+1}}{2L\Gamma\left(\frac{s}{2}\right)} \left[\frac{1}{s(s-1)} + \int_1^\infty \left(x^{-\frac{s}{2}-\frac{1}{2}} + x^{\frac{s}{2}-1} \right) \psi(x) dx \right], \tag{3.81}
\end{aligned}$$

which converges for all $\Re(s) \neq 1$. For easier recognition, let us write

$$\sum_{n=1}^{\infty} \frac{1}{n^s} = \zeta(s), \tag{3.82}$$

so the last procedure gives us

$$\zeta(s) = \frac{\pi^{s-\frac{1}{2}}}{\Gamma\left(\frac{s}{2}\right)} \Gamma\left(\frac{1-s}{2}\right) \zeta(1-s), \tag{3.83}$$

or

$$\zeta(s) = \vartheta(s) \zeta(1-s), \tag{3.84}$$

where we define

$$\vartheta(s) = \frac{\pi^{s-\frac{1}{2}}}{\Gamma\left(\frac{s}{2}\right)} \Gamma\left(\frac{1-s}{2}\right). \tag{3.85}$$

Equation (3.83), or equivalently Eq. (3.84), is known as the **reflection formula** (or functional equation) for the ζ -function, and $\zeta(s)$ is known as the **Riemann zeta function**, obtained by B. Riemann in 1859 (see Ref. [35]).

Back to the expression for the energy, in the new notation we have that

$$E(L; s) = \frac{\pi}{2L} \zeta(s) = \frac{\pi^{s+\frac{1}{2}}}{2L\Gamma\left(\frac{s}{2}\right)} \Gamma\left(\frac{1-s}{2}\right) \zeta(1-s), \tag{3.86}$$

and the Casimir energy follows for $s = -1$; therefore,

$$E_C = \frac{\pi}{2L} \zeta(-1) = -\frac{\pi}{24L}, \quad (3.87)$$

which recovers the force given by Eq. (3.74). The last procedure shows that using analytical continuation we can recover the Casimir force when we have Dirichlet boundary conditions. In fact, this is just an application of a more general theory of the Laplacian with Dirichlet boundary conditions, which allows us to renormalize zero-point energies. Let us now briefly discuss these properties, following the Ref.[36].

Consider the eigenfunctions and eigenvalues of the negative Laplacian operator $(-\Delta)$ on a bounded (open connected) domain D in Euclidean space $\mathbb{R}^d$. The eigenvalues form a countable sequence. Using λ_k for $k = 1, 2, \dots$, they are ordered as

$$0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_k \leq \dots \quad (3.88)$$

when $k \rightarrow \infty$, with possible multiplicities. The eigenfunctions $\{\phi_k\}_{k=1}^\infty$ form a basis in $\mathcal{L}^2(D)$ with the boundary conditions. For simplicity, let us assume the Dirichlet boundary conditions. Each ϕ_k has eigenvalue $\lambda_k(-\Delta) \equiv \lambda_k$.

In spectral theory, the asymptotic behaviour of the Dirichlet Laplacian eigenvalues in the analytic regularization procedure plays a fundamental role. This behavior was first investigated by Weyl [37]. Applying the Fredholm-Hilbert formalism of linear integral equations, it was proved that for $D \subset \mathbb{R}^d$, ($d = 2, 3$)

$$\lim_{k \rightarrow \infty} \frac{k}{\lambda_k} = \frac{\text{Vol}_d(D)}{4\pi}, \quad (3.89)$$

where $\text{Vol}_d(D)$ is the volume of the region D .

We begin our discussion by defining the density of eigenvalues as a sum of delta functions:

$$g(\lambda) = \sum_k \delta(\lambda - \lambda_k), \quad (3.90)$$

and the counting function $N(\lambda) := \#\{\lambda_m : \lambda_m < \lambda\}$, defined as

$$N(\lambda) = \int_0^\lambda g(\lambda') d\lambda', \quad (3.91)$$

which gives the number of elements in the sequence of eigenvalues that are smaller than λ . The asymptotic behavior of the counting function is given by

$$N(\lambda) = f(d) \mu_d(\Omega) \lambda^{\frac{d}{2}}, \quad (\lambda \rightarrow \infty), \quad (3.92)$$

where $f(d)$ is an entire function of d . Furthermore, the additional asymptotic terms also provide information about the boundary of the domain. For example, for $D \subset \mathbb{R}^3$, we obtain a contribution proportional to the surface area of D .

Our first observation concerns the renormalization of the zero-point energy. Let us define the Minakshisundaram-Pleijel bilocal zeta-function $\mathcal{Z}(x, y; s)$ for $s \in \mathbb{C}$ as

$$\mathcal{Z}(x, y; s) = \sum_{k=1}^{\infty} \frac{\phi_k(x)\phi_k(y)}{\lambda_k^s}, \quad (3.93)$$

which converges uniformly in x and y for $\Re(s) > s_0$ and was originally defined in a connected compact Riemannian manifold [38]. From this bilocal zeta-function, it is possible to define a spectral zeta-function associated with the eigenvalues of the Laplacian in $D \subset \mathbb{R}^d$. We define $Z(s) = \text{Tr}(-\Delta)^{-s}$, where

$$Z(s) = \sum_{k=1}^{\infty} \lambda_k^{-s} = \lim_{m \rightarrow \infty} \sum_{k=1}^m \lambda_k^{-s}. \quad (3.94)$$

Using the counting function $N(\lambda)$ and the definition of the Riemann-Stieltjes integral, we obtain

$$\sum_{n=1}^m \lambda_n^{-s} = \sum_{n=1}^{k-1} \lambda_n^{-s} + \int_a^b t^{-s} dN(t); \quad (3.95)$$

$$\lambda_{k-1} \leq a < \lambda_k, \quad \lambda_m \leq b < \lambda_{m+1}.$$

Thus, the spectral zeta-function can be expressed as

$$Z(s) = \sum_{n=1}^{k-1} \lambda_n^{-s} + \int_{\lambda_k}^{\infty} N(t)t^{-s} dt. \quad (3.96)$$

In principle, this formula is valid in the region of the complex plane where the original sum converges. As the sum on the right-hand side is analytic over the entire complex s -plane, the qualitative behavior of its analytic continuation is determined by the Riemann-Stieltjes integral expressed in terms of Weyl's counting function.

To determine the polar structure of the spectral zeta-function, let us consider an evolution equation in $\mathcal{L}^2(D)$, formulated as the following initial-boundary problem in $(0, \infty) \times D$. For $D \subset \mathbb{R}^d$, we have

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u, \\ u(0, x) = f(x), \\ u(t, x)|_{x \in \partial D} = 0. \end{cases} \quad (3.97)$$

The weak solution $u(t, x)$, which satisfies the diffusion equation in the sense of generalized functions, is given by

$$u(t, x) = \int p_D(t, x, y) f(y) d\mu(y), \quad (3.98)$$

where $d\mu(y)$ is the volume element of the domain, and $p_D(t, x, y)$ is the diffusion kernel, i.e., the positive fundamental solution to the heat equation. For a generic boundary condition, the spectral decomposition of the diffusion kernel can be represented as

$$p_D(t, x, y) = \sum_{k=1}^{\infty} e^{-t\lambda_k} \phi_k(x) \phi_k(y). \quad (3.99)$$

Using a Mellin transform and the definition of the Minakshisundaram-Pleijel zeta-function $\mathcal{Z}(x, y; s)$, we obtain

$$\Gamma(s) \mathcal{Z}(x, y; s) = \int_0^{\infty} t^{s-1} p_D(t, x, y) dt. \quad (3.100)$$

For $x \neq y$, $\Gamma(s) \mathcal{Z}(x, y; s)$ is a regular function of s in the entire complex plane. For $x = y$, there is a pole at $s = 1$. Since we are interested in global issues, let us define the trace of the diffusion kernel, written as $\Theta(t) = \text{Tr}(e^{t\Delta})$, where, using the Riemann-Stieltjes integral, we can write

$$\Theta(t) = \int_0^{\infty} e^{-\lambda t} dN(\lambda) = \sum_{k=1}^{\infty} e^{-\lambda_k t}, \quad t > 0. \quad (3.101)$$

The spectral zeta-function can be represented as

$$Z(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} t^{s-1} \Theta(t) dt. \quad (3.102)$$

Its polar structure in the extended complex plane is determined by the classical spectral invariants, which are the expansion coefficients at $t \rightarrow 0^+$ of the diffusion kernel trace.

When $\partial D \neq \emptyset$, the coefficients of the asymptotic expansion of the heat trace have been calculated for a variety of boundary conditions:

$$\lim_{t \rightarrow 0^+} \Theta(t) = (4\pi t)^{-\frac{d}{2}} \left[\sum_{p=0}^K c_p(D) t^{\frac{p}{2}} + o(t^{\frac{K+1}{2}}) \right], \quad (3.103)$$

where the coefficients $c_p(D)$ are related to the geometric characteristics of the bounded domain. Useful information on the heat kernel coefficients in mathematical and physical literature can be found in Ref. [39–41]. By a Tauberian

theorem, we are able to connect the first term of the above asymptotic expansion with Weyl's asymptotic behavior of the Laplace operator spectrum.

For the case of vacuum energy, Fulling has stressed the need to study the cylinder kernel [42, 43]. See, for example, [44]. To implement this idea, let us define the zeta-function $\zeta_{\sqrt{A}}(s)$ constructed with the energies ω_k of each normal mode:

$$\zeta_{\sqrt{A}}(s) = \sum_{k=1}^{\infty} \frac{1}{\omega_k^s}, \quad \Re(s) > s_1. \quad (3.104)$$

The renormalized vacuum energy is defined as $\langle E \rangle_r = \zeta_{\sqrt{A}}(s)|_{s=-1}$. Using a Mellin transform again, we obtain

$$\sum_{k=1}^{\infty} \frac{1}{\omega_k^s} = \frac{1}{\Gamma(\frac{s}{2})} \int_0^{\infty} t^{\frac{s}{2}-1} \sum_{k=1}^{\infty} e^{-\omega_k^2 t} dt. \quad (3.105)$$

The zeta-function $\zeta_{\sqrt{A}}(s)$ is a meromorphic function of s with simple poles. In the case where $s = -1$ is a pole, we can obtain a representation in a neighborhood of the pole, including some regular part known as the renormalized vacuum energy. We emphasize that the measurable Casimir energy is obtained from this mathematical formalism based on analytic continuation, where undesirable polar contributions must be removed through a renormalization procedure, as we have shown in Eq. (3.87). A straightforward calculation shows that the Casimir energy for the slab geometry in d dimensions ($\mathbb{R}^{d-1} \times [0, L]$) gives us the Casimir energy per unit of hyperarea of the surfaces:

$$\epsilon_d(L) = -\frac{\pi^{\frac{d}{2}} \Gamma(-\frac{d}{2})}{2(2L)^d} \zeta(-d). \quad (3.106)$$

At this point, it is clear that the Casimir energy depends on the geometry of the manifold. Different geometries have been considered in the literature; see, e.g., Ref. [45].

Now, let us obtain the Casimir energy for the electromagnetic field inside a perfect d -dimensional waveguide with sides a, b , with the same procedure of Ref. [46]. That is, our manifold is $\mathbb{R}^{d-2} \times [0, a] \times [0, b]$. Now we recast the speed of light, c , and the reduced Planck constant, $\hbar$. In a future application where we use this result, it will be useful to have c and $\hbar$ explicitly in the result. Using the equation of motion (Eq. (3.38)) and the spectral theorem, we have the energy denoted by $E_d(L_1, L_2, \dots, L_{d-2}, a, b)$, given by the Riemann-Stieltjes integral of the spectral measure of the Hamiltonian operator in such a domain. Assuming that $L_i \gg a, b$ for all $i = 1, \dots, d-2$, one can write this quantity as

$$E_d(L_1, \dots, L_{d-2}, a, b) = \frac{A_{d-2}}{(2\pi)^{d-2}} \int \sum_{m,n=1}^{\infty} \hbar \omega_{mn}(q) d^{d-2}q \quad (3.107)$$

where we have used the following definition of the hyper-area

$$A_{d-2} = \prod_{i=1}^{d-2} L_i, \quad (3.108)$$

with the frequencies given by

$$\omega_{mn}(q) = c \sqrt{q^2 + \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2}, \quad (3.109)$$

and the continuous momenta

$$q^2 = q_1^2 + \dots + q_{d-2}^2. \quad (3.110)$$

It is clear that we need to regularize expression (3.107). As in the previous example, we apply an analytic regularization procedure by introducing a parameter, $s \in \mathbb{C}$, and our Casimir energy will be given by an analytic extension. With some straightforward manipulations and inserting the parameter for analytic continuation, Equation (3.107) can be rewritten in a more illuminating form:

$$\begin{aligned} \epsilon_d(a, b; s) &= \frac{1}{A_{d-2}} E_d(L_1, \dots, L_{d-2}, a, b; s) \\ &= \frac{\hbar}{2(2\pi)^{d-2}} \int \left[\sum'_{m,n=-\infty}^{\infty} \omega_{mn}^{-s}(q) - 2 \sum_{n=1}^{\infty} \omega_{0n}^{-s}(q) - 2 \sum_{m=1}^{\infty} \omega_{m0}^{-s}(q) \right] d^{d-2}q, \end{aligned} \quad (3.111)$$

where the prime over the summation sign means that the term with $m = n = 0$ is removed from the double series. To proceed with the calculations, we perform a change of variables in the continuum momenta to a spherical coordinate system, with radial variable given by q and angular element $d\Omega_{d-2}$. The angular integration leads to the factor

$$\int d\Omega_{d-2} = \frac{2\pi^{\frac{d-2}{2}}}{\Gamma\left(\frac{d-2}{2}\right)}, \quad (3.112)$$

and the integration over q can also be performed, leading to

$$\begin{aligned} \epsilon_d(a, b; s) &= \frac{\hbar c \pi^{-\frac{d}{2}} \Gamma\left(1 + \frac{s}{2} - \frac{d}{2}\right)}{2^{d-1} \Gamma\left(\frac{s}{2}\right)} \left[Z_2\left(\frac{1}{a}, \frac{1}{b}; s - d + 2\right) \right. \\ &\quad \left. - \left(\frac{1}{a^{d-2-s}} + \frac{1}{b^{d-2-s}} \right) \zeta(s - d + 2) \right], \end{aligned} \quad (3.113)$$

where we have used the definition of the **Epstein zeta-function**

$$Z_2(x, y; s) = \sum'_{m,n=-\infty}^{\infty} [(xm)^2 + (yn)^2]^{-s/2}. \quad (3.114)$$

Using the reflection formula for the Epstein zeta-function [45], we can write

$$Z_2\left(\frac{1}{a}, \frac{1}{b}; s - d + 2\right) = \frac{ab}{\pi^{s+\frac{d-1}{2}}} \frac{\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(\frac{2-d+s}{2}\right)} Z_2(a, b; d - s), \quad (3.115)$$

and for the Riemann zeta-function, we use the reflection formula given in Eq. (3.83) to obtain

$$\Gamma\left(1 + \frac{s}{2} - \frac{d}{2}\right) \zeta(s - d + 2) = \frac{\Gamma\left(\frac{d-1-s}{2}\right)}{\pi^{-s+\frac{d}{2}+1}} \zeta(d - 1 - s). \quad (3.116)$$

One can derive a general expression for $\epsilon_d(a, b; s)$ employing the analytic extension procedure. The Casimir energy for the waveguide is obtained for $s = -1$:

$$\begin{aligned} \epsilon_d(a, b; -1) = & -\frac{\pi^{-\frac{d+1}{2}}}{2^d} \left[ab\pi^{1-\frac{d-1}{2}} \Gamma\left(\frac{d+1}{2}\right) Z_2(a, b; d+1) \right. \\ & \left. - \left(\frac{1}{a^{d-1}} + \frac{1}{b^{d-1}}\right) \frac{\Gamma\left(\frac{d}{2}\right)}{\pi^{\frac{d}{2}+2}} \zeta(d) \right]. \end{aligned} \quad (3.117)$$

This expression remains finite for $d \geq 3$. In the case of $d = 3$, we obtain

$$\epsilon_3(a, b; -1) = \frac{\hbar c}{16\pi^2} \left(\frac{1}{a^2} + \frac{1}{b^2}\right) \zeta(3) - \frac{\hbar c}{8\pi} ab Z_2(a, b; 4). \quad (3.118)$$

The sign difference between the two contributions ensures the well-known behavior of the change of sign of the Casimir force in a box geometry [47].

In the last two examples of explicit calculation of the Casimir force, we have assumed Dirichlet boundary conditions. In the electromagnetic case, this is equivalent to considering a perfect conductor. In the next section, we explore the case of non-ideal boundary conditions to approach a dielectric material.

3.2.2 Non-ideal Boundary Conditions

The Casimir effect in real materials is an important topic of modern research. In this context, the work of Lifshitz serves as a cornerstone that advanced the analysis of the Casimir effect in real material media [48]. The basic idea is to model vacuum quantum fluctuations as a stochastic fluctuating electromagnetic field and

to use the fluctuation-dissipation theorem to determine the frequency-dependent Casimir energy. The general result obtained by Lifshitz provides a formula for the Casimir energy density and pressure in a plane geometry filled with different dielectric media. Other approaches have enriched the discussion and reinforced Lifshitz's result. For instance, using the Green's function approach, Dzyaloshinskii et al. obtained the same result for the Casimir effect in dielectrics [49]. We also mention the approach proposed by Van Kampen et al., where the physical effect of the dielectric is carried by the so-called surface stationary modes of the electromagnetic field [50]. The discrepancy between the dissipationless plasma model of dielectric materials and the dissipative Drude model has also been discussed in the literature, e.g., Ref. [51].

In Ref.[36], we propose a new way to explore the finite conductivity scenario for the slab geometry and also for the bidimensional box. This approach is based on the spectral theory presented in the previous section and on approximate functional equations.

Later in this section, we introduce the Van Kampen method of surface modes to calculate the Casimir energy of a three-dimensional waveguide filled with a dielectric. This result has been obtained by the author and collaborators in Ref. [46]. Although finite-sized cavities with perfect conductors have been discussed before (see Ref. [45]), the inclusion of the dielectric leads to highly non-trivial problems. The case of a dielectric cylinder was discussed in Ref. [52]. However, the rectangular waveguide has not been discussed, we believe, because ensuring the consistency of boundary conditions at the corners is problematic.

Finite conductivity via approximate functional equations

Here, we present the calculations and results of Ref. [36].

Our main objective is to discuss the Casimir energy of a massless scalar field at zero temperature satisfying non-ideal boundary conditions. Due to the similarity between the quantized electromagnetic field and massless scalar fields satisfying Dirichlet and Neumann boundary conditions, our problem has formal similarities with the conductivity correction to the Casimir force of the quantized electromagnetic field. One initial approach is to describe finite conductivity using microscopic models. A microscopic approach has been extensively studied by G. Barton (see, e.g., Refs. [53–55]). The case of QED in a dielectric matter background has also been analyzed, with various quantization schemes proposed. For the nonlinear case, see Refs. [56–58], and for the dispersive case, see Ref. [59].

Instead of addressing the nonlinear problem of microscopic modeling of finite conductivity, i.e., non-ideal boundary conditions, we confine ourselves to using the spectral theory of elliptic differential operators. Corrections to the Casimir force can be discussed using an analytic regularization procedure and approxi-

mate functional equations of spectral zeta-functions. These functional equations express the Riemann and Epstein zeta-functions as finite sums outside their original domain of convergence. Connections between number theory and quantum field theory have been explored in the literature, as seen in arithmetic quantum theory [60–65].

Using our methodology, the total renormalized energy of scalar fields in the presence of bounded domains can always be derived using an analytic regularization procedure, where the Dirichlet and Neumann Laplacian are used, as presented in Sec. 3.2. In Eq.(3.86), we have shown that the vacuum energy in the slab geometry $\mathbb{R}^{d-1} \times [0, L]$ with Dirichlet boundary conditions can be written in terms of the Riemann zeta-function. To calculate its correction due to non-ideal boundary conditions, we represent the energy density using an asymptotic expansion derived by Hardy and Littlewood. They obtained an approximate functional equation for the Riemann zeta-function expressed as finite sums beyond their original domain of convergence [66]. Next, we generalize this result to the case of a field in the presence of a rectangular box with lengths L_1 and L_2 with non-ideal boundary conditions. Other generalizations of the Riemann functional equation have been presented in the literature. Recently, the introduction of different cut-offs in the integral representation of the zeta-function, which remain invariant under the transformation $x \mapsto 1/x$, has been discussed. It has been shown that the Riemann functional equation can be generalized with the same symmetry $s \rightarrow (1 - s)$ in the critical strip [67].

In the Lifshitz approach, the dispersion forces between dissipative media arise from the fluctuating electromagnetic field defined both within and outside the media. Using the fluctuation-dissipation theorem, the Lifshitz expression for the force between plates depends on the dielectric functions of the surfaces and the medium in which they are immersed. The finite conductivity correction to the ideal Casimir calculation is obtained using the frequency dependence of the dielectric function. The imperfect conductivity at high frequencies can be modeled by introducing only the plasma frequency ω_p of the plates. It is important to note that the Casimir result is recovered at distances larger than the plasma wavelength.

In our case, we discuss the vacuum energy of a quantized scalar field in the presence of classical surfaces, where the field satisfies non-ideal boundary conditions. These can be understood as finite conductivity conditions, which we refer to as *ideal high-pass Dirichlet boundary conditions*. To clarify, our boundary condition applies to frequencies: for frequencies smaller than some ω_{k_c} , we have the usual Dirichlet boundary conditions; otherwise, the plates are transparent to the field. However, a crucial point is that it is not convenient to simply calculate the correction to the renormalized vacuum energy by separating the effects of the low-energy vacuum modes from the high-energy modes using a sharp cut-

off. Since the energy density is a sum of positive terms, one always obtains a positive energy density.

$$\epsilon_d^{\text{f.c.}}(L) = \sum_{k=1}^{k_c} \omega_k > 0, \quad (3.119)$$

where ω_{k_c+1} is plasma frequency of the material.

We start by using an analytic regularization procedure and the fact that, for Dirichlet boundary conditions, the eigenvalues vary continuously under a smooth deformation of the domain (spectral stability of the elliptic operator under domain deformation). Moreover, the minimax principle states that the eigenvalues monotonically decrease when the domain is enlarged,

$$\sigma_m(D_1) \geq \sigma_m(D_2), \quad D_1 \subset D_2. \quad (3.120)$$

By the above arguments, we can use an approximate functional equation that expresses the Riemann zeta-function as finite sums outside its original domain of convergence.

Initially, we use a classical result by Hardy and Littlewood, following the derivation discussed in Ref. [68]. Let us write the Riemann zeta-function as

$$\begin{aligned} \zeta(s) &= \sum_{n \leq n_c} n^{-s} + \sum_{n > n_c} n^{-s} \\ &= \sum_{n \leq n_c} n^{-s} + \frac{1}{\Gamma(s)} \int_0^\infty x^{s-1} \left(\sum_{n > n_c} e^{-nx} \right) dx \\ &= \sum_{n \leq n_c} n^{-s} + \frac{1}{\Gamma(s)} \int_0^\infty \frac{x^{s-1} e^{-n_c x}}{e^x - 1} dx, \end{aligned} \quad (3.121)$$

where the absolute convergence justifies the inversion of the order of summation and integration. To proceed, we analyze the following integral $I(s)$. We have

$$I(s) = \int_C \frac{z^{s-1} e^{-n_c z}}{e^z - 1} dz, \quad (3.122)$$

where the contour C starts at infinity on the positive real axis, encircles the origin once in the positive direction, excluding the points $\pm 2\pi i, \pm 4\pi i, \dots$, and returns to infinity. We obtain

$$I(s) = (e^{2\pi i s} - 1) \int_0^\infty \frac{x^{s-1} e^{-n_c x}}{e^x - 1} dx. \quad (3.123)$$

Using the analytic continuation principle, we can write

$$\zeta(s) = \sum_{n \leq n_c} n^{-s} + \frac{e^{-\pi i s} \Gamma(1-s)}{2\pi i} \int_C \frac{z^{s-1} e^{-n_c z}}{e^z - 1} dz. \quad (3.124)$$

From the above equation, we find an approximate representation of the zeta-function in terms of finite sums. Once can prove that (see Ref. [68])

$$\zeta(s) = \sum_{n \leq x} \frac{1}{n^s} + \frac{(2\pi)^s \Gamma(1-s)}{\Gamma(1-\frac{s}{2}) \Gamma(\frac{s}{2})} \sum_{n \leq y} \frac{1}{n^{1-s}} + O(x^{-\sigma}) + O(t^{\frac{1}{2}-\sigma} y^{\sigma-1}), \quad (3.125)$$

for $0 \leq \sigma < 1$, which holds for given $x, y, t > C > 0$ satisfying $2\pi xy = t$ where $t \gg 1$. This is known as an approximate functional equation.

For simplicity, using the approximate functional equation, we discuss the case of a slab geometry $\mathbb{R}^{d-1} \times [0, L]$. Drawing a parallel with the electromagnetic case, in the scalar field scenario, we define the plasma frequency ω_p and the plasma wavelength $\lambda_p = 2\pi/\omega_p$. Next, we define a “critical” mode index n_c , which will be related to the plasma wavelength.

In order to find an adequate maximum number of states n_c for a single compactified direction, we first introduce the notion of the density of states $\rho(k)$ in the phase space and the number of states $dN = \rho(k) d^d k$ that lie between k and $k + dk$. In the d -dimensional space, where all the directions are finite and have lengths $L_1, L_2, \dots, L_{d-1}, L$, the density of states is simply

$$\rho(k) = \left(\frac{L}{\pi^d} \right) \prod_{i=1}^{d-1} L_i, \quad (3.126)$$

we can find the number of states inside a volume that possess the maximum value of momentum k_{max} as

$$N(k_{max}) = \int_{|k| < k_{max}} k \rho(k) dk = \rho \frac{\pi^{d/2}}{\Gamma(\frac{d}{2} + 1)} k_{max}^d, \quad (3.127)$$

where we have used the definition of the volume of a sphere in d dimensions. On the other hand, we are interested in obtaining the maximum number of states in a single compactified direction n_c . We have that

$$N(k_{max}) = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2} + 1)} n_c^d. \quad (3.128)$$

Therefore, we identify $n_c^d = \rho k_{max}^d$. Now, we relate the maximum wave number with the plasma frequency of the material in such a manner that $k_{max} = 2\pi/\lambda_p$. With all this, after some algebra, we conclude that

$$n_c = 2 \left(\frac{L^{1/d}}{\lambda_p} \right) \prod_{i=1}^{d-1} L_i^{1/d}, \quad (3.129)$$

since all the directions L_i from $i = \{1, 2, \dots, d-1\}$ are much larger than L . The only dependence of the maximum number of states is of the form

$$n_c(L) \equiv \left(\frac{L}{\lambda_p} \right)^{1/d}. \quad (3.130)$$

In the Hardy and Littlewood approximate functional equation, we choose

$$x = y = \left(\frac{L}{\lambda_p} \right)^{1/d} = n_c \quad \Rightarrow \quad t = 2\pi \left(\frac{L}{\lambda_p} \right)^{2/d} = 2\pi n_c^2. \quad (3.131)$$

Using the asymptotic expansion, Eq. (3.125), and the definition in Eq. (3.85), we obtain the Casimir energy as

$$\epsilon_d(L) = -\frac{\pi^{\frac{d}{2}} \Gamma\left(-\frac{d}{2}\right)}{2(2L)^d} \left[H_{n_c}(-d) + \vartheta(-d) H_{n_c}(d+1) \right]. \quad (3.132)$$

The quantities $H_n(s)$ are the generalized harmonic numbers, defined by

$$H_n(s) = \sum_{k=1}^n \frac{1}{k^s}. \quad (3.133)$$

Since Eq. (3.132) only makes sense as an analytic continuation, these finite sums must be understood in that context. Moreover, we emphasize that the equality holds by analytic continuation outside the strip $0 < \sigma < 1$. This can be demonstrated using an analytic continuation of the asymptotic expansion.

Each generalized harmonic number has an expression for its domain of interest in the complex plane. Let us start with the second term in the sum, $H_{n_c}(d+1)$. Formally, this quantity is given by

$$H_{n_c}(d+1) \equiv \sum_{n=1}^{n_c} \frac{1}{n^{d+1}}. \quad (3.134)$$

However, since we start from Eq. (3.106), which is an analytic continuation, the finite sum should be considered in the range of interest. In this situation, we can use a known expression:

$$H_{n_c}(d+1) = \zeta(d+1) + \frac{(-1)^d}{d!} \psi_d(n_c+1), \quad (3.135)$$

which holds for $n_c \in \mathbb{R} \setminus \{-1, -2, -3, \dots\}$ and $d \in \mathbb{N}$ (see, e.g., [69]). Here, $\psi_m(x)$ is the polygamma function. Using a recurrence relation and an expression for large arguments, we can write the polygamma function as

$$\psi_d(n_c+1) = \frac{(-1)^d d!}{n_c^{d+1}} + (-1)^{d+1} \sum_{k=0}^{\infty} \frac{(k+d-1)!}{k!} \frac{B_k}{n_c^{d+k}}, \quad (3.136)$$

where B_k are the Bernoulli numbers (we take the convention $B_1 = 1/2$). Using the definition of n_c and considering the limit $L/\lambda_p \gg 1$, we can write

$$\psi_d(n_c+1) \approx (-1)^{d+1} \left(\frac{\lambda_p}{L} \right) \left[(d-1)! - \frac{1}{2} d! \left(\frac{\lambda_p}{L} \right)^{\frac{1}{d}} \right], \quad (3.137)$$

which allows us to express $H_{n_c}(d+1)$ in powers of λ_p/L .

For the first term in Eq. (3.132), we formally have

$$H_{n_c}(-d) \equiv \sum_{n=1}^{n_c} \frac{1}{n^{-d}}. \quad (3.138)$$

Using elementary operations and the uniqueness of analytic continuation, it is straightforward to see that

$$H_{n_c}(-d) = \zeta(-d) - \zeta_H(-d; n_c+1), \quad (3.139)$$

where $\zeta_H(-d; n_c+1)$ is the **Hurwitz zeta-function**, defined by

$$\zeta_H(s; a) \equiv \sum_{n=0}^{\infty} \frac{1}{(n+a)^s}, \quad (3.140)$$

for $\Re(s) > 1$ and $a \neq 0, -1, -2, \dots$.

Let us define the Casimir energy per unit area with non-ideal boundary conditions, i.e., finite conductivity (f.c.), as

$$\epsilon_d^{\text{f.c.}}(L) \equiv -\frac{1}{L^d} \frac{\pi^{d/2}}{2^{d+1}} \Gamma\left(-\frac{d}{2}\right) \zeta_H(-d; n_c+1). \quad (3.141)$$

Once this is established, we can identify the contribution from the ideal boundary conditions, while the remaining term can be regarded as a correction due to the dielectric properties. We obtain

$$\epsilon_d^{\text{f.c.}}(L) = \epsilon_d(L) + \frac{\Gamma(1+d)\lambda_p}{2\Gamma\left(1+\frac{d}{2}\right)} \left(\frac{1}{4\sqrt{\pi}}\right)^d \left[\frac{1}{L^{d+1}d} - \frac{\lambda_p^{\frac{1}{d}}}{2L^{d+1+\frac{1}{d}}} \right]. \quad (3.142)$$

As observed, in the slab geometry, the Casimir force is a negative quantity ($\epsilon_d(L) < 0$), while the second contribution in the above equation is positive. We have successfully derived the Casimir energy per unit area with non-ideal boundary conditions. It is worth noting that the first finite conductivity correction to the electromagnetic Casimir energy has the same order as the correction obtained using the Lifshitz calculations. In contrast, the second correction is smaller: while the Lifshitz formula gives a second correction as L^{-5} , our approach yields $L^{-\frac{13}{3}}$. Fixing $d = 3$ and disregarding the second correction we find that

$$\mathcal{E}_3^{\text{f.c.}}(L) \approx -\frac{0.007}{L^3} + \frac{0.002\lambda_p}{L^4}, \quad (3.143)$$

where the correction term is slightly smaller than the one obtained in the Lifshitz's formula. This means that some refinement in the choice of n_c may be needed. However this does not shed shadows in the remarkable fact that the power law of the correction is obtained from the approximate functional equation. A fundamental aspect that requires careful investigation is the discussion of vacuum energy in a bounded domain.

Now let us apply the same set of ideas to the case of a finite volume box in the bidimensional case. To that end, let us now discuss the eigenvalues of a second-order elliptic self-adjoint partial differential operator acting on scalar functions on a bounded domain. We consider the eigenvalues of $-\Delta$ on a connected open set D in Euclidean space $\mathbb{R}^2$. We assume that the massless scalar field is confined in a rectangular box, with lengths L_1 and L_2 , obeying Dirichlet boundary conditions. The eigenfrequencies that we use to expand the field operator are given by

$$\omega_{n_1 n_2} = \left[\left(\frac{n_1 \pi}{L_1} \right)^2 + \left(\frac{n_2 \pi}{L_2} \right)^2 \right]^{\frac{1}{2}}; \quad n_1, n_2 = 1, 2, \dots \quad (3.144)$$

The unrenormalized vacuum energy in this case is

$$U(L_1, L_2) = \frac{1}{2} \sum_{n_1, n_2=1}^{\infty} \omega_{n_1 n_2}. \quad (3.145)$$

Using an analytic regularization procedure, the divergent expression can be written as

$$E(L_1, L_2, s) = \frac{1}{2} \sum_{n_1, n_2=1}^{\infty} \omega_{n_1 n_2}^{-2s}, \quad (3.146)$$

for $s \in \mathbb{C}$. Observe that the vacuum energy is obtained when $s = -\frac{1}{2}$. The above double series converges absolutely and uniformly for $\Re(s) > 1$. An analytic function, which plays an important role in algebraic number theory, is the Epstein zeta-function associated with quadratic forms [70]. Suppose that

$$\phi(a, b, c; x, y) = ax^2 + cxy + by^2, \quad (3.147)$$

where a, b and $c \in \mathbb{R}$, $a > 0$, and $\eta = 4ab - c^2 > 0$. Let us define the function $\mathcal{A}(s)$ by the series

$$\mathcal{A}(a, b, c; s) = \sum'_{n_1, n_2=-\infty}^{\infty} \phi^{-s}(a, b, c; n_1, n_2), \quad (3.148)$$

The above series defines an analytic function for $s = \sigma + it$, ($\sigma \in \mathbb{R}$ and $t \in \mathbb{R}$), with $\sigma > 1$, where we adopt the notation that the prime sign in the summation indicates that the contribution $n_1 = n_2 = 0$ (the origin of the mode space) must be excluded. This particular case of the **Epstein zeta-function** can be analytically continued to the whole complex plane, except for a simple pole at $s = 1$ [71]. This double series exhibits a functional equation that can be obtained using properties of the theta-function or the Poisson summation formula. The functional equation reads

$$\mathcal{A}(a, b, c; s) = \left(\frac{2\pi}{\sqrt{\eta}}\right)^{2s-1} \frac{\Gamma(1-s)}{\Gamma(s)} \mathcal{A}\left(\frac{1}{a}, \frac{1}{b}, \frac{1}{c}; 1-s\right) \quad (3.149)$$

We are interested in the case where $c = 0$. Let us define the function $Z\left(\frac{1}{L_1}, \frac{1}{L_2}; s\right)$ by

$$Z\left(\frac{1}{L_1}, \frac{1}{L_2}; s\right) = \sum'_{n_1, n_2=-\infty}^{\infty} \left(\frac{n_1^2}{L_1} + \frac{n_2^2}{L_2}\right)^{-s}, \quad (3.150)$$

We can find that the vacuum energy is written as

$$E(L_1, L_2; s) = \frac{1}{8} Z\left(\frac{\pi^2}{L_1^2}, \frac{\pi^2}{L_2^2}; s\right) - \frac{1}{4} \left[\left(\frac{\pi}{L_1}\right)^{-2s} + \left(\frac{\pi}{L_2}\right)^{-2s} \right] \zeta(2s). \quad (3.151)$$

As discussed, $E(L_1, L_2, s)$ is analytic in $s \in \mathbb{C} \setminus \{\frac{1}{2}, 1\}$. Using the analytic continuation of the Epstein and the Riemann zeta-functions, we obtain the vacuum

energy $U(L_1, L_2) = E(L_1, L_2; s = -1/2)$ for the system with Dirichlet boundary conditions. We get

$$U(L_1, L_2) = \frac{\pi}{48} \left(\frac{1}{L_1} + \frac{1}{L_2} \right) \frac{L_1 L_2}{32\pi} \sum'_{n_1, n_2=-\infty}^{\infty} (n_1^2 L_1^2 + n_2^2 L_2^2)^{-\frac{3}{2}}. \quad (3.152)$$

The next step involves discussing the scalar case, similar to the electromagnetic case of imperfect conductors, where there is a plasma frequency ω_p . Using the same approach discussed in the previous section, we aim to determine the approximate functional equation for the Epstein zeta-function.

Potter [72] has derived the following approximate functional equation for the Epstein zeta-function:

$$\mathcal{A}(a, b, c; s) = \sum'_{\phi \leq x} \phi^{-s}(a, b, c; n_1, n_2) + X(s) \sum'_{\phi \leq y} \phi^{s-1}(a, b, c; n_1, n_2), \quad (3.153)$$

for $t \gg 1$, and the condition $4\pi^2 xy = \eta t^2$ must be satisfied. The quantity $X(s)$ is defined by

$$X(s) = \left(\frac{2\pi}{\sqrt{\eta}} \right)^{2s-1} \frac{\Gamma(1-s)}{\Gamma(s)}. \quad (3.154)$$

Henceforth, we take $\mathcal{A}(a, b, 0; s) \equiv \mathcal{A}(a, b; s)$ and similarly for ϕ .

Of course, to obtain the correction to the Casimir energy via an asymptotic series, we will need to use the Potter approximate functional equation for the Epstein zeta-function, but also the Hatree-Littlewood approximate functional equation for the Riemann zeta-function. Let's start analyzing the Epstein zeta-function. It is convenient to introduce a λ_p term in the expression to only have dimensionless quantities and establish a parallel with the Casimir energy in a finite conductivity scenario. In this case, we have

$$\mathcal{A} \left(\frac{\pi^2 \lambda_p^2}{L_1^2}, \frac{\pi^2 \lambda_p^2}{L_2^2}; s \right) = \sum'_{\Phi \leq x} \Phi_{12}^{-s} + X(s) \sum'_{\Phi \leq y} \Phi_{12}^{s-1}, \quad (3.155)$$

where to lighten the notation, we defined

$$\Phi_{12} = \phi \left(\frac{\pi^2 \lambda_p^2}{L_1^2}, \frac{\pi^2 \lambda_p^2}{L_2^2}; n_1, n_2 \right) = \frac{\pi^2 \lambda_p^2}{L_1^2} n_1^2 + \frac{\pi^2 \lambda_p^2}{L_2^2} n_2^2, \quad (3.156)$$

once that $4\pi^2 xy = \eta t^2$ with

$$\eta = 4 \left(\frac{\pi^2 \lambda_p^2}{L_1 L_2} \right)^2 \Rightarrow xy = \left(\frac{\pi \lambda_p^2}{L_1 L_2} \right)^2 t^2. \quad (3.157)$$

Since

$$X(s) = \left(\frac{L_1 L_2}{\pi \lambda_p^2} \right)^{2s-1} \frac{\Gamma(1-s)}{\Gamma(s)}, \quad (3.158)$$

using a similar argument to the one we used before, but now all dimensions remain compact, we can define the quantities

$$\begin{aligned} n_c^{(1)} &\equiv \left(\frac{L_1}{\lambda_p} \right)^{1/2} \quad \text{and} \quad n_c^{(2)} \equiv \left(\frac{L_2}{\lambda_p} \right)^{1/2} \\ \Rightarrow xy &= \left[\frac{\pi}{(n_c^{(1)} n_c^{(2)})^2} \right]^2 t^2, \end{aligned} \quad (3.159)$$

which, considering the fact that we do not have a preferred direction, indicates that the natural choice for t should be

$$t = \frac{1}{\pi} (n_c^{(1)} n_c^{(2)})^2 \Rightarrow x = y = n_c^{(1)} n_c^{(2)}. \quad (3.160)$$

So, looking back at Eq. (3.155), we see that the sums are over all modes inside the ellipse defined by

$$\frac{n_1^2}{L_1 n_c^{(1)} n_c^{(2)}} + \frac{n_2^2}{L_2 n_c^{(1)} n_c^{(2)}} = \left(\frac{1}{\pi \lambda_p} \right)^2 = \text{constant}, \quad (3.161)$$

in the (n_1, n_2) -plane with the origin removed.

For the Riemann zeta-function contributions that are present in Eq. (3.151), we have

$$\zeta(2s) = \sum_{n \leq u} \frac{1}{n^{2s}} + \frac{(2\pi)^{2s} \Gamma(1-2s)}{\Gamma(1-s) \Gamma(s)} \sum_{n \leq v} \frac{1}{n^{1-2s}}, \quad (3.162)$$

for $\alpha \gg 1$ where $2\pi uv = \alpha$. Proceeding exactly as in the slab bag geometry case, we find that

$$u = v \equiv n_c^{(i)} = \left(\frac{L_i}{\lambda_p} \right)^{1/2} \Rightarrow \alpha = 2\pi \frac{L_i}{\lambda_p}; \quad i = 1, 2, \quad (3.163)$$

continuing from the previous case, we employ an analogous method. Using the same harmonic number definitions, once the range in the complex plane will be the same. Considering the case where $s = -1/2$ and manipulating the equations,

it is possible to find that

$$\begin{aligned}
 E(L_1, L_2; s) = & \frac{\lambda_p^{2s}}{8} \sum'_{\Phi \leq n_c^{(1)} n_c^{(2)}} \Phi_{12}^{-s} + \left(\frac{L_1 L_2}{\pi \lambda_p^2} \right)^{2s-1} \frac{\Gamma(1-s)}{\Gamma(s)} \frac{\lambda_p^{2s}}{8} \sum'_{\Phi \leq n_c^{(1)} n_c^{(2)}} \Phi_{12}^{s-1} \\
 & - \frac{\lambda_p^{2s}}{4} \sum_{i=1}^2 \left\{ \left(\frac{\lambda_p}{L_i} \right)^{-2s} \left[2\zeta(2s) - \zeta_H(2s; n_c^{(i)} + 1) \right] \right. \\
 & \left. + (-1)^{-4s+1} \frac{(2\pi)^{2s} \Gamma(1-2s)}{\Gamma(1-s) \Gamma(s)} \left[\frac{1}{2s} \left(\frac{\lambda_p}{L_i} \right)^{-3s} - \frac{1}{2} \left(\frac{\lambda_p}{L_i} \right)^{\frac{-6s+1}{2}} \right] \right\}. \quad (3.164)
 \end{aligned}$$

We define the vacuum energy for finite conductivity (f.c.) as

$$\begin{aligned}
 U^{\text{f.c.}}(L_1, L_2) &= E^{\text{f.c.}} \left(L_1, L_2, s = -\frac{1}{2} \right) \\
 &= \frac{1}{8\lambda_p} \sum_{\Phi \leq n_c^{(1)} n_c^{(2)}} \Phi_{12}^{\frac{1}{2}} - \frac{1}{4} \sum_{i=1}^2 \frac{1}{L_i} \left[\zeta_H(-1; n_c^{(i)} + 1) - \frac{1}{6} \right]. \quad (3.165)
 \end{aligned}$$

Therefore

$$\begin{aligned}
 U^{\text{f.c.}}(L_1, L_2) &= U(L_1, L_2) - \frac{\pi^2 \lambda_p^3}{32(L_1 L_2)^2} \sum_{\Phi \leq n_c^{(1)} n_c^{(2)}} \Phi_{12}^{-\frac{3}{2}} \\
 &\quad + \frac{1}{2\lambda_p (2\pi)^2} \sum_{i=1}^2 \left[\left(\frac{\lambda_p}{L_i} \right)^{3/2} - \frac{1}{2} \left(\frac{\lambda_p}{L_i} \right)^2 \right], \quad (3.166)
 \end{aligned}$$

is the Casimir energy for a rectangular box with non-ideal boundary conditions.

Finite conductivity in electromagnetic case via stationary modes

In order to present the stationary modes approach, we follow Ref. [73]. Here we use Gaussian units.

Let us consider a system composed of three dielectrics. The first dielectric, $\varepsilon_1(\omega)$, lies in the region $z < 0$, the second, $\varepsilon_2(\omega)$, in the region $z > d$, and the third dielectric, $\varepsilon_3(\omega)$, is in between the other two, that is, $0 < z < d$, as shown in Fig. 3.3.

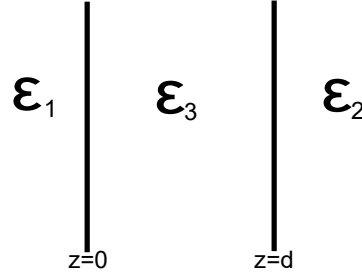


Figure 3.3: Configuration of three dielectrics in a slab geometry.

First, we must compute the relevant modes in the system. To achieve this, we note that a possible set of solutions to Maxwell's equations

$$\begin{aligned}
 \nabla \cdot \mathbf{D} &= 0, \\
 \nabla \cdot \mathbf{B} &= 0, \\
 \nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \\
 \nabla \times \mathbf{B} &= \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t},
 \end{aligned} \tag{3.167}$$

is

$$\begin{aligned}
 \mathbf{E}(\mathbf{r}, t) &= \mathbf{E}_0(\mathbf{r})e^{-i\omega t}, \\
 \mathbf{B}(\mathbf{r}, t) &= \mathbf{B}_0(\mathbf{r})e^{-i\omega t}.
 \end{aligned} \tag{3.168}$$

Assuming that the media are isotropic, we have $D(\mathbf{r}, t) = \varepsilon(\omega)E_0(\mathbf{r})e^{-i\omega t}$ for all the dielectrics. Maxwell's equations are satisfied if, in each dielectric, we have $\nabla \cdot \mathbf{E}_0 = \nabla \cdot \mathbf{B}_0 = 0$, which implies that

$$\begin{aligned}
 \Delta \mathbf{E}_0 + \frac{\omega^2}{c^2} \varepsilon(\omega) \mathbf{E}_0 &= 0, \\
 \Delta \mathbf{B}_0 + \frac{\omega^2}{c^2} \varepsilon(\omega) \mathbf{B}_0 &= 0.
 \end{aligned} \tag{3.169}$$

The boundary conditions require that the normal and tangential components of $\mathbf{E}$ and $\mathbf{B}$ are continuous, and the derivative of the transverse component of $\mathbf{E}$ is zero. We assume a solution of the following form:

$$\begin{aligned}
 \mathbf{E}_0(\mathbf{r}) &= [e_x(z)\hat{x} + e_y(z)\hat{y} + e_z(z)\hat{z}] e^{i(k_x x + k_y y)}, \\
 \mathbf{B}_0(\mathbf{r}) &= [b_x(z)\hat{x} + b_y(z)\hat{y} + b_z(z)\hat{z}] e^{i(k_x x + k_y y)},
 \end{aligned} \tag{3.170}$$

which implies that the momentum must satisfy the following equation:

$$\begin{aligned}\frac{de_i}{dz} - K^2 e_i &= 0, \\ \frac{db_i}{dz} - K^2 b_i &= 0,\end{aligned}\tag{3.171}$$

where we have defined $K^2 = k_x^2 + k_y^2 - \varepsilon(\omega)\frac{\omega^2}{c^2}$ and $i = \{x, y, z\}$. Let us assume a coordinate system where $k_y = 0$ and denote k_x by k . Requiring the continuity of the normal component of $\mathbf{D}(\mathbf{r})$, we find that $\varepsilon(\omega)e_z(z)$ must be continuous for all ω , and $\nabla \cdot \mathbf{E}_0 = 0$ implies that

$$ike_x + \frac{de_z}{dz} = 0.\tag{3.172}$$

Using the fact that $\nabla \times \mathbf{E}_0 = i\frac{\omega}{c}\mathbf{B}_0$, it is straightforward to obtain that $\nabla \cdot \mathbf{B}_0 = 0$ is satisfied, and the continuity of the normal component implies that e_y is continuous. Continuity of e_x follows from the last equation. To analyze the continuity of the tangential component of $\mathbf{B}$, we use the previous equation and Eq. (3.171) to obtain

$$ke_z + i\frac{de_x}{dz} = \frac{1}{k} \left[\varepsilon(\omega)\frac{\omega^2}{c^2} \right] e_z,\tag{3.173}$$

and the continuity of this quantity follows from the continuity of the normal component of $\mathbf{D}(\mathbf{r})$.

Therefore, to satisfy all the boundary conditions, it is sufficient to require the continuity of εe_z , $\partial_z e_z$, e_y , and $\partial_z e_y$. The solution to Eq. (3.171) can be written as

$$e_z(z) = A_1 e^{K_1 z} + A_2 e^{-K_1 z},\tag{3.174}$$

and by setting the constants of unphysical exponentially growing modes to zero, we can write the solution for all three regions as

$$e_z(z) = \begin{cases} Ae^{K_1 z}, & \text{if } z < 0, \\ Be^{K_3 z} + Ce^{-K_3 z}, & \text{if } 0 \leq z \leq d, \\ De^{-K_2 z}, & \text{if } z > d. \end{cases}\tag{3.175}$$

where $K_i = \sqrt{k^2 - \varepsilon_i(\omega)\frac{\omega^2}{c^2}}$, for $i = 1, 2, 3$. The continuity of εe_z and $\partial_z e_z$ leads to algebraic equations for A, B, C , and D . The nontrivial solutions of these equations impose that

$$\mathcal{F}_a(\omega) = \frac{(\varepsilon_3 K_1 + \varepsilon_1 K_3)(\varepsilon_3 K_2 + \varepsilon_2 K_3)}{(\varepsilon_3 K_1 - \varepsilon_1 K_3)(\varepsilon_3 K_2 - \varepsilon_2 K_3)} e^{2K_3 d} - 1 = 0.\tag{3.176}$$

The continuity of e_y and $\partial_z e_y$ is satisfied if

$$\mathcal{F}_b(\omega) = \frac{(K_1 + K_3)(K_2 + K_3)}{(K_1 - K_3)(K_2 - K_3)} e^{2K_3 d} - 1 = 0. \quad (3.177)$$

Usually, we cannot satisfy both equations simultaneously, but if we impose $e_y = 0$, we can satisfy Eq. (3.176). If we impose $e_z = 0$, we can satisfy Eq. (3.177). This leads to two types of modes:

- (a) Solutions of Eq. (3.176) with $e_y = 0$;
- (b) Solutions of Eq. (3.177) with $e_z = 0$.

These two kinds of modes are called **surface modes**. Now we can compute the vacuum energy associated with such modes, which will be given by

$$E(d) = \frac{\hbar L^2}{4\pi} \int_0^\infty k \left[\sum_n \omega_{na}(k) + \sum_n \omega_{nb}(k) \right] dk, \quad (3.178)$$

where ω_{na} are modes of type (a), ω_{nb} are modes of type (b), and L is the size of the x, y direction. We suppose that $L \gg d$. Using the argument principle of complex numbers, we can identify the sum of the modes as the sum of zeros of $F_{a,b}(\omega)$ subtracted from the sum of the poles of $F_{a,b}(\omega)$. The poles of $F_{a,b}(\omega)$ are independent of d , therefore they do not contribute to the force. Thus, we can write

$$E(d) = \frac{\hbar L^2}{4\pi} \frac{1}{2\pi i} \int_0^\infty k \left[\oint_C \omega \frac{\mathcal{F}'_a(\omega)}{\mathcal{F}_a(\omega)} d\omega + \oint_C \omega \frac{\mathcal{F}'_b(\omega)}{\mathcal{F}_b(\omega)} d\omega \right] dk, \quad (3.179)$$

where the curve C is given by the imaginary axis and a semicircle on the right side of the complex ω -plane (see Fig. 3.4). The integral along the semicircle is d -independent and does not contribute to the force. To analyze the integral along the imaginary axis, we define $\omega = i\xi$ and define $\mathcal{F}_{a,b}(i\xi) = F_{a,b}(\xi)$ to obtain

$$-i \int_{-\infty}^\infty \xi \frac{F'_{a,b}(\xi)}{F_{a,b}(\xi)} d\xi = -i \int_{-\infty}^\infty \xi \frac{d}{d\xi} \ln F_{a,b}(\xi) d\xi = i \int_{-\infty}^\infty \ln F_{a,b}(\xi) d\xi. \quad (3.180)$$

Therefore, our energy is given by

$$E(d) = \frac{\hbar L^2}{8\pi} \int_0^\infty k \left[\int_{-\infty}^\infty \ln F_a(\xi) d\xi + \int_{-\infty}^\infty \ln F_b(\xi) d\xi \right] dk, \quad (3.181)$$

Explicitly, we have

$$F_a(\xi) = \frac{(\varepsilon_3 K_1 + \varepsilon_1 K_3)(\varepsilon_3 K_2 + \varepsilon_2 K_3)}{(\varepsilon_3 K_1 - \varepsilon_1 K_3)(\varepsilon_3 K_2 - \varepsilon_2 K_3)} e^{2K_3 d} - 1, \quad (3.182)$$

$$F_b(\xi) = \frac{(K_1 + K_3)(K_2 + K_3)}{(K_1 - K_3)(K_2 - K_3)} e^{2K_3 d} - 1, \quad (3.183)$$

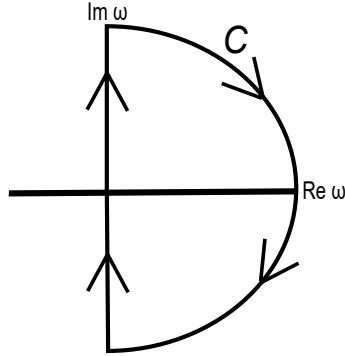


Figure 3.4: Contour of integration C .

with $\varepsilon_i = \varepsilon_i(i\xi)$ and the corresponding changes in the definition of K_i . With that, one can directly compute the force

$$F(d) = -\frac{\partial E(d)}{\partial d} = -\frac{\hbar}{2\pi^2} \int_0^\infty k \left\{ \int_0^\infty K_3 \left[\frac{1}{F_a(k, \xi)} + \frac{1}{F_b(k, \xi)} \right] d\xi \right\} dk. \quad (3.184)$$

Now let us rewrite the previous equation in terms of p , defined by $k^2 = \varepsilon_3(p-1)\xi^2/c^2$. From it, it follows that $K_3 = \sqrt{\varepsilon_3} p \xi / p$ and $K_{1,2}^2 = \varepsilon_3(\xi^2/c^2)[p^2 - 1 + \varepsilon_{1,2}/\varepsilon_3]$, then the force is written as

$$F(d) = -\frac{\hbar}{2\pi^2 c^3} \int_1^\infty p^2 \left\{ \int_0^\infty \xi^3 \varepsilon_3^{\frac{3}{2}} \left[\left(\frac{(\varepsilon_3 s_1 + \varepsilon_1 p)(\varepsilon_3 s_2 + \varepsilon_2 p)}{(\varepsilon_3 s_1 - \varepsilon_1 p)(\varepsilon_3 s_2 - \varepsilon_2 p)} e^{2\xi p \sqrt{\varepsilon_3} \frac{d}{c}} - 1 \right)^{-1} + \left(\frac{(s_1 + p)(s_2 + p)}{(s_1 - p)(s_2 - p)} e^{2\xi p \sqrt{\varepsilon_3} \frac{d}{c}} - 1 \right)^{-1} \right] d\xi \right\} dp, \quad (3.185)$$

which is the Lifshitz formula, obtained in 1956 by E. Lifshitz in Ref. [48].

With the general theory developed, we now present the results of Ref. [46], where we are able to generalize the Lifshitz formula to a dielectric waveguide. Now we consider a system with the geometry given by a waveguide along the z -direction that has a length a in the x -direction and b in the y -direction. That is, the waveguide is defined by the set of ordered pairs $\{(x, y); x \in [0, a], y \in [0, b]\}$. The non-perfect conducting materials have dielectric constants ε_1 inside and ε_2 outside the waveguide, as shown in Fig. (3.5).

Starting from Maxwell's equations (Eq. (3.167)), we again look for stationary mode solutions in the form of Eq. (3.168). By the translation symmetry along the z -axis, we expect that the electric and magnetic fields only depend on coordinates x and y , while in the z direction we expect a free plane wave term. Hence, we

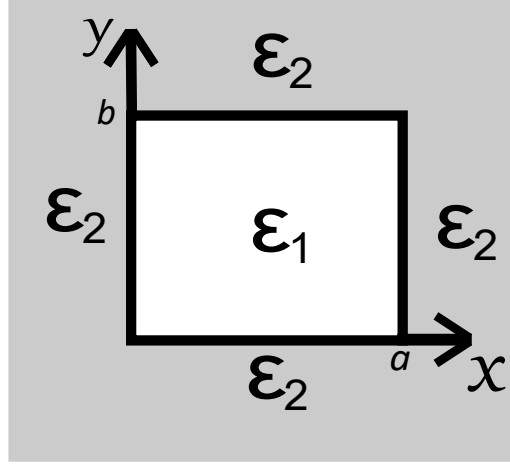


Figure 3.5: Top view of the rectangular waveguide filled with two distinct dielectrics.

look for a solution of the form

$$\mathbf{E}_0(\mathbf{r}) = (e_x(x, y)\hat{i} + e_y(x, y)\hat{j} + e_z(x, y)\hat{k})e^{ikz}, \quad (3.186)$$

$$\mathbf{B}_0(\mathbf{r}) = (b_x(x, y)\hat{i} + b_y(x, y)\hat{j} + b_z(x, y)\hat{k})e^{ikz}. \quad (3.187)$$

By using the Gauss law in the electric displacement field, one finds that

$$\frac{\partial e_x}{\partial x} + \frac{\partial e_y}{\partial y} + ik e_z = 0. \quad (3.188)$$

From the Faraday law, we have that the spatial dependence of the magnetic field is $\mathbf{B}_0 = -i(c/\omega)\nabla \times \mathbf{E}_0$, and therefore we can write

$$\mathbf{B}_0 = -i\left(\frac{c}{\omega}\right)\left\{\left(\frac{\partial e_z}{\partial y} - ik e_y\right)\hat{i} + \left(ike_x - \frac{\partial e_z}{\partial x}\right)\hat{j} + \left(\frac{\partial e_y}{\partial x} - \frac{\partial e_x}{\partial y}\right)\hat{k}\right\}e^{ikz}, \quad (3.189)$$

From this equation, it follows immediately that the Gauss law for the magnetic field is satisfied, i.e., $\nabla \cdot \mathbf{B}_0 = 0$. Also, after some manipulations, we have straightforward that $\nabla \times \mathbf{B}_0 = -i(c/\omega)\nabla \times (\nabla \times \mathbf{E}_0) = i(c/\omega)\Delta \mathbf{E}_0$. Replacing this into Ampère's law, we obtain the wave equation

$$\Delta \mathbf{E}_0 + \frac{\omega^2}{c^2}\epsilon(\omega)\mathbf{E}_0 = 0. \quad (3.190)$$

By substituting Eq. (3.187) into Eq. (3.190), we find that the components of the electric field must satisfy

$$\frac{\partial^2 e_i}{\partial x^2} + \frac{\partial^2 e_i}{\partial y^2} - K^2 e_i = 0, \quad (3.191)$$

where the index is $i = \{x, y, z\}$ and we have defined the wave number on the transverse section of the waveguide as

$$K^2 = k^2 - \frac{\omega^2}{c^2} \varepsilon(\omega). \quad (3.192)$$

Now we must analyze the boundary conditions. To do so, let us define the vertical and horizontal surfaces of the dielectric. The two vertical surfaces of the dielectric are defined by $V_1 = \{(x, y) \in [0, 0] \times [0, b]\}$ and $V_2 = \{(x, y) \in [a, a] \times [0, b]\}$, while the horizontal ones are the sets $H_1 = \{(x, y) \in [0, a] \times [0, 0]\}$ and $H_2 = \{(x, y) \in [0, a] \times [b, b]\}$.

Let us now start with the boundary conditions for the vertical surfaces V_1 and V_2 .

The normal component of the electric displacement vector $\mathbf{D}$ must be continuous across these surfaces. Therefore, this implies the continuity of $\varepsilon(\omega) e_x$ at the vertical surfaces V_1 and V_2 . The continuity of the tangential components of the electric field implies that e_y and e_z must also be continuous. The continuity of the z -component, together with Eq. (3.188), implies that $\partial_x e_x + \partial_y e_y$ must be continuous. This final result can be satisfied if, independently, we require that $\partial_x e_x$ and $\partial_y e_y$ are also continuous.

The continuity of the normal component of the magnetic field indicates that on the vertical surfaces, the term $(\partial_y e_z - i k e_y)$ must be continuous, which would add the continuity condition for $\partial_y e_z$. The continuity of the tangent component of the magnetic field in the z -direction implies that $(\partial_y e_x - \partial_x e_y)$ is continuous. We can satisfy this condition if $\partial_y e_x$ and $\partial_x e_y$ are continuous. The continuity of the tangent component of the magnetic field in the y -direction indicates that $(i k e_x - \partial_x e_z)$ must be continuous. We can rewrite this term by using Eq. (3.188), as follows:

$$\begin{aligned} i k e_x - \partial_x e_z &= i k e_x + \frac{1}{i k} \partial_x (\partial_x e_x + \partial_y e_y) \\ &= \frac{1}{i k} (-k^2 e_x + \partial_x^2 e_x + \partial_{x,y}^2 e_x) \\ &= \frac{1}{i k} \left(-\frac{\omega^2}{c^2} \varepsilon(\omega) e_x + \partial_y (\partial_x e_y - \partial_y e_x) \right), \end{aligned} \quad (3.193)$$

where we have used the wave equation Eq. (3.191). This last condition is satisfied since $\varepsilon(\omega) e_x$ is already continuous.

Now turning to the boundary conditions on the horizontal surfaces H_1 and H_2 .

The continuity of the normal component of $\mathbf{D}$ implies the continuity of $\varepsilon(\omega) e_y$ at the horizontal surfaces of the waveguide. The continuity of the tangential components of the electric field implies that e_x and e_z must also be continuous.

The continuity of the z -component, together with Eq. (3.188), implies that $\partial_x e_x + \partial_y e_y$ must also be continuous. This result can be satisfied if, independently, we require that $\partial_x e_x$ and $\partial_y e_y$ are continuous on the frontier.

For the magnetic field, the continuity of the normal component at the horizontal surfaces implies the continuity of $(i k e_x - \partial_x e_z)$, which would be satisfied only if $\partial_x e_z$. The continuity of the tangent component of the magnetic field in the z -direction implies that $(\partial_y e_x - \partial_x e_y)$ is continuous. We can satisfy this condition if, independently, $\partial_y e_x$ and $\partial_x e_y$ are continuous. The continuity of the tangent x -component of the magnetic field on the horizontal surfaces indicates that $(\partial_y e_z - i k e_y)$ must be continuous. We can rewrite this term using Eq. (3.188), as:

$$\begin{aligned} \partial_y e_z - i k e_y &= -\frac{1}{i k} \partial_y (\partial_x e_x + \partial_y e_y) - i k e_y \\ &= -\frac{1}{i k} (\partial_y^2 e_y - k^2 e_y + \partial_{x,y}^2 e_x) \\ &= \frac{1}{i k} \left(-\frac{\omega^2}{c^2} \varepsilon(\omega) e_y + \partial_x (\partial_y e_x - \partial_x e_y) \right), \end{aligned} \quad (3.194)$$

where we have used the wave equation Eq. (3.191). This last condition is satisfied since $\varepsilon(\omega) e_y$ is already continuous on these horizontal surfaces.

From the previous discussion about the boundary conditions, we conclude that there are some conditions that are incompatible. The origin of this problem lies in the impossibility of defining a normal and tangential component at the corners of the rectangular waveguide. For example, the y -component of the electric field is normal to the horizontal surfaces H_1 and H_2 , so that $\varepsilon(\omega) e_y$ must be continuous at those surfaces. However, the same y -direction is tangential when referring to the vertical surfaces V_1 and V_2 , where only e_y must be continuous. In this case, we conclude that, to satisfy both conditions at the four corners of the waveguide, $(x, y) \in \{(0, 0), (a, 0), (0, b), (a, b)\}$, it must be that the transverse components should vanish, i.e., $e_x = e_y = 0$. We can extend this observation and seek stationary solutions where $e_y(x, y) \equiv 0$ for all points in space, and this condition will define our X -mode solution. Similarly, we can search for and independently solve where $e_x(x, y) \equiv 0$, and these conditions will define the Y -mode.

First, let us discuss the surface stationary X -modes. For these modes, we assume that the electric field only has e_x and e_z components, while we set $e_y = 0$. By using Gauss' equation, Eq. (3.188), we note that the z -component is completely determined by the e_x component:

$$e_z = \frac{i}{k} \frac{\partial e_x}{\partial x}, \quad (3.195)$$

so that the only degree of freedom is e_x . By considering the boundary conditions on the waveguide surfaces, we find that for the vertical surfaces V_1 and V_2 ,

the components $\varepsilon(\omega)e_x$, $\partial_x e_x$, and $\partial_y e_x$ must be continuous. For the horizontal surfaces H_1 and H_2 , the components e_x , $\partial_x e_x$, and $\partial_y e_x$ must be continuous.

Here we note an apparent contradiction. From the continuity of the normal component of the electric field, we have that $\varepsilon(\omega)e_x$ must be continuous at the vertical surfaces V_1 and V_2 . However, from the continuity of the tangential component of the electric field, only e_x must be continuous at the horizontal surfaces H_1 and H_2 . But we know that it is impossible for both e_x and $\varepsilon(\omega)e_x$ to be continuous at the interface between dielectrics with different properties. In order to fulfill both requirements independently, we have two possibilities: these define the mode X_a solutions and the mode X_b solutions.

For the mode X_a solutions, the components $\varepsilon(\omega)e_x$, $\partial_x e_x$, and $\partial_y e_x$ must be continuous. Also, it is required that, at the horizontal surfaces of the waveguide, the transverse component of the electric field vanishes, i.e., $e_x(x, 0) = e_x(x, b) = 0$ for all values $0 \leq x \leq a$. The wave equation given by Eq. (3.191) can be solved by the separation of variables method. Hence, we look for solutions of the form $e_x(x, y) = f(x)g(y)$ such that these functions satisfy

$$\frac{f''(x)}{f(x)} + \frac{g''(y)}{g(y)} - K^2 = 0. \quad (3.196)$$

By considering explicitly the boundary conditions for X_a -modes and avoiding nonphysical exponentially growing solutions, we find oscillatory solutions in the y -direction and exponentially decaying functions in the x -direction. This means that the X_a -modes solutions are given by $e_x^{(n)}(x, y) = f_n(x)g_n(y)$ with

$$g_n(y) = \sin\left(\frac{n\pi}{b}y\right), \quad (3.197)$$

where $n = 1, 2, 3, \dots$. We have a surface-decaying behavior from the waveguide surfaces in the x -direction:

$$f_n(x) = \begin{cases} Ae^{\Lambda_2 x}, & x < 0, \\ Be^{-\Lambda_1 x} + Ce^{\Lambda_1 x}, & 0 < x < a, \\ De^{-\Lambda_2 x}, & x > a, \end{cases} \quad (3.198)$$

where we have defined the wave numbers

$$\Lambda_{1,2} = \sqrt{\left(\frac{n\pi}{b}\right)^2 + k^2 - \frac{\omega^2}{c^2}\varepsilon_{1,2}(\omega)}. \quad (3.199)$$

These wave numbers indeed depend on integer n , wave number k , and wave frequency ω . This means that $\Lambda_{1,2} = \Lambda_{1,2}(n, k, \omega)$. However, we have omitted an

explicit dependence on these parameters to emphasize the dependence of $\Lambda_{1,2}$ on the different dielectric constants of the materials $\varepsilon_{1,2}$.

Now, considering the continuity of $\varepsilon(\omega)e_x$ and the derivative $\partial_x e_x$ at the vertical surfaces V_1 and V_2 , we obtain the following condition in order to obtain non-trivial solutions for the X_a -modes:

$$\mathcal{F}_{X_a}(n, k, \omega) = e^{a\Lambda_1} \left(\frac{\Lambda_1 \varepsilon_2 + \Lambda_2 \varepsilon_1}{\Lambda_1 \varepsilon_2 - \Lambda_2 \varepsilon_1} \right)^2 - e^{-a\Lambda_1} = 0. \quad (3.200)$$

This equation gives us all the values of the allowed frequencies ω that contribute to the zero-point energy.

Let us now discuss the X_b -mode solutions. Now, the components e_x , $\partial_x e_x$, and $\partial_y e_x$ must be continuous, and the transverse electric field must vanish at the vertical surfaces of the waveguide, i.e., $e_x(0, y) = e_x(a, y) = 0$ for all values $0 \leq y \leq b$. As before, we look for solutions that are exponentially decaying from the waveguide surface. By using the separation of variables method, we note that it must refer to oscillatory solutions in the x -direction and exponentially decaying solutions in the y -direction. For the X_b -modes, we have solutions of the form $e_x^{(n)}(x, y) = f_n(x)g_n(y)$, where in this case

$$f_n(x) = \sin\left(\frac{n\pi}{a}x\right), \quad (3.201)$$

where $n = 1, 2, 3, \dots$, and in the y -direction, it is found an exponentially decaying behavior:

$$g_n(y) = \begin{cases} \mathcal{A}e^{K_2 y}, & y < 0, \\ \mathcal{B}e^{-K_1 y} + Ce^{K_1 y}, & 0 < y < b, \\ \mathcal{D}e^{-K_2 y}, & y > b. \end{cases} \quad (3.202)$$

Here we have defined the wave numbers

$$K_{1,2} = \sqrt{\left(\frac{n\pi}{a}\right)^2 + k^2 - \frac{\omega^2}{c^2}\varepsilon_{1,2}(\omega)}, \quad (3.203)$$

where $K_{1,2} = K_{1,2}(n, k, \omega)$. Now, considering that for the X_b -modes, we need to ensure the continuity of $e_x(x, y)$ and of $\partial_y e_x(x, y)$, we find the condition to have non-trivial solutions for the X_b -mode as

$$\mathcal{F}_{X_b}(n, k, \omega) = e^{bK_1} \left(\frac{K_1 + K_2}{K_1 - K_2} \right)^2 - e^{-bK_1} = 0, \quad (3.204)$$

This condition gives us some normal frequencies that contribute to the zero-point energy.

Now, let us focus on the surface stationary Y -modes. In this case, we look for stationary field solutions where the electric field has only e_y and e_z components, while $e_x = 0$. By using Gauss's law, Eq. (3.188), we see that e_z is not independent, and therefore, e_y is the only degree of freedom for the Y -modes. In turn, this component must satisfy the boundary conditions at the waveguide interface between the dielectrics. For the vertical surfaces V_1 and V_2 : the components e_y , $\partial_x e_y$, and $\partial_y e_y$ must be continuous. While for the horizontal surfaces H_1 and H_2 : the components $\varepsilon(\omega)e_y$, $\partial_x e_y$, and $\partial_y e_y$ must be continuous. In order to accomplish this, we need to add some supplementary conditions that define two kinds of modes for the Y -solutions.

Analogous to the X -modes case, the mode Y_a solution will be given by the components e_y , $\partial_x e_y$, and $\partial_y e_y$ being continuous, with the supplementary condition that the transverse component of the electric field is null at the horizontal surfaces of the waveguide, i.e., $e_y(x, 0) = e_y(x, b) = 0$ for all values $0 \leq x \leq a$. By using these conditions and looking for non-null solutions, one obtains an equation for the frequencies of the electromagnetic wave inside the waveguide,

$$\mathcal{F}_{Y_a}(n, k, \omega) = e^{a\Lambda_1} \left(\frac{\Lambda_1 + \Lambda_2}{\Lambda_1 - \Lambda_2} \right)^2 - e^{-a\Lambda_1} = 0. \quad (3.205)$$

Finally, for the mode Y_b solution, the components $\varepsilon(\omega)e_y$, $\partial_x e_y$, and $\partial_y e_y$ must be continuous with the additional condition $e_y(0, y) = e_y(a, y) = 0$, for all values $0 \leq y \leq b$. In this case, we find that the condition that defines the frequency for the surface modes of type Y_b is given by

$$\mathcal{F}_{Y_b}(n, k, \omega) = e^{bK_1} \left(\frac{K_1\epsilon_2 + K_2\epsilon_1}{K_1\epsilon_2 - K_2\epsilon_1} \right)^2 - e^{-bK_1} = 0, \quad (3.206)$$

where $\Lambda_{1,2}$ and $K_{1,2}$ have been defined in Eq. (3.199) and Eq. (3.203). As in the slab geometry case, we find that the expressions in Eq. (3.200) and Eqs. (3.204-3.206) give us all the possible values of the surface mode frequencies for the electromagnetic field inside the dielectric cavity. With this result, we are able to calculate the zero-point energy inside the waveguide and, consequently, analyze the Casimir effect.

The zero-point energy can be evaluated by a similar expression to the slab case, now considering that we have four types of surface modes. It follows that

$$E_{ZP} = \left(\frac{\hbar L_z}{4\pi} \right) \int_{-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_r (\omega_r^X(n, k) + \omega_r^Y(n, k)) dk, \quad (3.207)$$

where ω_N^X and ω_N^Y are all the allowed frequencies for the X -mode and Y -mode. Again, considering the argument principle, we interpret each sum over r as a

sum over the poles of $\mathcal{F}_{Y,X}$; therefore, it can be recast as a complex integral:

$$E_{ZP} = \left(\frac{\hbar L_z}{4\pi} \right) \frac{1}{2\pi i} \int_{-\infty}^{\infty} \sum_{n=1}^{\infty} \left[\oint_C \omega \frac{\mathcal{F}'_X(n, k, \omega)}{\mathcal{F}_X(n, k, \omega)} d\omega + \oint_C \omega \frac{\mathcal{F}'_Y(n, k, \omega)}{\mathcal{F}_Y(n, k, \omega)} d\omega \right] dk, \quad (3.208)$$

where the prime denotes the derivative with respect to ω . As in the slab geometry case, we assume that the contour C is given by Fig. 3.4. In the limit of infinite radius for the contour C , the only non-zero contribution to the complex integral above comes from the imaginary axis $\omega = i\xi$, where $\xi \in (+\infty, -\infty)$. By a change of variables, we define $F_X(\xi) = \mathcal{F}_X(i\xi)$.

Performing an integration by parts and some manipulations, we find

$$E_{ZP} = \left(\frac{\hbar L_z}{8\pi^2} \right) \int_{-\infty}^{\infty} \left\{ \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} [\ln F_X(n, k, \xi) + \ln F_Y(n, k, \xi)] d\xi \right\} dk. \quad (3.209)$$

Now, we have to consider that there are two contributions for each X -mode and Y -mode. Hence, by using explicitly the boundary equations for all the surface modes, Eq. (3.200) and Eqs. (3.204-3.206), we obtain the zero-point energy in the dielectric waveguide as

$$\begin{aligned} E_{ZP} = \left(\frac{\hbar L_z}{8\pi^2} \right) \int_{-\infty}^{\infty} \left\{ \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \left[\ln \left(e^{a\lambda_1} \left(\frac{\lambda_1 \epsilon_2 + \lambda_2 \epsilon_1}{\lambda_1 \epsilon_2 - \lambda_2 \epsilon_1} \right)^2 - e^{-a\lambda_1} \right) \right. \right. \\ \left. \left. + \ln \left(e^{bv_1} \left(\frac{v_1 + v_2}{v_1 - v_2} \right)^2 - e^{-bv_1} \right) + \ln \left(e^{bv_1} \left(\frac{v_1 \epsilon_2 + v_2 \epsilon_1}{v_1 \epsilon_2 - v_2 \epsilon_1} \right)^2 - e^{-bv_1} \right) \right. \right. \\ \left. \left. + \ln \left(e^{a\lambda_1} \left(\frac{\lambda_1 + \lambda_2}{\lambda_1 - \lambda_2} \right)^2 - e^{-a\lambda_1} \right) \right] d\xi \right\} dk, \end{aligned} \quad (3.210)$$

where we have denoted the wave numbers for imaginary frequencies by

$$\lambda_{1,2} = \sqrt{\left(\frac{n\pi}{b} \right)^2 + k^2 + \frac{\xi^2}{c^2} \epsilon_{1,2}(i\xi)}, \quad (3.211)$$

and

$$v_{1,2} = \sqrt{\left(\frac{n\pi}{a} \right)^2 + k^2 + \frac{\xi^2}{c^2} \epsilon_{1,2}(i\xi)}, \quad (3.212)$$

These variables depend on the integer n , the wave number in the z -direction, k , and on the imaginary frequency ξ . It is worth noting that, in general, the dielectric constant depends on the wave frequency.

The Eq. (3.210) is the main result of Ref. [46]. This equation generalizes the Lifshitz formula for a rectangular waveguide. The original Lifshitz result, in the case of two parallel plates, can be recovered from our result if we keep one direction of the waveguide fixed and allow the others to go to infinity. More specifically, in this limit, we can consider that a is finite while $L_z, b \gg a$. In order to take this limit, we use the following relation:

$$\lim_{b \rightarrow \infty} \sum_{n=1}^{\infty} f\left(\frac{n\pi}{b}\right) = \left(\frac{b}{2\pi}\right) \int_{-\infty}^{\infty} d\tilde{k} f(\tilde{k})$$

and define the variable

$$K_i = \sqrt{\tilde{k}^2 + k^2 + \frac{\xi^2}{c^2} \epsilon_i(i\xi)}.$$

In this manner, we can write

$$\begin{aligned} E_{ZP}^{plates} = N \int & \left\{ \ln \left(\left(\frac{K_1 + K_2}{K_1 - K_2} \right)^2 e^{2aK_1} - 1 \right) \right. \\ & \left. + \ln \left(\left(\frac{K_1 \epsilon_2 + K_2 \epsilon_1}{K_1 \epsilon_2 - K_2 \epsilon_1} \right)^2 e^{2aK_1} - 1 \right) \right\} dk d\tilde{k} d\xi. \end{aligned} \quad (3.213)$$

where $N = \hbar L_z b / 16\pi^3$. This expression is obtained by considering the limits of the contributions of the first and fourth terms inside the integral of the general result Eq. (3.210). This is because the dependence of the second and third terms inside the integral in Eq. (3.210) only depends on the length b through the exponential factor, which gives us an infinite (constant) term in the limit $b \rightarrow \infty$. In the above integral, we have that all the limits of integration are from $-\infty$ to $+\infty$. By considering k and $\tilde{k}$ as coordinates of a two-dimensional space, defining $\kappa = \sqrt{k^2 + \tilde{k}^2}$, and performing the angular integration, we obtain

$$\begin{aligned} E_{ZP}^{plates} = \tilde{N} \int_0^{\infty} & \left\{ \kappa \int_{-\infty}^{\infty} \left[\ln \left(\left(\frac{K_1 + K_2}{K_1 - K_2} \right)^2 e^{2aK_1} - 1 \right) \right. \right. \\ & \left. \left. + \ln \left(\left(\frac{K_1 \epsilon_2 + K_2 \epsilon_1}{K_1 \epsilon_2 - K_2 \epsilon_1} \right)^2 e^{2aK_1} - 1 \right) \right] d\xi \right\} d\kappa, \end{aligned} \quad (3.214)$$

where $\tilde{N} = \hbar L_z b / 8\pi^2$. The above equation is exactly the Lifshitz formula, for the case of two parallel plates (separated by a finite distance a) with a medium of dielectric constant ϵ_1 between two media of dielectric constant ϵ_2 in a slab configuration.

Let us discuss the general result given by Eq. (3.210) for the case where the surfaces are perfect conductors. To do this, one can first rewrite the expression for the zero-point energy in a more compact way:

$$E_{ZP} = \left(\frac{\hbar L_z}{8\pi^2} \right) \int_{-\infty}^{\infty} \left\{ \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \left[\ln(\mathcal{X}_1 e^{a\lambda_1} - e^{-a\lambda_1}) + \ln(\mathcal{X}_2 e^{bv_1} - e^{-bv_1}) \right. \right. \\ \left. \left. + \ln(\mathcal{Y}_1 e^{bv_1} - e^{-bv_1}) + \ln(\mathcal{Y}_2 e^{a\lambda_1} - e^{-a\lambda_1}) \right] d\xi \right\} dk, \quad (3.215)$$

where the reflectivity indices are defined as follows:

$$\mathcal{X}_1 = \left(\frac{\lambda_1 \epsilon_2 + \lambda_2 \epsilon_1}{\lambda_1 \epsilon_2 - \lambda_2 \epsilon_1} \right)^2, \quad \mathcal{X}_2 = \left(\frac{v_1 + v_2}{v_1 - v_2} \right)^2, \\ \mathcal{Y}_1 = \left(\frac{v_1 \epsilon_2 + v_2 \epsilon_1}{v_1 \epsilon_2 - v_2 \epsilon_1} \right)^2, \quad \mathcal{Y}_2 = \left(\frac{\lambda_1 + \lambda_2}{\lambda_1 - \lambda_2} \right)^2. \quad (3.216)$$

In the ideal case, the medium inside the waveguide is a perfect vacuum with $\epsilon_1 = 1$, whereas the boundaries are perfect reflecting surfaces with $\epsilon_2 \rightarrow \infty$. From this follows that the wave numbers inside the waveguide are given by $\lambda_1 \rightarrow \lambda^{(0)}$ and $v_1 \rightarrow v^{(0)}$, with

$$\lambda^{(0)} = \sqrt{\left(\frac{n\pi}{b} \right)^2 + k^2 + \frac{\xi^2}{c^2}}, \\ v^{(0)} = \sqrt{\left(\frac{n\pi}{a} \right)^2 + k^2 + \frac{\xi^2}{c^2}}. \quad (3.217)$$

Outside the waveguide, one has a perfect conductor with $\epsilon_2 \rightarrow \infty$, and consequently, $\lambda_2, v_2 \rightarrow \infty$. It can be shown that in this limit all the reflectivity indexes, Eq. (3.216), tend to unity, and hence, the zero-point energy for the ideal conducting waveguide is given by

$$E_{ZP}^{Ideal} = \left(\frac{\hbar L_z}{4\pi^2} \right) \int_{-\infty}^{\infty} \left\{ \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \left[a\lambda^{(0)} + bv^{(0)} + \ln(1 - e^{-2a\lambda^{(0)}}) \right. \right. \\ \left. \left. + \ln(1 - e^{-2bv^{(0)}}) \right] d\xi \right\} dk. \quad (3.218)$$

The above expression is symmetric under the permutation of the cavity length, so we can write

$$E_{ZP}^{Ideal} = \left(\frac{\hbar c L_z}{4\pi^2} \right) \left(I(a, b) + I(b, a) \right), \quad (3.219)$$

with the integral

$$I(a, b) = \sum_{n=1}^{\infty} \int \left[a \sqrt{\left(\frac{n\pi}{b}\right)^2 + \rho^2} + \ln \left(1 - e^{-2a \sqrt{\left(\frac{n\pi}{b}\right)^2 + \rho^2}} \right) \right] d^2 \rho, \quad (3.220)$$

where we have defined the bidimensional vector $\vec{\rho} = (k, \xi/c)$ with $\rho^2 = k^2 + \xi^2/c^2$. The ideal result of the zero-point energy given by Eq. (3.218) needs to be regularized. Here we use dimensional regularization [74–76]⁷. In this manner, let us define the s -dimensional integrals

$$\begin{aligned} J_s(a, b) &= a \sum_{n=1}^{\infty} \int \sqrt{\left(\frac{n\pi}{b}\right)^2 + \rho^2} d^s \rho, \\ K_s(a, b) &= \sum_{n=1}^{\infty} \int \ln \left(1 - e^{-2a \sqrt{\left(\frac{n\pi}{b}\right)^2 + \rho^2}} \right) d^s \rho, \end{aligned} \quad (3.221)$$

from these expressions, we see that the zero-point energy Eq. (3.218) can be recovered when $s = 2$, since it is clear that $I(a, b) = J_2(a, b) + K_2(a, b)$. The terms in Eq. (3.221) only depend on the modulus of the s -dimensional vector $\vec{\rho}$. One can perform the general solid angle integration with Eq. (3.112). On the other hand, the integration over the modulus ρ can be realized by using the Beta function representations

$$B(x, y) = \frac{\Gamma(\alpha)\Gamma(\gamma)}{\Gamma(\alpha + \gamma)} = \int_0^{\infty} y^{\alpha-1} (1+y)^{-\alpha-\gamma} dy. \quad (3.222)$$

Finally, by using the reflection formula of the Riemann zeta function, analogous to Eq. (3.116), one can prove that

$$J_s(a, b) = -\frac{a}{2b^{s+1}} \pi^{s/2-1} \Gamma\left(\frac{s+2}{2}\right) \zeta(s+2). \quad (3.223)$$

The second regularized integral K_s , in Eq. (3.221), can be rewritten by using the Taylor expansion of the logarithm function as follows:

$$\ln(1-x) = -\sum_{k=1}^{\infty} \frac{x^k}{k}, \quad \text{for } |x| < 1. \quad (3.224)$$

Hence, we can write

$$K_s(a, b) = -\frac{2\pi^{s/2}}{\Gamma(s/2)} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{m} \int_0^{\infty} \rho^{s-1} e^{-2ma \sqrt{\left(\frac{n\pi}{b}\right)^2 + \rho^2}} d\rho. \quad (3.225)$$

⁷A more detailed application of this technique is given in Sec. 4.3

In order to perform the integration above, we use the integral representation of the modified Bessel function [77]

$$K_\nu(xz) = \frac{\sqrt{\pi}}{\Gamma(\nu + \frac{1}{2})} \left(\frac{x}{2z}\right)^\nu \int_0^\infty t^{2\nu} \frac{e^{-x\sqrt{t^2+z^2}}}{\sqrt{t^2+z^2}} dt, \quad (3.226)$$

hence, one obtains that

$$K_s(a, b) = \frac{2\pi^{\frac{3s-1}{2}}}{b^s} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{m} \frac{d}{d\lambda} \left(K_{\frac{s-1}{2}}(\lambda n) \left(\frac{2n}{\lambda}\right)^{\frac{s-1}{2}} \right),$$

where we have defined $\lambda = 2m\pi a/b$. Now, by using the following recursion formula of the modified Bessel function

$$\left(\frac{1}{z} \frac{d}{dz}\right)^m K_0(z) = (-1)^m z^{-m} K_m(z), \quad (3.227)$$

and also considering the series expansion

$$\sum_{n=1}^{\infty} K_0(\lambda n) = \frac{1}{2} \left(C + \ln \left(\frac{\lambda}{4\pi} \right) \right) + \frac{\pi}{2\lambda} + \pi \sum_{p=1}^{\infty} \left(\frac{1}{\sqrt{\lambda^2 + (2\pi p)^2}} - \frac{1}{2\pi p} \right), \quad (3.228)$$

one can obtain that

$$K_s(a, b) = 2\pi^{\frac{s-1}{2}} \left\{ \frac{1}{4a^s} \Gamma\left(\frac{s+1}{2}\right) \zeta(s+1) + \frac{1}{4\sqrt{\pi}} \Gamma\left(\frac{s+2}{2}\right) \zeta(s+2) \frac{a}{b^{s+1}} - \frac{1}{8\sqrt{\pi}} \Gamma\left(\frac{s+2}{2}\right) ab Z_2(a, b; s+2) \right\}, \quad (3.229)$$

where we have used the definition of the Epstein zeta function, Eq. (3.114). Now, putting everything together, one can recast Eq. (3.219) as

$$E_C^{Ideal} = \frac{\hbar c L_z}{8\pi^2} \left(\frac{\pi}{2} \zeta(3) \left(\frac{1}{a^2} + \frac{1}{b^2} \right) - ab Z_2(a, b, 4) \right), \quad (3.230)$$

which is the Eq. (3.118). By using the variable $r = a/b$, one can express this energy as

$$E_C^{Ideal} = \left(\frac{\hbar c L_z}{a^2} \right) E(r), \quad (3.231)$$

with the dimensionless function

$$E(r) = \frac{1}{16\pi} \zeta(3) (1 + r^2) - \frac{r^3}{8\pi^2} Z_2(r, 1, 4). \quad (3.232)$$

With the Casimir energy at hand, one can find the Casimir force

$$F_C^{Ideal} = -\frac{\partial E_C^{Ideal}}{\partial a}. \quad (3.233)$$

We can write it in terms of the adimensional variable r as

$$F_C^{Ideal} = \left(\frac{\hbar c L_z}{a^3} \right) f(r), \quad (3.234)$$

where

$$f(r) = \frac{\zeta(3)}{8\pi} - \frac{\zeta(4)}{\pi^2 r} + \frac{r^3}{8\pi^2} Z_2(r, 1, 4) - \frac{2r^3}{\pi^2} z(r), \quad (3.235)$$

and we have defined the function $z(r)$ given by

$$z(r) = \sum_{m,p=1}^{\infty} \frac{(mr)^2}{[(mr)^2 + p^2]^3}. \quad (3.236)$$

In Fig. 3.6, we show the graph of the Casimir energy and the Casimir force for a perfectly conducting waveguide of rectangular cross-section. The Casimir energy is always negative but exhibits a maximum value for some critical value r_c of the ratio between the waveguide lengths, $r = a/b$. Near that point, the Casimir force is null and changes its behavior from attractive for $r < r_c$ to repulsive for $r > r_c$. The dependence of the attractive-repulsive nature of the Casimir force on the length ratio of the cavity shape is well-known in the literature and is recovered in the limit of perfect conductivity [78, 79].

We conclude this section by presenting the corrections to the zero-point energy due to the finite conductivity of the waveguide material. First, we define some useful variables. Instead of working with the variables $\lambda_{1,2}$ and $\nu_{1,2}$, see Eq. (3.211) and Eq. (3.212), we define the variables p and $\tilde{p}$ given by

$$\begin{aligned} \left(\frac{n\pi}{b} \right)^2 + k^2 &= \varepsilon_1 \frac{\xi^2}{c^2} (p^2 - 1), \\ \left(\frac{n\pi}{a} \right)^2 + k^2 &= \varepsilon_1 \frac{\xi^2}{c^2} (\tilde{p}^2 - 1), \end{aligned} \quad (3.237)$$

and we define the variables s and $\tilde{s}$ as

$$\begin{aligned} p^2 - 1 + \frac{\varepsilon_2}{\varepsilon_1} &= s^2, \\ \tilde{p}^2 - 1 + \frac{\varepsilon_2}{\varepsilon_1} &= \tilde{s}^2. \end{aligned} \quad (3.238)$$

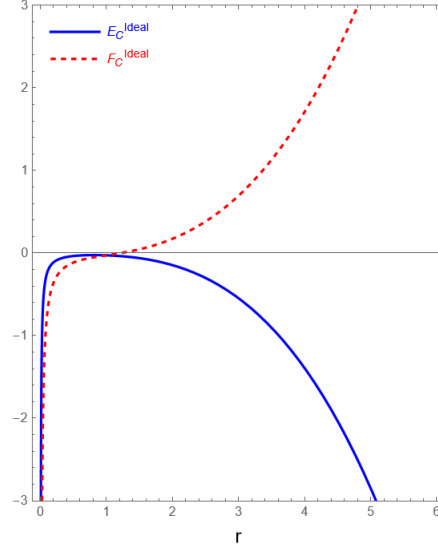


Figure 3.6: Casimir energy and force in the case of a waveguide with perfect conducting surfaces. These quantities are plotted as a function of the ratio $r = a/b$ between the lengths of the waveguide cross-section. The energy is measured in units of $\hbar c L_z / a^2$, while force units are $\hbar c L_z / a^3$. Graph taken of Ref. [46].

With these variables, one can show that $\lambda_1 = \sqrt{\epsilon_1} \xi p / c$, $\lambda_2 = \sqrt{\epsilon_1} \xi s / c$, $v_1 = \sqrt{\epsilon_1} \xi \tilde{p} / c$, and $v_2 = \sqrt{\epsilon_1} \xi \tilde{s} / c$. Hence, the reflectivity index, Eq. (3.216), can be rewritten as

$$\begin{aligned} \mathcal{X}_1 &= \left(\frac{p\epsilon_2 + s\epsilon_1}{p\epsilon_2 - s\epsilon_1} \right)^2, & \mathcal{X}_2 &= \left(\frac{\tilde{p} + \tilde{s}}{\tilde{p} - \tilde{s}} \right)^2, \\ \mathcal{Y}_1 &= \left(\frac{\tilde{p}\epsilon_2 + \tilde{s}\epsilon_1}{\tilde{p}\epsilon_2 - \tilde{s}\epsilon_1} \right)^2, & \mathcal{Y}_2 &= \left(\frac{p + s}{p - s} \right)^2. \end{aligned} \quad (3.239)$$

We showed in the previous section that these reflectivity indexes tend to unity in the case of a vacuum waveguide with perfect conductors on the outside: $\mathcal{X}_{1,2}, \mathcal{Y}_{1,2} \rightarrow 1$. For the case of an imperfect conducting surface, we expect a behavior that gives us some finite corrections to the ideal perfect conducting case, such as

$$\mathcal{X}_{1,2} = 1 + \Delta\mathcal{X}_{1,2}, \quad \mathcal{Y}_{1,2} = 1 + \Delta\mathcal{Y}_{1,2}. \quad (3.240)$$

Considering small corrections, we can expand the zero-point energy for the imperfect conductor case as

$$E_{ZP} = E_{ZP}^{Ideal} + \Delta E_{ZP}, \quad (3.241)$$

where the ideal case is given by Eq. (3.218) or equivalently by Eq. (3.230). The correction due to finite conductivity of the dielectric is given by the term ΔE_{ZP} .

Explicitly, in this case, we assume vacuum inside the waveguide with dielectric constant $\varepsilon_1 = 1$, while for the outside, we consider that the dielectric constant follows the plasma model and is given by $\varepsilon_2 = \varepsilon(\omega)$, where

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \quad (3.242)$$

and the plasma frequency ω_p is a specific characteristic of the material. Considering this, we have that in terms of the imaginary frequency, $\varepsilon_2 = 1 + \omega_p^2/\xi^2$.

Since inside the waveguide we have vacuum, the wave number there is $\lambda_1 \rightarrow \lambda^{(0)}$, see Eq. (3.217), and one can define p_0 such that $\lambda^{(0)} = \xi p_0/c$, and $s = \sqrt{p_0^2 + \omega_p^2/\xi^2}$. By expanding s up to first order in ξ/ω_p , we obtain

$$s \approx \frac{\omega_p}{\xi} + \frac{p_0^2 \xi}{2\omega_p}. \quad (3.243)$$

By using the above expansion together with Eq. (3.242) and that $\varepsilon_1 \rightarrow 1$ with $p \rightarrow p_0$, one finds the corrections to the reflectivity indexes:

$$\Delta\mathcal{X}_1 \approx \frac{4\xi}{p_0 \omega_p}, \quad \Delta\mathcal{Y}_2 \approx \frac{4p_0 \xi}{\omega_p}. \quad (3.244)$$

In a very similar way, we have that inside the waveguide, $v_1 \rightarrow v^{(0)}$, and with this, we define the variable $\tilde{p}_0$ such that $v^{(0)} = \xi \tilde{p}_0/c$, and $\tilde{s} = \sqrt{\tilde{p}_0^2 + \omega_p^2/\xi^2}$. Performing the expansion, one obtains the first corrections to the reflectivity indexes:

$$\Delta\mathcal{Y}_1 \approx \frac{4\xi}{\tilde{p}_0 \omega_p}, \quad \Delta\mathcal{X}_2 \approx \frac{4\tilde{p}_0 \xi}{\omega_p}. \quad (3.245)$$

By considering these finite conductivity corrections, one can write the zero-point energy correction as given by

$$\begin{aligned} \Delta E_{ZP} = \left(\frac{\hbar L_z}{8\pi^2} \right) \int_{-\infty}^{\infty} \left\{ \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \left[(\Delta\mathcal{X}_1 + \Delta\mathcal{Y}_2) \left(1 - e^{-2a\lambda^{(0)}} \right)^{-1} \right. \right. \\ \left. \left. + (\Delta\mathcal{X}_2 + \Delta\mathcal{Y}_1) \left(1 - e^{-2b\lambda^0} \right)^{-1} \right] d\xi \right\} dk. \end{aligned} \quad (3.246)$$

By exploring the symmetry of this energy correction under the permutation of the cavity lengths a and b , one can express this as a function of only the scale a and the ratio $r = a/b$. Also, considering that the plasma wavelength of the material is $\lambda_p = 2\pi c/\omega_p$, we can write

$$\Delta E_{ZP} = \hbar L_z c \lambda_p \left(\frac{U(r)}{a^3} + \frac{U(r^{-1})}{b^3} \right). \quad (3.247)$$

where we have defined the dimensionless function

$$U(r) = \frac{1}{2\pi^2} \sum_{n=1}^{\infty} \int_0^{\infty} \chi \left(\sqrt{(n\pi r)^2 + \chi^2} + \frac{\chi^2}{2\sqrt{(n\pi r)^2 + \chi^2}} \right) \left(\frac{1}{1 - e^{-2\sqrt{(n\pi r)^2 + \chi^2}}} \right) d\chi, \quad (3.248)$$

as expected, this integral needs to be regularized. We use dimensional regularization in the same manner as done previously for the case of the ideal perfect conducting waveguide. We find that

$$U(r) = -\frac{3\zeta(3)}{32\pi^2} + \frac{\zeta(4)}{16\pi^3 r} + \frac{r^3}{2\pi^3} z(r), \quad (3.249)$$

and one can express

$$\Delta E_{ZP} = \left(\frac{\hbar L_z c \lambda_p}{a^3} \right) \Delta E(r), \quad (3.250)$$

where $\Delta E(r) = U(r) + r^3 U(r^{-1})$.

This allows us to write the Casimir-Lifshitz energy for the dielectric waveguide in the plasma model as

$$E_C = \left(\frac{\hbar c L_z}{a^2} \right) \left(E(r) + \frac{\lambda_p}{a} \Delta E(r) \right). \quad (3.251)$$

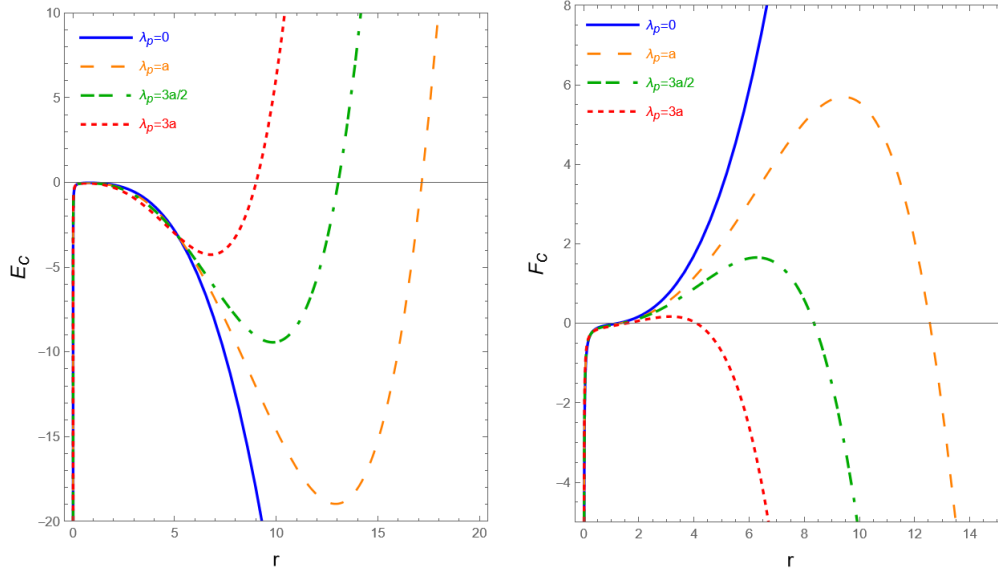
The Casimir-Lifshitz energy is shown in Fig. (3.7a) for different values of the plasma wavelength λ_p , measured in units of the length a . In this figure, we note that the effect of the finite conductivity correction is to change the concavity of the Casimir energy for large values of r . This leads to the appearance of a local minimum of the zero-point energy near some value r^* . Near this point, the Casimir-Lifshitz energy behaves as an effective potential well. In this case, the Casimir force is shown in Fig. (3.7b). In that figure, a second inversion in the attractive-repulsive nature of the Casimir force occurs at r^* . This second point is also an equilibrium point with zero Casimir force, but it corresponds to a stable equilibrium, whereas the initial critical point, r_c , is an unstable equilibrium.

3.2.3 Phonons

For future convenience, we assume Gaussian units in this section.

Before introducing interactions between the fields, let us explore a useful theory of quasi-particles. To introduce these quasi-particles, let us start with an ideal fluid obeying the free Euler's equation

$$\frac{\partial}{\partial t} \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p \quad (3.252)$$



(a) The final Casimir energy corrected by the finite dielectric properties of the material. The correction depend on the plasma wave length λ_p with respect to a .

(b) The final Casimir force corrected by the finite dielectric properties of the material. The correction depend on the plasma wave length λ_p with respect to a .

Figure 3.7: Plots for the anharmonic Casimir oscillator. The energies and forces are in units of $\hbar c L_z / a^2$ and $r = a/b$ is the ratio between the length of the cross-section. Both graphs have been taken of Ref. [46].

where $\rho(\mathbf{x}, t)$ is the mass density, $p(\mathbf{x}, t)$ is the local pressure, and $\mathbf{v}(\mathbf{x}, t)$ is the local velocity. Assuming there is no loss of mass, the fluid also obeys the continuity equation

$$\frac{\partial}{\partial t} \rho = -\nabla \cdot (\rho \mathbf{v}). \quad (3.253)$$

We know that small perturbations, like sound, inside liquids or solids, can propagate without generating significant changes in the mean values of the medium. Therefore, let us consider a small perturbation propagating in this ideal fluid. This small perturbation is characterized by the following local variations:

$$p(\mathbf{x}, t) = p_0 + \delta p(\mathbf{x}, t), \quad (3.254)$$

$$\rho(\mathbf{x}, t) = \rho_0 + \delta \rho(\mathbf{x}, t), \quad (3.255)$$

$$\mathbf{v}(\mathbf{x}, t) = \delta \mathbf{v}(\mathbf{x}, t), \quad (3.256)$$

where we denote by the index 0 the mean quantities that are static in time and position-independent. Making this change of variables in Eq. (3.252), using a Taylor expansion to first order in $1/(\rho_0 + \delta \rho)$, and disregarding products of small

perturbations, i.e., contributions of order $O(\delta^2)$, we obtain

$$\frac{\partial}{\partial t} \delta \mathbf{v} = -\frac{1}{\rho_0} \nabla \delta p, \quad (3.257)$$

Now we observe that, in a fixed volume, any variation in the pressure can be directly related to a variation in the density of the system, and that the square root of the variation of pressure in terms of the density is the speed of sound, c_s , inside a material. Therefore, we have

$$\nabla \delta p = \frac{\partial p_0}{\partial \rho_0} \nabla \delta \rho = c_s^2 \nabla \delta \rho, \quad (3.258)$$

which implies that the perturbations satisfy the following equation:

$$\frac{\partial}{\partial t} \delta \mathbf{v} = -\frac{c_s^2}{\rho_0} \nabla \delta \rho. \quad (3.259)$$

With an analogous procedure in the continuity equation (Eq. (3.253)), we obtain

$$\frac{\partial}{\partial t} \delta \rho = -\rho_0 \nabla \delta \mathbf{v}. \quad (3.260)$$

Now let us consider that the perturbation of the velocity is a gradient of a scalar potential, i.e., $\delta \mathbf{v} = \nabla \phi(\mathbf{x}, t)$. In terms of the scalar potential, the previous two equations become

$$\frac{\partial}{\partial t} \nabla \phi = -\frac{c_s^2}{\rho_0} \nabla \delta \rho, \quad (3.261)$$

$$\frac{\partial}{\partial t} \delta \rho = -\rho_0 \Delta \phi. \quad (3.262)$$

Taking the time derivative of Eq. (3.261) and using Eq. (3.262), we get

$$\left(\frac{1}{c_s^2} \frac{\partial^2}{\partial t^2} - \Delta \right) \phi = 0, \quad (3.263)$$

and, taking the gradient of Eq. (3.262) and using Eq. (3.261), we obtain

$$\left(\frac{1}{c_s^2} \frac{\partial^2}{\partial t^2} - \Delta \right) \delta \rho = 0. \quad (3.264)$$

Thus, $\phi(\mathbf{x}, t)$ and $\delta \rho(\mathbf{x}, t)$ satisfy wave equations. With this remarkable result, we now can construct the associated Lagrangian, the Hamiltonian, then impose the canonical commutation relation (Eq. (3.4)), and then proceed with the analogous

procedure discussed in Sec. 3.1.1, but now we have the speed of sound instead of the speed of light⁸. Following similar steps that lead us to Eq. (3.11), we obtain the following expansion of the operator $\delta\rho$:

$$\delta\rho(t, \mathbf{x}) = \sum_{\mathbf{k}} \sqrt{\frac{\hbar\rho_0\omega}{2Vc_S^2}} \left(c_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} - c_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right), \quad (3.265)$$

where V is some quantization volume, $k = \|\mathbf{k}\|$, $\omega = c_S k$, and $c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger$ are the **phonon** annihilation and creation operators. Therefore, we have obtained a quantum description of the perturbations in the fluid. These collective behaviors that we call phonons are quasi-particles and are important for many transport properties of materials [80, 81].

The correlation function of the phonons can be directly calculated, renaming $\delta\rho$ as ρ_1 ⁹ and transitioning to the continuous momentum, we have

$$\begin{aligned} \langle \rho_1(\mathbf{x}, t) \rho_1(\mathbf{x}', t') \rangle &= (\rho_1(\mathbf{x}', t') \rho_1(\mathbf{x}, t) \Omega, \Omega) = \frac{\hbar\rho_0}{12\pi^3 c_S^2} \int c_S k e^{i(\mathbf{k}\cdot(\mathbf{x}'-\mathbf{x})-c_S k(t'-t))} d^3k \\ &= \frac{\hbar\rho_0}{2\pi^2 c_S} \frac{(\mathbf{x}' - \mathbf{x})^2 + 3c_S^2(t' - t)^2}{[(\mathbf{x}' - \mathbf{x}) + c_S(t' - t)]^3 [c_S(t' - t) - (\mathbf{x}' - \mathbf{x})]^3}, \end{aligned} \quad (3.266)$$

this is the same form of the correlation function for the time derivative of a massless scalar field, apart from the factor ρ_0 and changing the speed of sound by the speed of light.

Using a limit of the previous expression, Ref. [82] showed that phonons in the vacuum state induce a correction in the cross-section of light scattering, proportional to the fifth power of the light frequency. Compared to scattering by thermal density fluctuations, it is found that this correction can be of order 0.5% for water at room temperature and optical frequencies. Many studies have considered the previous equation and its implications. Since near a boundary, the correlation function of the phonons resembles the behavior of the electric and magnetic fields, it was proposed that the phononic Casimir effect [83] could be used to search for an observable effect related to quantum fields near boundaries. Some geometries and their effects on the correlation function have also been investigated [84].

More recently, it has become clear that the space and time average of the phonon-phonon correlation function plays a fundamental role in its understanding and potential observation. Additionally, it is argued that the comprehension

⁸Remember that in Sec. 3.1.1 we had $c = 1$.

⁹Therefore, the total density is given by $\rho = \rho_0 + \rho_1$.

of zero-point fluctuations may shed light on the measurement problem in quantum mechanics; see Ref. [85] and the references therein.

Zero-point fluctuations sensor

As we said, light scattering can be affected by the zero-point fluctuations due to the phonons in a material. However, such a measurement may be difficult to realize due to the non-static behaviors of the fluctuations. Therefore, instead of trying to “see” the fluctuations directly, we may use some kind of external sensor to measure their effects remotely. First, let us set up our model.

A charge in the vicinity of a diluted dielectric, let's say at some distance d along the z -axis, can have its dynamics computed using the image method [86]. Alternatively, we can decompose the dielectric into the sum of electric dipoles. Denoting the polarizability of one molecule by α_m , the mass density of the dielectric by ρ , the mass of the molecule by m , and $|d\hat{z} - \mathbf{x}'| = r$ as the distance between the charge and the dipole, the force of one dipole on the electric charge q is given by

$$\mathbf{F}_{1d} = -2q^2\alpha_m \left(\frac{\rho(\mathbf{x}', t)}{m} \right) \frac{(d\hat{z} - \mathbf{x}')}{r^6}, \quad (3.267)$$

using that $\rho(\mathbf{x}', t) = \rho_0 + \rho_1(\mathbf{x}', t)$, with ρ_1 given by Eq. (3.265), and integrating over the semi-infinite dielectric $V = \{(\mathbf{x}', y', z') | -\infty < x' < \infty, -\infty < y' < \infty, -\infty < z' \leq 0\}$, we obtain the electric force due to the diluted dielectric

$$\mathbf{F} = -\frac{\pi\alpha_m q^2}{2d^2} \left(\frac{\rho_0}{m} \right) - 2q^2 \frac{\alpha_m}{m} \int_V \rho_1(\mathbf{x}', t) \frac{(d\hat{z} - \mathbf{x}')}{r^6} dV = \mathbf{F}_0 + \mathbf{F}_1. \quad (3.268)$$

Thus, using the phonons and the diluted dielectric approximation, we expect to obtain a correction to the classical force due to the zero-point fluctuations. Since this force is now an operator, we need to compute its average. However, it follows directly that $\langle \mathbf{F}_1 \rangle = 0$, but $\langle \mathbf{F}_1^2 \rangle \neq 0$. Therefore, the effects of the phonons are on the root mean square of the force.

The effects of the fluctuations need to be averaged for a proper description of the observable effect, since the time-energy uncertainty principle allows large fluctuations in a short time. Therefore, we need to choose a sampling function, say $g(t)$, such that

$$\begin{cases} \int g(t) dt = \mathbb{E}[1] = 1, \\ \int g(t) e^{i\omega t} dt = \tilde{g}(\omega), \\ |\tilde{g}(\omega)| \rightarrow 0, \quad \text{if } \omega \gg 1, \end{cases} \quad (3.269)$$

to evaluate our time averages, denoted by $\mathbb{E}[\cdot]$. Since in $\mathbf{F}_1^2$ only ρ_1 is time-dependent, we shall compute the time average of $\rho_1(\mathbf{x}', t)\rho_1(\mathbf{x}', t)$. But first, we

notice that we expect the momentum that contributes to the integral of ρ_1 to be of order $k \geq d^{-1}$. Therefore, we have a typical time scale in our system given by $\tau \approx d/c_S$. Thus, any high-momentum divergences that may appear are suppressed by the time average. Then we have that

$$\langle \mathbb{E} [\rho_1^2(\mathbf{x}, t)] \rangle = \sum_{\mathbf{k}} \frac{\hbar \omega \rho_0}{2V c_S^2} |\tilde{g}(\omega)|^2, \quad (3.270)$$

in the continuous momentum, it follows

$$\begin{aligned} \langle \mathbb{E} [\rho_1^2(\mathbf{x}, t)] \rangle &= \frac{\hbar \rho_0}{2(2\pi)^3 c_S^2} \int \omega |\tilde{g}(\omega)|^2 d^3k \\ &= \frac{\hbar \rho_0}{4\pi^2 c_S^5} \int_0^\infty \omega^3 |\tilde{g}(\omega)|^2 d\omega \\ &= \frac{\hbar \rho_0}{4\pi^2 \tau^4 c_S^5} C_g, \end{aligned} \quad (3.271)$$

where we have defined $C_g = \tau^4 \int_0^\infty \omega^3 |\tilde{g}(\omega)|^2 d\omega$. Therefore, we can recast the root mean square of the force of one dipole, $\sqrt{\langle \mathbf{F}_1^2 \rangle} = |\mathbf{F}_1|$, as

$$\begin{aligned} |\mathbf{F}_1| &= \frac{\alpha_m q^2}{\pi \tau^2 m} \sqrt{\frac{\hbar \rho_0 C_g}{c_S^5}} \int_V \frac{1}{r^5} dV \\ &= \frac{\alpha_m q^2}{3d^2 \tau^2 m} \sqrt{\frac{\hbar \rho_0 C_g}{c_S^5}}. \end{aligned} \quad (3.272)$$

Defining $\tau = ad/c_S$, for some $a \geq 1$, we find

$$|\mathbf{F}_1| = \frac{\alpha_m q^2}{3d^4 a^2 m} \sqrt{\frac{\hbar \rho_0 C_g}{c_S}}. \quad (3.273)$$

Now, we can divide the root mean square of the force due to the phonons by the root mean square of the classical force to compare its intensity. Thus, we have

$$\frac{|\mathbf{F}_1|}{|\mathbf{F}_0|} = \frac{2}{3\pi} \sqrt{\frac{\hbar}{\rho_0 c_S}} \frac{C_g}{a^2 d^2}. \quad (3.274)$$

In order to properly estimate the fluctuations, we need to fix a dielectric, an electric charge, and the function $\tilde{g}(\omega)$. Let's say that we have an electron as the test charge and the diluted dielectric is He^4 , so we still need the specifics of

$\tilde{g}(\omega)$. There are many choices of the sampling function that satisfy the desired properties of Eq. (3.269). For example, if we set $\tau = 1$, then $g = e^{-\omega^2/4}$ gives us $C_g \approx 8$. Instead of picking a Gaussian distribution, we choose the function that gives the best numeric fitting from Ref. [87]. This function is given by the sum of

$$\begin{aligned} \tilde{g}_{\text{fit}}(\omega\tau) = & 1 - 0.0378271 (\omega\tau)^2 - 0.000429218 (\omega\tau)^4 + 0.000875262 (\omega\tau)^6 \\ & - 0.0000485667 (\omega\tau)^8 - 2.61062 \times 10^{-10} (\omega\tau)^{10} + 1.9601 \times 10^{-13} (\omega\tau)^{12}, \end{aligned} \quad (3.275)$$

for $\omega\tau < 9.92$, and

$$\tilde{g}_{\text{asy}}(\omega\tau) = 2.9324e^{-\sqrt{2\omega\tau}}, \quad \text{for } \omega\tau \geq 9.92 \quad (3.276)$$

If we set $\tilde{g}(\omega\tau) = \tilde{g}_{\text{fit}}(\omega\tau) + \tilde{g}_{\text{asy}}(\omega\tau)$, we obtain $C_g = 9.3$. Fixing $a = 1$, it follows

$$\frac{|\mathbf{F}_1|}{|\mathbf{F}_0|} = 1.352 \times 10^{-15} \text{cm}^2 \frac{1}{d^2}. \quad (3.277)$$

For the phonon description to be valid, we need the characteristic distances of the system to be greater than the interatomic distances of the dielectric. Therefore, assuming that the interatomic distance is of the order of $1 \text{ \AA}$ (10^{-8} cm), the minimum value that we can allow for d is around $10 \text{ \AA}$. In this minimum distance, the force due to the phonons is maximum and contributes around 10% of the total force on the charge. Even in the more conservative scenario, with $d = 100 \text{ \AA}$, the contribution of the phonon force is around 1% of the total force. Therefore, it may have an observable effect on the charge.

Associated with these fluctuating forces due to the phonons, our electric charge will acquire a velocity $v_1 = |\mathbf{F}_1|\tau/m_q$, with m_q being the mass of the charge. The ratio between this velocity and the thermal velocity¹⁰ of the charge is given by

$$\frac{v_1}{v_T} = \frac{q^2 \alpha_m a}{3m} \sqrt{\frac{\hbar \rho_0}{k_B T m_q c_S^3}} \frac{C_g}{d^3}, \quad (3.278)$$

Now, with the charge as an electron, the dielectric as He^4 at $T = 4\text{K}$, $a = 1$, and $C_g = 9.3$, we obtain

$$\frac{v_1}{v_T} = 1.476 \times 10^{-19} \text{cm}^3 \frac{1}{d^3}, \quad (3.279)$$

Therefore, in the case of $d = 10 \text{ \AA}$, we have the velocity induced by the fluctuations around a hundred times greater than the thermal velocity, and at $d = 100$

¹⁰Remember that $v_T = \sqrt{\frac{k_B T}{m_q}}$, with k_B as the Boltzmann constant.

$\text{\AA}$, v_1 is around 10 times greater than v_T . The implications of this are immediate. The electron will exhibit an effective temperature greater than the 4 K at which the system is maintained.

In the case of a free electron near the diluted dielectric, the fluctuations may induce a classically unexpected deviation from the z -axis. Let the force due to the fluctuations be denoted by $\mathbf{F}_1 = \mathbf{F}_\perp + \mathbf{F}_z$, where $\mathbf{F}_\perp$ contains the contribution of the force in the x and y directions. If we compute separately the root mean square of each contribution, we can obtain the following ratio:

$$\frac{|\mathbf{F}_\perp|}{|\mathbf{F}_z|} = \frac{\pi}{4}, \quad (3.280)$$

which means that the perpendicular contributions to the mean root square of the fluctuating force are non-vanishing, raising the possibility of movement out of the z -plane.

3.3 Interacting Fields

Up to now, we have discussed only linear equations of motion, which arise from a Lagrangian that is at most quadratic in the field variables. Such theories are able to describe fields in free space, without interaction with themselves or other fields. From a particle perspective, this corresponds to the description of a free quantum particle. In this section, we will introduce interactions into the theory, following Refs. [22–24, 88].

Let us suppose that any interacting theory can be written as the sum of a free Hamiltonian and an interacting part, i.e.

$$H = H_0 + H_I, \quad (3.281)$$

where H_0 is the free Hamiltonian, which we have considered so far, and H_I is the interacting part. Now, we mimic the case of quantum mechanics and define the evolution of an operator as

$$A(t) = e^{iH_0 t} A e^{-iH_0 t}, \quad (3.282)$$

where $A = A(t = 0)$. This relation is called the **interaction picture**. The connection with the Heisenberg picture follows directly:

$$A(t) = e^{iH_0 t} e^{-iH t} A_H e^{iH t} e^{-iH_0 t}, \quad (3.283)$$

where A_H is the operator A in the Heisenberg picture. If $t = 0$, it follows directly that all three pictures (Schrödinger, Heisenberg, and interaction) are the same.

Since all pictures are linked by unitary transformations, they all have the same expectation value.

The expansion of the scalar field given by Eq. (3.11) can be obtained by¹¹

$$\phi(\mathbf{x}, t) = e^{iH_0 t} \phi(\mathbf{x}) e^{-iH_0 t}. \quad (3.284)$$

Before we continue with the discussion of fields, let us take a step back and analyze the interaction picture in a state, ψ , of a Hilbert space. To connect the state $\psi(t_0)$ at time t_0 to the state $\psi(t_1)$ at time t_1 , we can use the interaction picture for the states, which follows directly from the definition:

$$\psi(t_1) = U(t_1, t_0) \psi(t_0), \quad (3.285)$$

Formally, the solution to this equation is

$$U(t_1, t_0) = e^{iH_0 t_1} e^{-iH(t_1 - t_0)} e^{-iH_0 t_0}, \quad (3.286)$$

Note that, in general, H_0 and H do not commute. From the previous relation, it follows directly that the operator U satisfies:

- (i) $U(t, t_0)$ is unitary;
- (ii) $U(t_0, t_0) = I$;
- (iii) $U(t_2, t_1)U(t_1, t_0) = U(t_2, t_0)$;
- (iv) $U^\dagger(t_0, t_1) = U(t_1, t_0)$.

We notice that $U(t, 0)$ is the operator that links the interaction picture and the Heisenberg picture in Eq. (3.283). $U(t, t_0)$ is called the **time-evolution operator** and it satisfies

$$i \frac{\partial}{\partial t} U(t, t_0) = H_I(t) U(t, t_0), \quad (3.287)$$

which can be recast as the following integral equation:

$$U(t, t_0) = I + (-i) \int_{t_0}^t H_I(t') U(t', t_0) dt'. \quad (3.288)$$

Now, let us pick a time $t_2 \in [t_0, t]$. Applying the previous reasoning, we get

$$U(t, t_0) = I + (-i) \int_{t_0}^t H_I(t') dt' + (-i)^2 \int_{t_0}^t \int_{t_0}^{t'} H_I(t') U(t'', t_0) dt' dt'', \quad (3.289)$$

¹¹This is just an application of the Baker-Campbell-Hausdorff relation.

If we go further and divide the interval $[t_0, t]$ into $n + 1$ intervals, we are left with the identity plus $n + 1$ multiple integrals, where the n -th term is given by

$$(-i)^n \int_{t_0}^t \left[\int_{t_0}^{t_1} \dots \int_{t_0}^{t_{n-1}} H_I(t_1) H_I(t_2) \dots H_I(t_n) dt_n dt_{n-1} \dots dt_2 \right] dt_1, \quad (3.290)$$

Solving this integral is quite complicated. However, we can introduce the **temporal ordering** to simplify the computation. The temporal ordering is defined as

$$\mathcal{T}(A(x)A(y)) = \theta(x_0 - y_0)A(x)A(y) + \theta(y_0 - x_0)A(y)A(x), \quad (3.291)$$

Thus, if $t_1 \geq t_2 \geq \dots \geq t_n$, we have

$$\mathcal{T}(H(t_1)H(t_2) \dots H(t_n)) = H(t_1)H(t_2) \dots H(t_n). \quad (3.292)$$

Let us analyze the $n = 2$ contribution. Changing the order of integration and renaming the variables, we have

$$\begin{aligned} \int_{t_0}^t \int_{t_0}^{t_1} H_I(t_1) H_I(t_2) dt_2 dt_1 &= \int_{t_0}^t \int_{t_0}^{t_1} H_I(t_1) H_I(t_2) dt_1 dt_2 = \int_{t_0}^t \int_{t_0}^{t_1} H_I(t_2) H_I(t_1) dt_2 dt_1 \\ \Rightarrow 2 \int_{t_0}^t \int_{t_0}^{t_1} H_I(t_1) H_I(t_2) dt_2 dt_1 &= \int_{t_0}^t \int_{t_0}^{t_1} H_I(t_1) H_I(t_2) dt_2 dt_1 + \int_{t_0}^t \int_{t_1}^t H_I(t_1) H_I(t_2) dt_2 dt_1 \\ &= \int_{t_0}^t \int_{t_0}^t \mathcal{T}(H_I(t_1) H_I(t_2)) dt_2 dt_1, \end{aligned} \quad (3.293)$$

Thus, the time-ordering allows us to rewrite the integrals over the entire interval. Generalizing the previous result to all n , we can rewrite the *perturbative series for the time-evolution operator* as the following Neumann series (see Eq. (A.165)):

$$U(t, t_0) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t \mathcal{T}(H_I(t_1) \dots H_I(t_n)) dt_1 \dots dt_n. \quad (3.294)$$

Formally, we can sum this series to write

$$U(t, t_0) = \mathcal{T} \left(e^{-i \int_{t_0}^t H_I(t') dt} \right), \quad (3.295)$$

If we are dealing with Hamiltonian density, as is usual in quantum field theory, the integral is taken over spacetime, and the Hamiltonian is the respective density.

Here we do not discuss the properties and difficulties of the S -matrix; we limit ourselves to saying that the elements of such a matrix are spacetime integrals of

the expectation values of the time-ordered products of the fields. Therefore, our observables are elements of the S -matrix. Next, we explicitly compute some time-ordered expectation values.

Now we notice that the divergence of the energy from the last section (see Eq. (3.66)) can be solved in another way. Let us define the **normal ordering**, $:\bullet:$, of the field operators by moving all annihilation operators to the right in the frequency decomposition, Eq. (3.11). This leads us to define it as

$$:\phi(x)\phi(y): = \phi(x)\phi(y) - (\phi(x)\phi(y)\Omega, \Omega), \quad (3.296)$$

equivalently, for the bosonic case¹², we have

$$\begin{aligned} :\phi(x)\phi(y): &= :\phi_-(x)\phi_-(y): + :\phi_-(x)\phi_+(y): + :\phi_+(x)\phi_+(y): + :\phi_+(x)\phi_-(y): \\ &= \phi_-(x)\phi_-(y) + \phi_-(x)\phi_+(y) + \phi_-(x)\phi_+(y) + \phi_-(y)\phi_+(x), \end{aligned} \quad (3.297)$$

therefore, it follows that the normal-ordered Hamiltonian, $:H:$, has zero expected value: $\langle :H: \rangle = 0$. This means that the normal ordering procedure is equivalent to the subtraction of a (formally) infinite energy.

Assume that $x_0 > y_0$, so by direct computation, we have that

$$\begin{aligned} \mathcal{T}(\phi(x)\phi(y)) &= \phi_-(x)\phi_-(y) + \phi_-(x)\phi_+(y) + \phi_-(x)\phi_+(y) + \phi_-(y)\phi_+(x) \\ &\quad + [\phi_+(x), \phi_-(y)], \end{aligned} \quad (3.298)$$

it follows that

$$\mathcal{T}(\phi(x)\phi(y)) = :\phi(x)\phi(y): + [\phi_+(x), \phi_-(y)]. \quad (3.299)$$

Now let us define the **contraction** (or **Wick contraction**) as

$$\overline{\phi(x)\phi(y)} = \begin{cases} [\phi_+(x), \phi_-(y)], & \text{if } x_0 > y_0, \\ [\phi_+(y), \phi_-(x)], & \text{if } y_0 > x_0. \end{cases} \quad (3.300)$$

From direct computation, it follows that

$$\langle \mathcal{T}(\phi(x)\phi(y)) \rangle = \langle \overline{\phi(x)\phi(y)} \rangle = G_F(x, y), \quad (3.301)$$

where $G_F(x, y)$ is the causal propagator, given by Eq. (3.30).

Theorem 3.5. (Wick's theorem) The time-ordered product of a set of operators can be decomposed into the corresponding sum of contractions of the normal-ordered products. All contractions of the operators must be considered.

¹²Note that for a fermionic field, we must use the anti-commutator. This leads us to a minus sign in the last term of Eq. (3.297)

Proof. We use mathematical induction. We have shown that it is true in the case of the product of two operators. Therefore, we suppose that it is true for the product of $m - 1$ operators. Suppose that $x_1^0 > x_2^0 > \dots > x_m^0$ and denote by $\phi_i = \phi(x_i)$ for all $i = 1, 2, \dots, m$. So

$$\begin{aligned}
 \mathcal{T}(\phi_1 \phi_2 \dots \phi_m) &= \phi_1 \phi_2 \dots \phi_m = \phi_1(\phi_2 \dots \phi_m) \\
 &= \phi_1 \left(: \phi_2 \dots \phi_m : + : \overbrace{\phi_2 \phi_3} \dots : + : \overbrace{\phi_2 \phi_3 \phi_4} \dots : + \dots \right. \\
 &\quad + : \overbrace{\phi_2 \phi_3 \phi_4 \phi_5 \phi_6} \dots : + : \overbrace{\phi_2 \phi_3 \phi_4 \phi_5 \phi_6} \dots : + \dots \\
 &\quad \left. + : \text{all triple contractions} : + : \text{all quadruple contractions} : + \dots \right) \\
 &= (\phi_{1+} + \phi_{1-})(: \phi_2 \dots \phi_m : + \dots), \tag{3.302}
 \end{aligned}$$

we note that $\phi_{1-} : \phi_2 \dots \phi_m : = : \phi_{1-} \phi_2 \dots \phi_m :$, while

$$\begin{aligned}
 \phi_{1+} : \phi_2 \dots \phi_m : &= : \phi_2 \dots \phi_m : \phi_{1+} + [\phi_{1+}, : \phi_2 \dots \phi_m :] \\
 &= : \phi_{1+} \phi_2 \dots \phi_m : + : [\phi_{1+}, \phi_{2-}] \phi_3 \dots \phi_m : \\
 &\quad + : \phi_2 [\phi_{1+}, \phi_{3-}] \dots \phi_m : + \dots + : \phi_2 \phi_3 \dots [\phi_{1+}, \phi_{m-}] : \\
 &= : \phi_{1+} \phi_2 \dots \phi_m : + : \overbrace{\phi_1 \phi_2 \phi_3} \dots \phi_m : \\
 &\quad + : \overbrace{\phi_1 \phi_2 \phi_3} \dots \phi_m : + : \overbrace{\phi_1 \phi_2 \phi_3} \dots \phi_m : . \tag{3.303}
 \end{aligned}$$

Thus, $\phi_{1+} : \phi_2 \dots \phi_m :$ generates all the single contractions that involve the field ϕ_1 . Using the same procedure, it is direct to obtain that $\phi_{1+} : \overbrace{\phi_2 \phi_3} \dots :$ generates all the double contractions with ϕ_1 , and so on. Therefore, we obtain that

$$\mathcal{T}(\phi_1 \phi_2 \dots \phi_m) = : \phi_1 \phi_2 \dots \phi_m : + : \text{all possible contractions} : . \tag{3.304}$$

■

The simplest case of a non-linear theory is the so-called **$\lambda\phi^4$ theory**. Such a theory is described by a Lagrangian given by

$$L = \frac{1}{2} \partial^\mu \phi(x) \partial_\mu \phi(x) - \frac{1}{2} m^2 \phi^2(x) + \frac{\lambda}{4!} \phi^4(x) = L_0 + L_I. \tag{3.305}$$

The interaction Hamiltonian density is $H_I = -L_I$. In order to appreciate Wick's

theorem, let us compute the time-ordered product of four fields:

$$\begin{aligned}
 \mathcal{T}(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) = & : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : \\
 & + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : \\
 & + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : \\
 & + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : \\
 & + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : + : \overbrace{\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)} : ,
 \end{aligned} \tag{3.306}$$

taking its expected value, it follows that

$$\begin{aligned}
 \langle \mathcal{T}(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) \rangle = & G_F(x_1, x_2)G_F(x_3, x_4) + G_F(x_1, x_4)G_F(x_2, x_3) \\
 & + G_F(x_1, x_3)G_F(x_2, x_4).
 \end{aligned} \tag{3.307}$$

Now let us analyze the time evolution of a state with two scalar particles propagating through the space from the point $\mathbf{x}$ to the point $\mathbf{y}$ in the interval $[0, t]$, with the Lagrangian of Eq. (3.305). Up to the first order in perturbation theory, it will be given by

$$\begin{aligned}
 (U(t, 0)\phi(x)\phi(y)\Omega, \Omega) = & \left(\mathcal{T} \left[\phi(x)\phi(y) + \phi(x)\phi(y) \left(-i \int H_I(z) d^4 z \right) \right] \Omega, \Omega \right) \\
 = & (\mathcal{T} [\phi(x)\phi(y)] \Omega, \Omega) \\
 & + \left(\mathcal{T} \left[\phi(x)\phi(y) \left(\frac{-i\lambda}{4!} \right) \int \phi(z)\phi(z)\phi(z)\phi(z) dz \right] \Omega, \Omega \right) \\
 = & G_F(x, y) + 3 \left(\frac{-i\lambda}{4!} \right) G_F(x, y) \int G_F(z, z) G_F(z, z) d^4 z \\
 & + 12 \left(\frac{-i\lambda}{4!} \right) \int G_F(x, z) G_F(z, z) G_F(y, z) d^4 z,
 \end{aligned} \tag{3.308}$$

where, in the last equality, we use the fact that only fully contracted terms are non-vanishing and the factors of 3 and 12 arise from equal contractions.

Let us suppose that we have four fixed points in space, as shown in Fig. 3.8, then we can schematically represent Eq. (3.307) as

$$\langle \mathcal{T}(\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)) \rangle = \begin{array}{c} \begin{array}{cc} 1 & 2 \\ \hline 3 & 4 \end{array} \\ + \begin{array}{c} 1 \\ \hline 3 \end{array} \end{array} + \begin{array}{c} \begin{array}{cc} 2 & 1 \\ \hline 4 & 3 \end{array} \\ + \begin{array}{c} 2 \\ \hline 4 \end{array} \end{array} + \begin{array}{c} \begin{array}{cc} 1 & 2 \\ \hline 3 & 4 \end{array} \end{array}, \tag{3.309}$$

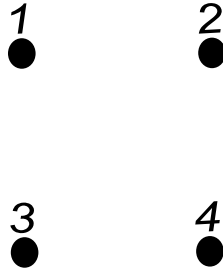


Figure 3.8: Four fixed points in space.

where each line represents a G_F . Using these diagrams, Eq. (3.308) can be written as

$$(U(t, 0)\phi(x)\phi(y)\Omega, \Omega) = \langle U(t, 0)\phi(x)\phi(y) \rangle$$

$$= \text{diagram 1} + \text{diagram 2} + \text{diagram 3} \quad (3.310)$$

again, each full line represents G_F while the intersection of four lines contains the prefactor $\left(\frac{-i\lambda}{4!}\right)$, and each loop is an integral. Each diagram carries a multiplicity factor that encapsulates the number of ways we can obtain each diagram. These diagrams are called **Feynman diagrams**, and the rules to compute them explicitly are called **Feynman rules**. In the next chapter, it will be clear that the first diagram in Eq. (3.310) must be canceled in order to obtain physical observables. Also, we will obtain these diagrams in the momentum representation, which has some computational advantages.

Before finishing this section, we must comment that, mathematically, the interaction picture does not exist. This result is a consequence of the so-called Haag's Theorem [89]. Roughly speaking, this theorem says that the basis of the Hilbert space of an interacting theory cannot be the same, nor unitarily equivalent, to the basis of the Hilbert space of the free theory. A nice review of the history and discussions about Haag's theorem can be found in Ref. [90].

However, it is a matter of fact the success of perturbation theory in many models in quantum field theory. This apparent contradiction raises some intriguing questions about the mathematics and philosophy of quantum field theory. My interpretation to reconcile these two results is as follows: we know that every Hilbert space has an orthonormal basis (Theorem A.62), the basis of the interacting theory in the coordinate representation can, in principle, be obtained; it corresponds to the Hermite polynomials. However, the computations become messy and sometimes ill-defined. Therefore, the role of perturbation theory is to smoothly deform the basis of the free theory in order to obtain the basis of the interacting theory.

Chapter 4

Constructive Quantum Field Theory

As we have mentioned before, quantum field theory has two main formulations. In the last chapter, we discussed the axiomatic formulation, and in this chapter, we discuss constructive field theory. While there are many computational advantages in the constructive scenario, discussions about it are common in many books on quantum field theory [91–95]. Here, we provide a brief construction of functional integrals and emphasize their computational advantages. Unless stated otherwise, we assume the natural system of units in this chapter ($c = \hbar = k_B = 1$).

We begin this section with a discussion on how to obtain quantum mechanics in the functional integral representation and then generalize the results to field theory. We primarily follow Refs. [93, 95].

4.1 Functional Integrals and Quantum Mechanics

As discussed in Sec. 2.2, the quantity $(\psi, A\psi)$ defines the probability amplitude of the observable A in the state ψ . Now, let us suppose that we wish to compute the amplitude probability of a state with momenta q_a at time t_a , $\psi_{q_a}(t_a)$, evolving to the momenta q_b at time t_b , $\psi_{q_b}(t_b)$. To compute $(\psi_{q_a}(t_a), \psi_{q_b}(t_b))$, we use the time evolution operator defined in Sec. 2.2:

$$(\psi_{q_a}(t_a), \psi_{q_b}(t_b)) = (e^{-iH(t_b-t_a)}\psi_{q_a}, \psi_{q_b}), \quad (4.1)$$

If we assume that the variation of the momenta from q_a to q_b is continuous, we can divide the interval of time $[t_a, t_b]$ into $N + 1$ intervals with equal length ε and

associate some momenta to each interval. This allows us to write

$$(\psi_{q_a}(t_a), \psi_{q_b}(t_b)) = \int (\psi_{q_a}(t_a), \psi_{q_1}(t_1)) (\psi_{q_1}(t_1), \psi_{q_2}(t_2)) \dots (\psi_{q_N}(t_N), \psi_{q_b}(t_b)) \prod_{i=1}^N dq_i. \quad (4.2)$$

Let us now examine any inner product of the integral. Using the fact that $t_{i+1} - t_i = \varepsilon$, we have, to first order in ε ,

$$(\psi_{q_{i+1}}(t_{i+1}), \psi_{q_i}(t_i)) = ((I - iH\varepsilon) \psi_{q_{i+1}}, \psi_{q_{i+1}}) = (I - i\varepsilon H) (\psi_{q_{i+1}}, \psi_{q_{i+1}}), \quad (4.3)$$

using that $(\psi_{q_{i+1}}, \psi_{q_{i+1}}) = \delta(q_{i+1} - q_i)$ and the Fourier transform of the generalized function δ [34], we find, to first order, that

$$(\psi_{q_{i+1}}(t_{i+1}), \psi_{q_i}(t_i)) = \frac{1}{2\pi} \int (I - i\varepsilon H(q_i, p_i)) e^{ip_i(q_{i+1} - q_i)} dp_i. \quad (4.4)$$

Thus, defining $q_0 = q_a$ and $q_{N+1} = q_b$, we obtain

$$(\psi_{q_a}(t_a), \psi_{q_b}(t_b)) = \frac{1}{2\pi} \prod_{i=1}^N \int \prod_{i=0}^N e^{i\varepsilon \sum_{i=0}^N [p_i(q_{i+1} - q_i)\varepsilon^{-1} - H(q_i, p_i)]} dp_i dq_i, \quad (4.5)$$

Now, taking the limit $N \rightarrow \infty$ while the size of the interval $[t_a, t_b]$ remains finite, we define $[dq] = \prod_{q \in \mathbb{R}} dq$ and $[dp] = \prod_{p \in \mathbb{R}} dp / (2\pi)$, and we can write

$$(\psi_{q_a}(t_a), \psi_{q_b}(t_b)) = \int e^{i \int_{t_a}^{t_b} [p\dot{q} - H(p, q)] dt} [dp][dq], \quad (4.6)$$

where $\dot{}$ represents the time derivative. Clearly, the previous integral is meaningless, as the measures do not converge. To be precise, $[dp]$ and $[dq]$ are not the usual Lebesgue measures; rather, they are *functional measures*. Functional integrals can only be performed symbolically; however, to obtain a convergent result, we need a well-defined function of the variables. This is not the case for the integral in Eq. (4.6). To make this meaningful, we perform the change of variables $t \rightarrow \tau = it$, which allows us to obtain

$$(\psi_{q_a}(t_a), \psi_{q_b}(t_b)) = \int e^{-\int_{\tau_a}^{\tau_b} [p\dot{q} - H(p, q)] d\tau} [dp][dq]. \quad (4.7)$$

Now, suppose the Hamiltonian has the form $\frac{p^2}{2m} + V(Q)$. The functional integral over p can be evaluated¹ to yield

$$(\psi_{q_a}(t_a), \psi_{q_b}(t_b)) = \int e^{-\int_{\tau_a}^{\tau_b} L(q, \dot{q}) d\tau} [dq] = \int e^{-S[L; \tau_a, \tau_b]} [dq], \quad (4.8)$$

¹This is just a Gaussian integral. We absorb the numerical factor into the measure.

where $L(q, \dot{q})$ is the *classical* Lagrangian and S is the *classical*² action functional (see Eqs.(2.1) and (2.3)). We note that the change of variables $t \rightarrow \tau = it$ has a deeper meaning. This change of variables is an analytic continuation from the Lorentzian metric of Minkowski space to the Euclidean space with the usual metric. That is, it transforms the Lorentz group into the Euclidean group. Such an analytic continuation is called **Wick rotation**, and in the literature, τ is referred to as *Euclidean time* or *imaginary time* [91, 93, 95]. If one applies the same analytic continuation to the Schrödinger equation (Eq. (2.104)) with the free-particle Hamiltonian, one recovers the diffusion equation, which is solved by the Wiener paths. To deal with meaningful quantities, we assume that we always use Euclidean time in the context of path integrals. For this reason, *we use the letter t instead of τ in this thesis*.

From the classical theory, we know that the equations of motion are unaffected if we add a total time derivative or a constant contribution to the Lagrangian. Therefore, we define the following:

$$Z[J] = \int e^{-S[L; t_a, t_b] + \int_{t_a}^{t_b} J(t)q(t)dt} [dq]. \quad (4.9)$$

Now, let us compute the expectation value of the position operator $Q(t)$. Using the same reasoning that led to Eq. (4.6), but with $t_a \rightarrow -\infty$ and $t_b \rightarrow +\infty$, we obtain

$$\langle Q(t) \rangle = (Q(t)\Omega, \Omega) = \int q(t) e^{-S[L]} [dq], \quad (4.10)$$

therefore, we can write

$$\left. \frac{\delta Z[J]}{\delta J(t)} \right|_{J(t)=0} = \langle Q(t) \rangle. \quad (4.11)$$

where $\delta/\delta J(t)$ denotes the functional derivative with respect to $J(t)$. It follows directly that the expectation value of any time-ordered product of $Q(t)$ is given by

$$\langle \mathcal{T}(Q(t_n) \dots Q(t_1)) \rangle = \left. \frac{\delta^n Z[J]}{\delta J(t_n) \dots \delta J(t_1)} \right|_{J(t)=0}, \quad (4.12)$$

therefore, all the expected values of products of Q are generated by $Z[J]$, and for this reason, $Z[J]$ is sometimes called the **generating functional**.

Before finishing this section, we will link the generating functional with the partition function in statistical mechanics. The partition function is defined as

$$Z_\beta = \sum_n e^{-\beta E_n} = \sum_n (e^{-\beta H} \psi_n, \psi_n) = \text{Tr } e^{-\beta H}. \quad (4.13)$$

²This means that the variables $q, \dot{q}$ are classical variables and commute with each other.

With the partition function, we can obtain thermal averages. For example, the average free energy is given by

$$\langle E \rangle_\beta = -\frac{\partial}{\partial \beta} \ln Z_\beta, \quad (4.14)$$

and the free energy

$$F_\beta = -\frac{1}{\beta} \ln Z_\beta. \quad (4.15)$$

Now notice that if we take $q_a = q_b$ and choose $t_b - t_a = \beta$ in Eq. (4.1), and integrate it in q_a , it becomes the same expression as in Eq. (4.13). For the correspondence to be complete, we must impose that the Euclidean time is periodic with period β , to satisfy the Kubo-Martin-Schwinger (KMS) condition, which is derived in the context of quantum statistical mechanics [96–98]. For this reason, sometimes we may refer to $Z[J]$ as the partition function as well. We return to this link between quantum fields and statistical mechanics in the next chapter.

4.2 Quantum Field Theory

As we have discussed in Sec. 3.3, the many observables of quantum field theory are given by the expectation value of the time-ordered products of the fields. Therefore, by an analogous construction to the preceding section, we can write

$$G^{(n)}(x_1, \dots, x_n) = \langle \mathcal{T}(\phi(x_1) \dots \phi(x_n)) \rangle = \frac{\delta^n Z[J]}{\delta J(t_n) \dots \delta J(t_n)} \Big|_{J(t)=0}. \quad (4.16)$$

But we know that this expected value is the n -point Green's function³. Now, we can express the generating functional of *all Green's functions* as

$$Z[J] = \sum_{n=0}^{\infty} \frac{1}{n!} \int G(x_1, \dots, x_n) J(x_1) \dots J(x_n) d^4 x_1 \dots d^4 x_n. \quad (4.17)$$

Through derivatives of the previous equations, one can obtain the Euclidean version of Eqs. (3.307) and (3.308). It is usual to call these Green's functions by *Schwinger functions*, which are the Euclidean counterpart of the Wightman functions of the previous chapter.

Analysing Eqs. (3.309 - 3.310), we notice that the expectation value of the time-ordered products gives rise to two types of diagrams: those that can be divided into subdiagrams (Eq. (3.309)) and the second diagram of Eq. (3.310), called

³Remember that we are in Euclidean time, therefore $dp_0 \rightarrow -idp_0$, and the d'Alembert operator becomes just the 4-Laplacian, $\square \rightarrow \Delta$.

disconnected or **reducible diagrams**), and those that cannot be divided into subdiagrams, called **irreducible** or **connected diagrams**. From the expressions that generate such diagrams, Eqs. (3.307 - 3.308), we observe that disconnected diagrams are simple products of Green's functions and their integrals, while connected diagrams are the Green's function and the integral of the product of Green's functions. Therefore, disconnected diagrams can be reconstructed from the connected ones. From a direct computation of the relation (4.16), we observe that we obtain all (connected and disconnected) Green's functions.

In order to obtain only the connected Green's functions, we define

$$W[J] = \ln Z[J]. \quad (4.18)$$

For practical purposes, let us fix the free scalar field; then we have a Gaussian functional integral that can be directly evaluated:

$$\begin{aligned} Z[J] &= \int e^{-S[\phi, J]} [d\phi] = \int e^{-\frac{1}{2} \int [\phi(x)(-\Delta + m^2)\phi(x) - J(x)\phi(x)] d^4x} [d\phi] \\ &= e^{-\frac{1}{2} \text{Tr} \ln(\Delta + m^2)} e^{-\frac{1}{2} \int [J(x')(-\Delta + m^2)^{-1} J(x)] d^4x' d^4x} \\ &= N e^{-\frac{1}{2} \int [J(x') G_F(x', x) J(x)] d^4x' d^4x}, \end{aligned} \quad (4.19)$$

where we have used that $e^{-\frac{1}{2} \text{Tr} \ln(\Delta + m^2)} = \text{Det}(-\Delta + m^2)^{-1/2} = N$. Now, taking the second functional derivative of $W[J]$ and setting $J = 0$, we obtain

$$\begin{aligned} \left. \frac{\delta^2 W[J]}{\delta J(x_1) \delta J(x_2)} \right|_{J=0} &= \left[\frac{1}{Z[J]} \frac{\delta^2 Z[J]}{\delta J(x_1) \delta J(x_2)} - \frac{1}{Z^2[J]} \frac{\delta Z[J]}{\delta J(x_1)} \frac{\delta Z[J]}{\delta J(x_2)} \right]_{J=0} \\ &= \frac{1}{Z[0]} \langle \mathcal{T}(\phi(x_1) \phi(x_2)) \rangle - \frac{1}{Z[0]} \langle \mathcal{T}(\phi(x_1)) \rangle \frac{1}{Z[0]} \langle \mathcal{T}(\phi(x_2)) \rangle \\ &= \frac{1}{Z[0]} \langle \mathcal{T}(\phi(x_1) \phi(x_2)) \rangle = G_C(x_1, x_2) = G_F(x_1, x_2). \end{aligned} \quad (4.20)$$

Therefore, from the second line of the last equation, we see that the disconnected pieces are subtracted from the expected value of the time-ordered product⁴. We will also verify this explicitly for the $\lambda\phi^4$ theory at the end of this chapter. The prefactor $Z^{-1}[0]$ can be chosen to ensure that $W[0] = 1$. By our previous discussion, we also know that $Z[0]$ is the vacuum-vacuum transition; therefore, the division by $Z[0]$ also cancels out the contribution due to this kind of transition.

For this reason, $W[J]$ is called the **generating functional of the connected Green's functions**, since sometimes the connected Green's functions are referred to as *correlation functions*. Thus, $W[J]$ can also be called the generating functional of the correlation functions.

⁴The free scalar theory is a special case where the only non-vanishing Green's function is the even ones.

Now, if we exponentiate Eq. (4.18), we can define the following functional of $J(x)$:

$$\phi_c(x) = \frac{\delta W[J]}{\delta J(x)}, \quad (4.21)$$

therefore, the vacuum-expectation value of any field, ϕ (not necessarily a scalar field), can be obtained by

$$\langle \phi \rangle = \lim_{J(x) \rightarrow 0} \phi_c(x). \quad (4.22)$$

By a Legendre transform from the variables $J(x)$ to the variables $\phi_c(x)$, we obtain

$$\Gamma[\phi_c(x)] = W[J] - \int J(x)\phi_c(x)d^4x, \quad (4.23)$$

which is the **effective action**. We note that, by comparing Eq. (4.18) with Eq. (4.15), we see that $W[J]$ is a non-thermal *free energy*, and comparing the last equation with the thermodynamic internal energy ($E = F + TS$), we observe a clear correspondence between them. The effective action is also called the **generating functional of the one-particle irreducible Green's functions**. We note that in the case of $\langle \phi \rangle = 0$, the effective action and the free energy coincide.

In the case of the free scalar field, from our definitions it follows that

$$\phi_c(x) = - \int G_F(x, x') J(x') d^4x', \quad (4.24)$$

then we have

$$(-\Delta + m^2)\phi_c(x) = J(x), \quad (4.25)$$

which is the classical equation of motion in the presence of the source $J(x)$. This justifies calling $\phi_c(x)$ the **classical field**. In the case of the free scalar field, the effective action is

$$\Gamma[\phi_c] = -\frac{1}{2} \int \phi_c(x) [-\Delta + m^2] \phi_c(x) d^4x, \quad (4.26)$$

which is the action of the free field.

For interacting theories, we are unable to compute the effective action exactly, so we use a Taylor functional expansion:

$$\Gamma[\phi_c] = \sum_{n=1}^{\infty} \int \Gamma^{(n)}(x_1, \dots, x_n) \phi_c(x_1) \dots \phi_c(x_n) d^4x_1 d^4x_n. \quad (4.27)$$

Each coefficient $\Gamma^{(n)}$ is an n -point one-particle irreducible Green's function. All the Feynman diagrams generated by these Green's functions are connected. In scalar free theory, only the two-point Green's function is non-vanishing.

Performing a Fourier representation, we have

$$\tilde{\Gamma}[\tilde{\phi}_c(p)] = \sum_{n=0}^{\infty} \frac{1}{n!} \int \delta(p_1 + \dots + p_n) \tilde{\Gamma}^{(n)}(p_1, \dots, p_n) \tilde{\phi}_c(p_1) \dots \tilde{\phi}_c(p_n) d^4 p_1 \dots d^4 p_n. \quad (4.28)$$

Performing a Fourier transform in the two-point Green's function of the free scalar field in Euclidean space (see Eq. (4.79)), we have

$$\tilde{G}(p) = \frac{1}{p^2 + m^2}. \quad (4.29)$$

An expansion of the effective action in terms of the derivatives of ϕ_c gives us

$$\Gamma[\phi_c(x)] = \int \left[-V_{\text{eff}}(\phi_c) + \frac{1}{2} \partial_i \phi_c \partial^i \phi_c + \dots \right] d^D x, \quad (4.30)$$

where V_{eff} is function of ϕ_c . V_{eff} is referred to as the **effective potential**. It follows directly that

$$\left. \frac{\partial V}{\partial \phi_c} \right|_{J=0} = 0. \quad (4.31)$$

For the free scalar field, we have

$$V(\phi_c) = \frac{1}{2} m^2 \phi_c^2, \quad (4.32)$$

which is consistent with the fact that the free scalar field has a vacuum expectation value of zero.

Supposing that the classical field is invariant under translations, we can expand the effective potential in terms of the zero-momentum Green's function:

$$V_{\text{eff}}(\phi_c) = - \sum_{n=0}^{\infty} \frac{1}{n!} \phi_c^n \Gamma^{(n)}(p^2 = 0). \quad (4.33)$$

In the interacting case, we can see that the effective potential will be the sum of the classical potential (coming from the Lagrangian) and radiative corrections.

One should notice that a more formal development of constructive field theory is possible in terms of random functionals and by exploring the idea of Wiener measures [99, 100]. As emphasized by A. S. Wightman in Ref. [101], the Euclidean/constructive formulation of field theory was “almost single-handedly carried” by K. Symanzik [102]. However, we must also emphasize the work of K. Osterwalder and R. Schrader, who provided the necessary conditions for the Schwinger functions of the theory to be analytically continued to the Wightman functions [103, 104].

We should notice that, in this chapter, we did not impose the canonical commutation relation on our field variables. Within this framework, the probabilities obtained from derivatives of $W[J]$ (or $Z[J]$) are classical probabilities, in the sense that they are not probability amplitudes. Therefore, the quantization process occurs in the evaluation of the functional integral, and the tools of probability theory can be applied.

4.2.1 Casimir Effect

Since we claim that constructive field theory can recover the results of axiomatic field theory, the simplest case to check is to impose some boundary conditions on the free massless scalar field. In this case, using Eq. (4.19), we write

$$Z[0] = \text{Det}(-\Delta)^{-\frac{1}{2}}, \quad (4.34)$$

however we need to give a meaning for the *functional determinant* of an operator is. Since Δ is a self-adjoint operator, its eigenvalues, λ_i , are real, and by analogy with matrices, we may define

$$\text{Det}(-\Delta) = \prod_i \lambda_i. \quad (4.35)$$

However, the range of i is continuous; therefore, the last equation diverges. To make sense of it, we notice that if we take the spectral zeta function defined in Eq. (3.104), one can show that

$$\left. \frac{d}{ds} \zeta_\Delta(s) \right|_{s=0} = - \sum_{i=1}^{\infty} \ln \lambda_i. \quad (4.36)$$

Thus, it follows that [105]

$$Z[0] = \exp \left(-\frac{1}{2} \sum_{i=1}^{\infty} \ln \lambda_i \right) = \exp \left(\frac{1}{2} \left. \frac{d}{ds} \zeta_D(s) \right|_{s=0} \right). \quad (4.37)$$

So, the value of the determinant follows from the evaluation of the spectral zeta function. To obtain the spectral zeta function, we must know the spectrum of the theory. Let us fix the manifold as a slab geometry with one compactified dimension, $\Omega_L \equiv \mathbb{R}^{d-1} \times [0, L]$. For simplicity, we assume Dirichlet boundary conditions:

$$\phi(x_1, \dots, x_{d-1}, 0) = \phi(x_1, \dots, x_{d-1}, L) = 0. \quad (4.38)$$

To proceed with the calculations, we must construct the appropriate $\zeta_\Delta(s)$. It can be constructed using the appropriate spectral measure in the Riemann-Stieltjes integral. All the information about the domain Ω_L and the boundary conditions is taken into account by the spectral measure. So, in the continuous limit, one obtains $\zeta_\Delta(s)$ as:

$$\zeta_\Delta(s) = \frac{2A_{d-1}}{(2\pi)^{d-1}} \int \sum_{n=1}^{\infty} \left[p^2 + \left(\frac{\pi n}{L} \right)^2 \right]^{-s} d^{d-1}p, \quad (4.39)$$

where $p^2 = p_1^2 + \dots + p_{d-1}^2$ and A_{d-1} is the area of the hypersurface in $d-1$ dimensions:

$$A_{d-1} \equiv \prod_{i=1}^{d-1} \lim_{L_i \rightarrow \infty} L_i, \quad (4.40)$$

where this limit must be understood as $L_i \gg L$, $\forall i = 1, \dots, d-1$. From here, one could proceed with the exact calculations of Ref. [106]; see also Ref. [107]. In the following, we introduce in the calculation a method that we will use later.

Such a method will reproduce the result in the literature via direct calculations. To proceed, let us use that

$$d^{d-1}p = \frac{2\pi^{\frac{d-1}{2}}}{\Gamma\left(\frac{d-1}{2}\right)} p^{d-2} dp, \quad (4.41)$$

and the Mellin representation of a^{-s} ,

$$a^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-ta} dt, \quad (4.42)$$

to rewrite Eq. (4.39) as

$$\begin{aligned} \zeta_\Delta(s) &= \frac{A_{d-1} \pi^{\frac{d-1}{2}}}{(2\pi)^{d-1} \Gamma\left(\frac{d-1}{2}\right) \Gamma(s)} \left(\frac{L^2}{\pi} \right)^s \int_0^\infty \left\{ t^{s-1} \sum_{n=1}^{\infty} e^{-tn^2\pi} \right. \\ &\quad \times \left. \int_0^\infty dp p^{d-2} \exp\left[\frac{-tL^2}{\pi} (p^2) \right] \right\} dt. \end{aligned} \quad (4.43)$$

The integration over the continuum modes can be readily performed. Performing the integral, one obtains:

$$\zeta_\Delta(s) = C_d(L, s) \int_0^\infty t^{s-\frac{1}{2}(d+1)} \psi(t) dt, \quad (4.44)$$

where we define the following quantities:

$$C_d(L, s) \equiv \frac{A_{d-1}}{(2L)^{d-1}\Gamma(s)} \left(\frac{L^2}{\pi} \right)^s, \quad (4.45)$$

$$\psi(t) \equiv \sum_{n=1}^{\infty} e^{-tn^2\pi}. \quad (4.46)$$

As one can see, the contribution of $\psi(t)$ decreases rapidly as $t \rightarrow \infty$. However, depending on the values of s and d , singularities arise at $t \rightarrow 0$ that need to be addressed. As discussed in Ref. [106], the singularity can be removed by assuming the system is confined to a large but finite box, which introduces an infrared cutoff in the p -integrals above. Rather than introducing an explicit infrared cutoff, we extract the finite part of the integral using the relations between $\psi(t)$ and the weight $1/2$ modular form given in Eq. (3.80).

Following similar steps as in Eq. (3.81), we obtain

$$\zeta_{\Delta}(s) = \frac{C_d(L, s)}{2} [2I_{1,d}(s) + I_{2,d}(s) - I_{3,d}(s)], \quad (4.47)$$

with $I_{1,d}, \dots$ being the integrals:

$$I_{1,d}(s) = \int_0^{\infty} t^{\frac{d}{2}-s-1} \psi(t) dt, \quad (4.48)$$

$$I_{2,d}(s) = \int_0^{\infty} t^{\frac{d}{2}-s-1} dt, \quad \text{and}, \quad (4.49)$$

$$I_{3,d}(s) = \int_0^{\infty} t^{\frac{d}{2}-s-\frac{3}{2}} dt. \quad (4.50)$$

The integral $I_{1,d}(s)$ is convergent for any values of s and d , while $I_{2,d}(s)$ diverges for $\text{Re}(2s) < d$ and $I_{3,d}(s)$ diverges for $\text{Re}(2s) < d - 1$. As seen in Eq. (4.45), we have that $C_d(L, s) \rightarrow 0$ as $s \rightarrow 0$, implying that

$$\left. \frac{d\zeta_{\Delta}(s)}{ds} \right|_{s=0} = \frac{1}{2} \left. \frac{dC_d(L, s)}{ds} \right|_{s=0} [2I_{1,d}(0) + I_{2,d}(0) - I_{3,d}(0)]. \quad (4.51)$$

The integral $I_{1,d}(0)$ is finite, positive definite, and independent of the plate separation L ; it depends only on the dimension d and can be performed analytically. On the other hand, the divergent integrals $I_{2,d}(0)$ and $I_{3,d}(0)$ are independent of the plate separation and can be dropped considering that we have a large box, which implies a large but finite wavelength, as argued in Ref. [106]

and mentioned above. These divergences would not arise if $m_0 \neq 0$. After some simplifications, one obtains that

$$\begin{aligned} \left. \frac{d\zeta_\Delta(s)}{ds} \right|_{s=0} &= \frac{A_{d-1}}{(2L)^{d-1}} I_{1,d}(0) = \frac{A_{d-1}}{(2L)^{d-1}} \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n^d} \\ &= \frac{A_{d-1}}{(2L)^{d-1}} \frac{\zeta(d)}{2\pi}. \end{aligned} \quad (4.52)$$

Using that $F = E - TS$ and the fact that $T = 0$ in our case, one concludes that

$$Z = e^{-F} = e^{-E} \Rightarrow E = -\frac{1}{2} \left. \frac{d\zeta_\Delta(s)}{ds} \right|_{s=0}. \quad (4.53)$$

Now we can define the energy density and find that

$$\frac{E}{A_{d-1}} \equiv \epsilon_d(L) = -\frac{1}{2(2L)^{d-1}} \frac{\zeta(d)}{2\pi}, \quad (4.54)$$

which evidently has the correct sign and power law with L , agreeing with previous results.

For $d = 3$, Eq. (4.54) results in

$$\epsilon_3(L) = -\frac{\zeta(3)}{16\pi L^2}, \quad (4.55)$$

which is the “universal” amplitude of the Goldstone modes [108]. The reason for the quotation marks will become clear in a further application. The Casimir force per unit of area (Casimir pressure) can be calculated as the negative derivative with respect to L of Eq. (4.54).

4.3 Interacting Fields

One of the biggest advantages of the constructive approach to quantum fields is its applicability to interacting theories. Taking a theory in which the Lagrangian allows decomposition into free and interacting parts, that is,

$$S[L] = \int L(\phi) d^4x = \int L_0(\phi) d^4x + \int L_I(\phi) d^4x = S_0[L_0] + S_I[L_I], \quad (4.56)$$

we obtain that the partition function with the source J is given by

$$Z[J] = \int e^{-S_0 - S_I + \int J(x)\phi(x) d^4x} [d\phi]. \quad (4.57)$$

Since the functional integral is just a formal integration, the non-Gaussian case (interacting theories) cannot be evaluated directly. However, we can construct a perturbation theory similar to that of Sec. 3.3.

We know that

$$e^{-S_I} = I + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} S_I^n = I - \int L_I(\phi(x)) d^4x + \frac{1}{2!} \int L_I(\phi(x)) L_I(\phi(y)) d^4x d^4y + \dots, \quad (4.58)$$

which implies that

$$Z[J] = \int \left[e^{-S_0 + \int J(x)\phi(x) d^4x} - \int L_I(\phi(x)) e^{-S_0 + \int J(x)\phi(x) d^4x} d^4x \right. \quad (4.59)$$

$$\left. + \frac{1}{2!} \int L_I(\phi(x)) L_I(\phi(y)) e^{-S_0 + \int J(x)\phi(x) d^4x} d^4x d^4y + \dots \right] [d\phi]. \quad (4.60)$$

Now let us suppose that any interaction of the field is given by a polynomial in the field variable, that is,

$$L_I(\phi) = P(\phi) = \sum_{n=1}^N c_n \phi^{n+2}(x), \quad (4.61)$$

then Eq. (4.59) turns into a series of expectation values of products of ϕ^5 . However, we know that such expectation values can be generated by applying functional derivatives over the partition function. Therefore, we can represent each $\phi(x)$ of L_I as $\delta/\delta J(x)$, so the previous equation becomes

$$L_I \left(\frac{\delta}{\delta J(x)} \right) = \sum_{n=1}^N c_n \frac{\delta^{n+2}}{\delta J(x)^{n+2}} = P \left(\frac{\delta}{\delta J(x)} \right). \quad (4.62)$$

Since that now the interacting Lagrangian is independent of the field variable, it can be taken out of the functional integral. Resumming the series of polynomials of L_I as $\delta/\delta J(x)$, we can rewrite Eq. (4.59) as

$$Z[J] = e^{-P \left(\frac{\delta}{\delta J(x)} \right)} Z_0[J], \quad (4.63)$$

where $Z_0[J]$ is the partition function of the free theory. Note that if we consider an interaction given by $c_n \phi^{n+2}(x)$, where $c_n < 1$, we can truncate the exponential series to a finite order for an approximation, as is the case in many theories. Also, it is worth noting that if we wish to deal with the interaction of two or more different fields, we must introduce a source J for each field, and then the polynomial interaction will be a product of derivatives with respect to different sources.

⁵Note that contributions of $\phi(x)$ and $\phi^2(x)$ can be absorbed into the free Lagrangian by a redefinition of variables.

4.3.1 The $\lambda\phi^4$ Theory

Let us apply the previous construction to the simplest case of an interacting theory, the $\lambda\phi^4$ theory. The Euclidean action of such a theory is given by

$$S = \int \left[\phi(x)(-\Delta + m^2)\phi(x) + \frac{\lambda}{4!}\phi^4(x) \right] d^D x. \quad (4.64)$$

Instead of dealing with a four-dimensional Euclidean space, let us consider the D -dimensional case.

Let us start the perturbative computation at first order in λ . The partition function of the interacting theory is given by

$$Z[J] = Z_0[J] - \frac{\lambda}{4!} \int \left(\frac{\delta}{\delta J(x)} \right)^4 Z_0[J] d^D x. \quad (4.65)$$

Using Eq. (4.19), the derivative with respect to $J(x)$ follows directly and reads

$$\frac{\delta Z_0[J]}{\delta J(x)} = - \int G_F(x', x) J(x) dx Z_0[J], \quad (4.66)$$

which allows us to express the first-order correction to the partition function as follows:

$$\begin{aligned} Z[J] = Z_0[J] & \left\{ 1 - \frac{\lambda}{4!} \int \left[3 (G_F(x, x))^2 + 6 G_F(x, x) \int G_F(x, y_1) G_F(x, y_2) J(y_1) J(y_2) dy_1 dy_2 \right. \right. \\ & \left. \left. + \int G_F(x, y_1) G_F(x, y_2) G_F(x, y_3) G_F(x, y_4) J(y_1) J(y_2) J(y_3) J(y_4) dy_1 dy_2 dy_3 dy_4 \right] dx \right\}. \end{aligned} \quad (4.67)$$

Now, we remember that the correlation functions of the model are given by functional derivatives of the partition function, setting $J = 0$ (see Eq. (4.16)). Defining

$Z_0[0] = 1$, we have

$$G^{(0)} = Z[0] = 1 - \frac{3\lambda}{4!} \int (G_F(x, x))^2 dx, \quad (4.68)$$

$$G^{(1)}(x) = \left. \frac{\delta Z[J]}{\delta J} \right|_{J=0} = 0, \quad (4.69)$$

$$G^{(2)}(x_1, x_2) = \left. \frac{\delta^2 Z[J]}{\delta J(x_1) \delta J(x_2)} \right|_{J=0} = G_F(x_1, x_2) - \frac{12\lambda}{4!} \int G_F(x_1, x) G_F(x, x) G_F(x, x_2) dx, \quad (4.70)$$

$$G^{(3)}(x_1, x_2, x_3) = \left. \frac{\delta^3 Z[J]}{\delta J(x_1) \delta J(x_2) \delta J(x_3)} \right|_{J=0} = 0, \quad (4.71)$$

$$\begin{aligned} G^{(4)}(x_1, x_2, x_3, x_4) &= \left. \frac{\delta^4 Z[J]}{\delta J(x_1) \delta J(x_2) \delta J(x_3) \delta J(x_4)} \right|_{J=0} \\ &= G_F(x_1, x_2) G_F(x_3, x_4) + G_F(x_1, x_3) G_F(x_2, x_4) + G_F(x_1, x_4) G_F(x_2, x_3) \\ &\quad - \frac{12\lambda}{4!} \left[G_F(x_1, x_2) \int G_F(x_3, x) G_F(x, x) G_F(x, x_4) dx + \text{all permutations of } \{1, 2, 3, 4\} \right] \\ &\quad - \frac{24\lambda}{4!} \int G_F(x_1, x) G_F(x_2, x) G_F(x_3, x) G_F(x_4, x) dx. \end{aligned} \quad (4.72)$$

⁶ Notice also that the product $G^{(0)}G^{(2)}(x_1, x_2)$ is also a Green's function. Therefore, we have that Eq. (4.70) corresponds to the first and second contributions of Eq. (3.310) and that the product $G^{(0)}G^{(2)}(x_1, x_2)$, at first order in λ , is the second contribution. Thus, such a contribution is not a new one. Also, the second line of Eq. (4.72) is the same as Eq. (3.309). The diagrammatic representation of the previous equations follows just like in Eqs. (3.309 - 3.310).

As we have argued before, not all Green's functions obtained by the derivatives of $Z[J]$ are independent. Therefore, we must now compute the independent ones up to first order. For that, we must take the derivatives of the generating functional of connected Green's functions, which is the free energy (Eq. (4.18)).

⁶Remember that $G_F(x, y) = G_F(y, x)$.

Up to first order in λ , we obtain

$$\begin{aligned}
 G_C^{(0)} &= W[0] = \ln \left[1 - \frac{3\lambda}{4!} \int (G_F(x, x))^2 dx \right] = \frac{3\lambda}{4!} \int (G_F(x, x))^2 dx, \quad (4.73) \\
 G_C^{(2)}(x_1, x_2) &= \frac{\delta^2 W[J]}{\delta J(x_1) \delta J(x_2)} \Big|_{J=0} = \left[\frac{1}{Z[J]} \frac{\delta^2 Z[J]}{\delta J(x_1) \delta J(x_2)} - \frac{1}{Z^2[J]} \frac{\delta Z[J]}{\delta J(x_1)} \frac{\delta Z[J]}{\delta J(x_2)} \right] \Big|_{J=0} \\
 &= \frac{1}{Z[0]} G^{(2)}(x_1, x_2) + \frac{1}{Z[0]} G^{(1)}(x_1) \frac{1}{Z[0]} G^{(1)}(x_2) \\
 &= G^{(2)}(x_1, x_2) = G_F(x_1, x_2) - \frac{12\lambda}{4!} \int G_F(x_1, x) G_F(x, x) G_F(x, x_2) dx. \quad (4.74)
 \end{aligned}$$

For $G_C^{(4)}$, the calculations become messy, with a total of 15 contributions to be evaluated. After taking the limit $J \rightarrow 0$, the nonvanishing contributions are

$$\begin{aligned}
 G_C^{(4)}(x_1, x_2, x_3, x_4) &= \frac{\delta^4 W[J]}{\delta J(x_1) \delta J(x_2) \delta J(x_3) \delta J(x_4)} \Big|_{J=0} = -\frac{2}{Z^3[0]} G^{(2)}(x_1, x_2) G^{(2)}(x_3, x_4) \\
 &\quad - \frac{2}{Z^2[0]} G^{(2)}(x_1, x_3) G^{(2)}(x_2, x_4) - \frac{2}{Z^2[0]} G^{(2)}(x_1, x_4) G^{(2)}(x_2, x_3) \\
 &\quad - \frac{1}{Z^2[0]} G^{(4)}(x_1, x_2, x_3, x_4). \quad (4.75)
 \end{aligned}$$

Up to order λ , it becomes

$$G_C^{(4)}(x_1, x_2, x_3, x_4) = -\frac{24\lambda}{4!} \int G_F(x_1, x) G_F(x_2, x) G_F(x_3, x) G_F(x_4, x) dx. \quad (4.76)$$

There are significant computational advantages to working with Green's functions in momentum space. Thus, similarly to Eq. (4.28), we can write

$$\tilde{G}^{(n)}(p_1, \dots, p_n) = \frac{1}{(2\pi)^D} \int G^{(n)}(x_1, \dots, x_n) e^{-i(p_1 x_1 + \dots + p_n x_n)} dx_1 \dots dx_n, \quad (4.77)$$

Since Green's functions in coordinate space are invariant under translations, the sum of the momenta must vanish, i.e., $\sum_n p_n = 0$. In momentum space, it follows that

$$\tilde{G}^{(2)}(p) = \frac{1}{p^2 + m^2} - \frac{\lambda}{2} \frac{1}{(2\pi)^D} \int \frac{1}{p^2 + m^2} \frac{1}{k^2 + m^2} \frac{1}{p^2 + m^2} dk. \quad (4.78)$$

In momentum space, the Feynman rules for constructing diagrams are as follows: for the **propagator**, we have

$$\text{---} = \frac{1}{p^2 + m^2} \quad (4.79)$$

and each **vertex** is given by

$$\text{X} = -\frac{\lambda}{4!} \quad (4.80)$$

It follows that at each vertex, the total momentum must be zero. Additionally, one must integrate each closed loop with the factor $(2\pi)^{-D}$. Therefore, we can recast the two-point correlation function at order λ as

$$G^{(2)}(p) = \text{---} + \text{---} \text{O} \text{---}. \quad (4.81)$$

From the definition of the classical field, Eq. (4.21), we obtain

$$\begin{aligned} \phi_c(x) = & \int G_F(x, y_1) J(y_1) dy_1 + \frac{\lambda}{2} \int G_F(x, y_1) G_F(y_1, y_1) G_F(y_1, y_2) J(y_2) dy_1 dy_2 \\ & - \frac{\lambda}{6} \int G_F(x, y_1) G_F(y_1, y_2) G_F(y_1, y_3) G_F(y_1, y_4) J(y_2) J(y_3) J(y_4) dy_1 dy_2 dy_3 dy_4, \end{aligned} \quad (4.82)$$

Thus, the generating functional of the one-particle irreducible Green's function at first order in λ ⁷, given by Eq. (4.23), is

$$\begin{aligned} \Gamma[\phi_c] = & \ln N - \frac{\lambda}{8} [G_F(x, x)]^2 dx - \frac{1}{2} \int \phi_c(x) (-\Delta + m^2) \phi_c(x) \\ & - \frac{\lambda}{4} \int [G_F(x, x) \phi_c(x)]^2 - \frac{\lambda}{4!} \int [\phi_c(x)]^4, \end{aligned} \quad (4.83)$$

which results in the following one-particle irreducible Green's function up to order λ in momentum space:

$$\tilde{\Gamma}^{(2)}(p) = p^2 + m^2 - \frac{\lambda}{2} \frac{1}{(2\pi)^D} \int \frac{1}{k^2 + m^2} dk, \quad (4.84)$$

$$\tilde{\Gamma}^{(4)}\left(\sum_{i=1}^4 p_i = 0\right) = -\lambda. \quad (4.85)$$

If we compare Eq. (4.84) with Eq. (4.78), we notice that the difference is that the one-particle irreducible Green's function does not contain the propagator of the external (out of any loop) legs. For this reason, some textbooks state that the effective action “amputates” the external legs of the Feynman diagrams. In

⁷Solve Eq. (4.82) perturbatively in $J(x)$ and then perform some integration by parts. Use the result in Eq. (4.23).

the literature, it is common to use the generating functional of the connected correlation function to build the theory and then ignore the external legs, without explicitly calculating the effective action. We follow this same procedure, and for this reason, we use $G^{(n)}(p)$ to refer to the n -point one-particle irreducible Green's function, without distinguishing it from $\tilde{\Gamma}^{(n)}$.

Each diagram has a **symmetry factor**, which corresponds to the number of ways one can construct the same diagram. Consider, for example, the second diagram of the two-point Green's function in Eq. (4.82). This diagram, known as a *tadpole*, is directly constructed from the vertex. Consider the vertex of Eq. (5.29) and label each leg from one to four, as in Eq. (3.309). To construct a two-point diagram, we must fix two legs. First, we have four legs to choose from; let us fix leg 4. Then, we need to fix one of the three remaining legs—say, leg 3. To complete the tadpole, we must link the remaining legs to each other, connecting 1 to 2. Multiplying all these choices, we obtain $4 \times 3 \times 1 = 12$. Dividing by the $4!$ factor from the Feynman rule for the vertex, we obtain the factor $1/2$ present in Eq. (4.78). For a complete discussion on symmetry factors, see Ref. [109].

If now we wish to compute the second-order contribution in λ for the two-point function, we must ask ourselves how many ways we can link the legs of two vertices, keeping two of them fixed. The result of this is two diagrams:

$$\text{Diagram 1} \quad \text{and} \quad \text{Diagram 2} \quad (4.86)$$

This demonstrates the remarkable usefulness of the diagrammatic representation: we are able to construct all the perturbation contributions without getting lost in a sea of functional derivatives and series expansions.

An inspection of Eq. (4.84) reveals that the tadpole contribution may diverge. In fact, we have:

$$\text{Diagram 1} = \frac{\lambda}{2} \frac{1}{(2\pi)^D} \int \frac{1}{p^2 + m^2} d^D p \propto \int_0^\infty \frac{p^{D-1}}{p^2 + m^2} dp, \quad (4.87)$$

and it follows that, depending on the dimension D , it may diverge as $p \rightarrow \infty$. Such a divergence is called *ultraviolet*. If we have the massless scalar field ($m^2 = 0$), it would also diverge at $p = 0$; this divergence is called *infrared*. There are many ways to regularize this algebraic divergence, for example, see Sec. A.4. One can also use a cut-off in the integral. Another way to deal with such a divergence is using dimensional regularization [74]. As a matter of fact, we have already used it to regularize Eq. (3.221); here we just present it in more detail for those who are not familiar with this technique. Using a polar representation of

the last integral, we can write:

$$I(D) = \frac{1}{(2\pi)^D} \int \frac{1}{p^2 + m^2} d^D p = \frac{1}{(4\pi)^{D/2} \Gamma(D/2)} \int_0^\infty \frac{p^{D-1}}{p^2 + m^2} dp, \quad (4.88)$$

so, using the Beta function (see Eq. (3.222)), defining $p^2 = ym^2$, we have:

$$\begin{aligned} I(D) &= \frac{(m^2)^{D/2-1}}{(4\pi)^{D/2} \Gamma(D/2)} \int_0^\infty y^{D/2-1} (1+y)^{-1} dy \\ &= \frac{(m^2)^{D/2-1}}{(4\pi)^{D/2} \Gamma(D/2)} \frac{\Gamma(D/2) \Gamma(1-D/2)}{\Gamma(1)} \\ &= \frac{(m^2)^{D/2-1}}{(4\pi)^{D/2}} \Gamma(1-D/2), \end{aligned} \quad (4.89)$$

From this equation, we see that this diagram diverges for even dimensions. In order to regularize it, let us suppose that D is even. Then, the dimensional regularization is applied by considering $D \rightarrow D - 2\varepsilon$. To avoid changing the units of the diagram, we also need to simultaneously make $\lambda \rightarrow \lambda \mu^{2\varepsilon}$, where μ has the same units as mass and is called the **renormalization parameter**. It follows that:

$$\text{tadpole} = \frac{\lambda \mu^{2\varepsilon}}{2} \frac{(m^2)^{D/2-\varepsilon-1}}{(4\pi)^{D/2-\varepsilon}} \Gamma(1-D/2+\varepsilon). \quad (4.90)$$

From the last result, we may fix a number of dimensions and then expand the expression around $\varepsilon = 0$. For concreteness, let us take $D = 2$. Then it follows:

$$\text{tadpole} = \frac{\lambda}{8\pi\varepsilon} + \frac{\lambda}{8\pi} \left[\ln(4\pi) + \ln\left(\frac{\mu^2}{m^2}\right) - \gamma_E + O(\varepsilon) \right]. \quad (4.91)$$

where the $\gamma_E \approx 0.577216$ is the Euler-Mascheroni constant. We note that, as expected, the diagram diverges if $\varepsilon = 0$. However, such a divergence can be *renormalized* if we add to the theory a contribution that generates a term in the 2-point function of the form $-\frac{\lambda}{8\pi\varepsilon}$. Such an additional contribution is called **counterterms**. Using the counterterms, we can also eliminate constants like $\frac{\lambda}{8\pi} \ln 4\pi$ and γ_E . Therefore, the renormalized tadpole is given by:

$$\text{tadpole} = \frac{\lambda}{8\pi} \ln\left(\frac{\mu^2}{m^2}\right). \quad (4.92)$$

This procedure shares many similarities with the one discussed in Sec. A.4. Both methods can be used for the same type of divergences (algebraic), and in both cases, we subtract the divergences term-by-term.

The divergences and the renormalization procedure are consequences of field theory. Different theories are classified in terms of their divergences and, therefore, by the possibility of renormalization. Analyzing the units of the model (we are in natural units, so we use length as the fundamental unit), a model in which the coupling constant is some negative power of L is said to be **super-renormalizable**. If the units of the coupling constant are L^0 , the theory is said to be **renormalizable**, and if the units of the coupling constant are a positive power of length, the theory is said to be **non-renormalizable**. It is straightforward to verify that the $\lambda\phi^4$ theory is super-renormalizable in 2 and 3 dimensions, renormalizable in 4 dimensions, and non-renormalizable for $D > 4$ dimensions. Detailed calculations of second-order diagrams in $\lambda\phi^4$ theory can be found in Ref. [110].

As one can observe, the finite result for the tadpole is given with a dependence on the renormalization parameter. While observables are given by the Green's function of the theory, such objects should not depend on this parameter once it is introduced “by hand”. Therefore, we must have:

$$\mu \frac{d\Gamma^{(n)}(m^2, \lambda, \mu)}{d\mu} = 0, \quad (4.93)$$

or, equivalently:

$$\mu \frac{\partial \Gamma^{(n)}}{\partial \mu} + \gamma(m^2, \lambda) \frac{\partial \Gamma^{(n)}}{\partial m^2} + \beta(m^2, \lambda) \frac{\partial \Gamma^{(n)}}{\partial \lambda} = 0, \quad (4.94)$$

where:

$$\beta(m^2, \lambda) = \mu \frac{\partial \lambda}{\partial \mu}, \quad (4.95)$$

$$\gamma(m^2, \lambda) = \mu \frac{\partial m^2}{\partial \mu}. \quad (4.96)$$

The Eq. (4.94) is known as the *Callan-Symanzik equation* [111–113]. One way to interpret the parameter μ is that it fixes the energy scale of the theory. With this interpretation in mind and using the β -function given in Eq. (4.95), D. Gross, F. Wilczek, and H. Politzer proved that quantum chromodynamics (QCD) has a regime of high energies in which it is perturbatively well-behaved. Nowadays, this result is known as asymptotic freedom [114, 115].

We must emphasize that even in renormalizable theories, there can be high energy regimes where the theory is not perturbatively well-behaved. Such divergent behavior is known as a *Landau pole*, and it has been found in various cases, *e.g.*, quantum electrodynamics (QED) [116] and in the $\lambda\phi^4$ theory [117].

A lot more can be discussed in the context of interacting theories and in the constructive approach. However, to keep the chapter as brief as possible, we leave these discussions to the references cited at the beginning of this chapter.

Chapter 5

Disordered Fields Theory

The statistical physics is one of the most successful theories in physics and it relies on the average treatment of systems, instead of dealing with the properties of every single component of it. The main achievement of statistical physics is beginning with a microscopic description of a system, given by some Hamiltonian, and being able to predict its macroscopic behavior. Among the successful predictions of statistical physics, phase transitions are one of the most important. However, even in the simplest model with a phase transition, the exact treatment of it can be cumbersome, and in some cases, impossible. Therefore, a way to approximate its behavior is necessary. It is in this scenario that the Landau theory of phase transitions emerges [118]. Furthermore, the Landau theory also allows us to build a bridge between the discrete models of traditional statistical mechanics and the constructive approach of quantum field theory.

After advancing our comprehension about homogeneous systems, the statistical physicists turned their attention to systems with impurities, as such impurities introduce many difficulties in the physical reasoning and mathematical framework of the theory.

In this chapter, we investigate the long-known connection between statistical physics systems and quantum field theory [80]. After that, we introduce disordered systems and the distributional zeta function method to deal with such systems, and then we discuss some original results. Here we follow Ref. [119–121]. Unless stated otherwise, we have a natural system of units, $\hbar = c = k_B = 1$.

5.1 Statistical Field Theory

Our aim in this section is to tighten the relation between constructive field theory and statistical field theory more than we have briefly discussed at the end of Sec 4.1. We assume that the reader is familiar with the basic results and properties

of statistical mechanics and take their validity as given.

We will show, with some details, how to start with the **Ising model** and obtain its corresponding quantum field theory. The Ising model is given by spins $s_i = \pm 1$ located on a lattice with N sites. Its Hamiltonian is written as

$$H = - \sum_{i,j} s_i J_{ij} s_j - \sum_i h_i s_i, \quad (5.1)$$

where h_i is an external magnetic field at site i and J_{ij} is the coupling between the spins. If J is positive, we have a ferromagnetic coupling. If J is negative, we have an antiferromagnetic coupling.

The probability of a given configuration s_i is given by the Boltzmann weight

$$P(s_i) = e^{-\beta H}, \quad (5.2)$$

where $\beta = T^{-1}$, and follows that the partition function is

$$Z = \sum_{s_i} e^{-\beta H}, \quad (5.3)$$

where the sum is taken over all configurations. From the usual statistical mechanics, we know that all the statistical averages (correlation functions) are obtained from derivatives of the partition function.

Now, consider the following Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-\frac{1}{4} \sum_{ij} \psi_i V_{ij}^{-1} \psi_j + \sum_i s_i \psi_i} \prod_{i=1}^N d\psi_i = C e^{\sum_{ij} s_i V_{ij} s_j}, \quad (5.4)$$

therefore, the partition function of the Ising model can be rewritten as

$$\begin{aligned} Z &= \sum_{s_i} e^{-\beta (\sum_{i,j} s_i J_{ij} s_j + \sum_i h_i s_i)} = \sum_{s_i} \int_{-\infty}^{\infty} e^{-\frac{1}{4\beta} \sum_{ij} \psi_i J_{ij}^{-1} \psi_j + \sum_i (\psi_i + \beta h_i) s_i} \prod_{i=1}^N d\psi_i \\ &= \int_{-\infty}^{\infty} e^{-\frac{1}{4\beta} \sum_{ij} (\psi_i - \beta h_i) J_{ij}^{-1} (\psi_j - \beta h_j)} \sum_{s_i} e^{\psi_i s_i} \prod_{i=1}^N d\psi_i, \end{aligned} \quad (5.5)$$

we note that, since the spins s_i are independent, the sum over the configurations can be performed:

$$\sum_{s_i} e^{\psi_i s_i} = \prod_i (2 \cosh \psi_i) = C e^{\sum_i \ln(\cosh \psi_i)}. \quad (5.6)$$

Defining $\phi_i = \frac{1}{2}J_{ij}^{-1}\psi_i$, we can write

$$Z = C e^{\frac{\beta}{4} h_i J_{ij}^{-1} h_j} \int e^{\beta \sum_{ij} (-\phi_i J_{ij} \phi_j) + \sum_i \ln \cosh(2J_{ij} \phi_j) + \beta \sum_i h_i \phi_i} \prod_{i=1}^N d\phi_i, \quad (5.7)$$

where C is a normalization constant.

As one can expect, we wish to rewrite the argument of the exponential as some Lagrangian. For that, we write the following Fourier representations:

$$\phi_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{p}} e^{-i\mathbf{p} \cdot \mathbf{x}_i} \phi(\mathbf{p}) \quad (5.8)$$

$$J_{ij} = \frac{1}{N} \sum_{\mathbf{p}} e^{-i\mathbf{p} \cdot (\mathbf{x}_i - \mathbf{x}_j)} J(\mathbf{p}), \quad (5.9)$$

In terms of the Fourier representation, and using a series expansion for $\ln \cosh x = \frac{1}{2}x^2 - \frac{1}{12}x^4$, we have that

$$\phi_i J_{ij} \phi_j = \sum_{\mathbf{p}} \phi(\mathbf{p}) J(\mathbf{p}) \phi(-\mathbf{p}) \quad (5.10)$$

$$\sum_i \ln \cosh(2J_{ij} \phi_i) = 2 \sum_{\mathbf{p}} \phi(\mathbf{p}) J(\mathbf{p}) J(-\mathbf{p}) \phi(-\mathbf{p}) - \frac{4}{3} \sum_{\mathbf{p}} \phi^2(\mathbf{p}) J^2(\mathbf{p}) J^2(-\mathbf{p}) \phi^2(-\mathbf{p}). \quad (5.11)$$

Now expand the $J(\mathbf{p})$ up to second order in $p = \|\mathbf{p}\|$:

$$J(\mathbf{p}) = J(1 - \rho^2 p^2), \quad (5.12)$$

where, assuming that we have only first-neighborhood interactions, $J = \gamma \beta J_0$, and γ is the number of nearest neighbors. Now, for the p^2 term in the first-neighborhood approximation, we get

$$J \rho^2 p^2 \approx J a^2 p^2, \quad (5.13)$$

therefore, $\rho \approx a$, the lattice spacing constant. This results in the following Lagrangian:

$$\begin{aligned} \beta L &= \beta \sum_{\mathbf{p}} \phi(\mathbf{p}) J [(1 - 2J) + (4J - 1)a^2 p^2] \phi(-\mathbf{p}) \\ &\quad - \frac{4\beta}{3} \sum_{\mathbf{p}} \phi^2(\mathbf{p}) J^4 (1 - 4a^2 p^2) \phi^2(-\mathbf{p}) \\ &= \beta L_0 - \beta L_I, \end{aligned} \quad (5.14)$$

analyzing only the free Lagrangian, we see that for $T_0 = 2\gamma J_0$, the theory becomes unstable. Therefore, if we expand each contribution of the free Lagrangian in powers of T_0 to first order, we get

$$1 - 2\beta J = \frac{T - T_0}{T_0}, \quad (5.15)$$

$$4\beta J - 1 = 1, \quad (5.16)$$

$$\beta J = \frac{1}{2}, \quad (5.17)$$

Therefore, it follows that

$$\beta L_0 = \frac{1}{2} \sum_{\mathbf{p}} \phi(\mathbf{p}) \left(\frac{T - T_0}{T_0} + a^2 p^2 \right) \phi(-\mathbf{p}), \quad (5.18)$$

performing the change of variables $m^2 = \frac{1}{a^2} \frac{T - T_0}{T_0}$ and $\phi \rightarrow a^2 \phi$ we obtain

$$\beta L_0 = \beta \frac{1}{2} \sum_{\mathbf{p}} \phi(\mathbf{p}) (p^2 + m^2) \phi(-\mathbf{p}), \quad (5.19)$$

It is straightforward to note that, up to the β pre-factor, it is a momentum representation of the following Lagrangian

$$L_0 = \frac{1}{2} \phi(x) (\Delta + m^2) \phi(x), \quad (5.20)$$

which is the Euclidean Lagrangian of the free scalar theory. To deal with the interacting Lagrangian

$$\beta L_I = \frac{4\beta}{3} \sum_{\mathbf{p}} \phi^2(\mathbf{p}) J^4 (1 - 4a^2 p^2) \phi^2(-\mathbf{p}), \quad (5.21)$$

we notice that the contribution of the momenta arises from a Laplacian acting over the $\phi(x)$, and since we are interested in using J^4 as a perturbative parameter, the contribution $J^4 \Delta \phi(x)$ is subleading and therefore can be disregarded. So by the change of variables $\frac{4}{3} J^4 = \lambda/4!$, we have that

$$\beta L_I = -\beta \frac{\lambda}{4!} \phi^4(x). \quad (5.22)$$

Then it follows that the partition function can be written as

$$Z[h] = \int e^{-\beta \int \left[\frac{1}{2} \phi(x) (\Delta + m^2) \phi(x) + \frac{\lambda}{4!} \phi^4(x) \right] dx + \int h(x) \phi(x) dx} [d\phi], \quad (5.23)$$

which, up to the factor of β , is the partition function of the $\lambda\phi^4$ theory discussed in Sec. 3.3 and in Sec.4.3.1. We note that, as expected, the resulting Lagrangian has the same symmetries as the Ising model, that is, the symmetry $\mathbb{Z}_2$. This field theoretical description of the statistical/condensed matter systems is usually referred to as the **soft spin approach** or **soft model**.

By a direct computation, we have that $\langle\phi\rangle = 0$, and comparing this to the results of the Ising model, we see that the field variable, in this case, represents the magnetization of the system, and its expected value going to zero corresponds to a system without *persistent magnetization*. For a system that presents persistent magnetization, we have that $\langle\phi\rangle \neq 0$, which means that the ground state (vacuum) of the theory must be shifted in order to ensure that we have a minimum value. Such a situation is achieved if we have $m^2 < 0$. Then we have $\langle\phi\rangle = v = \sqrt{-m^2/\lambda}$ as the ground state. Defining a new variable, $\varphi = \phi - v$, which has zero expected value, we obtain an effective $m_2^2 = 3\lambda v^2 + m^2$, and the interacting Lagrangian is modified to

$$L_I^{(2)} = -\rho\varphi^3(x) + \frac{\lambda}{4!}\varphi^4(x), \quad (5.24)$$

where we defined $\rho_0 = 4!\lambda v$. Such a procedure is called **spontaneous symmetry breaking**. We notice that both theories, with and without persistent magnetization, have the same $\mathbb{Z}_2$ symmetry. The difference is that to ensure we have the ground state, one of the field variables must be shifted. The change in the potential of the theory can be verified in the Figs. 5.1.

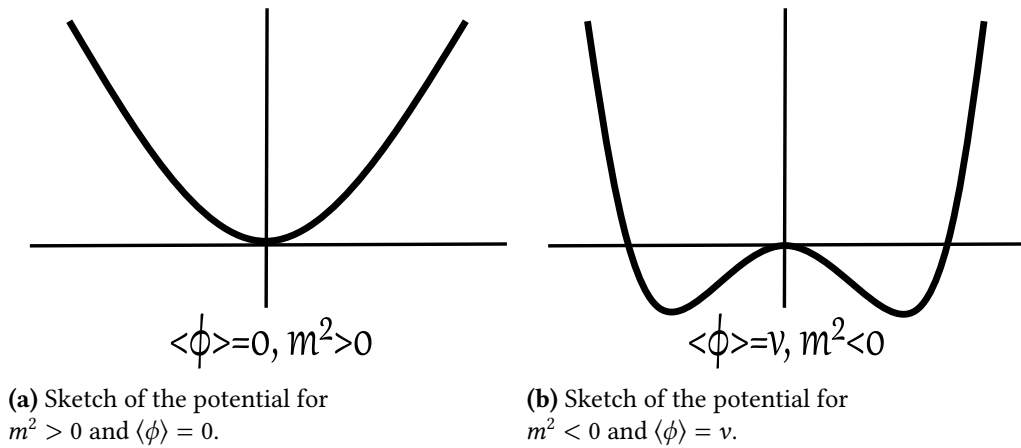


Figure 5.1: Two potentials, without and with persistent magnetization.

One may be puzzled by the previous fact, since we have shown that all representations of quantum systems should be unitarily equivalent to the canonical commutation relations, and, therefore, the vacuum should be the same (see the

Stone-von Neumann theorem, theorem 2.18). But the previous two vacuums are not the same and are not unitarily equivalent, and we are talking about the same system in different starting points (without and with persistent magnetization). However, we remark that the Stone-von Neumann theorem holds only in a finite number of dimensions of the phase space. In quantum field theory, we deal with an infinite number of degrees of freedom, which leads us to an infinite-dimensional phase space, and the Stone-von Neumann theorem cannot be used to ensure the uniqueness of the vacuum (up to unitary transformations).

The many possible vacuums of quantum fields are an interesting feature that leads to different fascinating phenomena. Among them are: phase transitions, the Unruh effect [122] (see also, Ref. [123]), and Hawking radiation [124].

Before we end this section, we note that if we have a bidimensional Heisenberg spin $\mathbf{S} = \{s_x, s_y\}$ instead of the Ising spin in Eq. (5.1), the same steps can be performed to obtain the following soft version action:

$$S(\phi_1, \phi_2) = \int \left[\sum_{i=1}^2 \phi_i(x)(-\Delta + m^2)\phi_i + \frac{\lambda}{4!}(\phi_1^2(x) + \phi_2^2(x))^2 \right] dx. \quad (5.25)$$

This model is invariant under the group $\mathcal{O}(2)$, that is, it is invariant under bidimensional rotations. Like in the Ising model, we can have the case of persistent magnetization. Performing the same steps as before, assuming $m^2 < 0$ and renaming the variables as $\varphi = \phi_1 - v$, $v^2 = 4!m^2/\lambda$, m_1^2 , $\psi = \phi_2$, and $\rho = \lambda v$, we obtain

$$S(\varphi, \psi) = \int \left[\frac{1}{2}\varphi(x)(-\Delta + m_0^2)\varphi(x) + \frac{\lambda}{4!}(\varphi^2(x) + \psi^2(x))^2 + \frac{1}{2}\psi(x)(-\Delta)\psi(x) + \frac{\rho}{4!}\varphi(x)(\varphi^2(x) + \psi^2(x)) \right] dx. \quad (5.26)$$

We readily notice that the spontaneous symmetry breaking introduces a massless field, ψ , in our description. Such a field is commonly referred to as the **Goldstone field** or **Goldstone modes**. In general, one can prove that *the breaking of a continuous symmetry introduces a Goldstone field in the theory*. Such a result is known as the **Goldstone theorem**.

5.1.1 Second order phase transition in the $\lambda\phi^4$ theory

As we know, a second-order phase transition in a system is characterized by the divergence of the free energy or by its on-shell 2-point correlation function (sometimes referred just as *mass*). In the case of the Ising or Heisenberg model, it

is the magnetization, becoming zero or increasing smoothly from zero in terms of some parameter. If this parameter has a thermodynamical origin (temperature, pressure, ...), we have a thermal phase transition. However, we can also have phase transitions due to non-thermal parameters, like the self-interaction of a theory raised by quantum fluctuations, see for example Refs. [110, 125, 126] and the references therein.

The usual phase transitions are closely related to the symmetries of a system. For example, consider a ferromagnet system without any persistent magnetization at some temperature T . Such a system is invariant under all rotations in the space and, therefore, is invariant under the group $\mathcal{O}(3)$. If we slowly lower the temperature, the spins of the system start to align, generating a non-zero magnetization. This magnetized system is invariant under rotations around the magnetization axis, that is, it is invariant under the group $\mathcal{O}(2)$, and we say that a symmetry breaking occurs. Conversely, if we start with a system with persistent magnetization and then raise the temperature, the magnetization becomes zero and we have restored the symmetry.

If we wish to obtain the field variables depending on the temperature, we must recover the Euclidean time explicitly, $\phi(x, \tau)$, also splitting the laplacian to separate the Euclidean time, $\Delta_D \rightarrow \partial^2/\partial\tau^2 + \Delta_{D-1} = \partial^2/\partial\tau^2 + \Delta$, and impose the KMS condition over the field variables, that is $\phi(x, \tau + \beta) = \phi(x, \tau)$. For more details about field theory in finite temperature scenario, see Ref. [127]. With this explicit dependence, we write the action functional, in a slightly different notation, as

$$S(\phi) = \frac{1}{2} \int_0^\beta \int \left[\phi(\tau, \mathbf{x}) \left(-\frac{\partial^2}{\partial\tau^2} - \Delta + \mu_0^2 \right) \phi(\tau, \mathbf{x}) + \frac{\lambda}{2} \phi^4(x, \tau) \right] dx d\tau. \quad (5.27)$$

Now we suppose that the system has some persistent magnetization making the $\mu_0^2 \rightarrow -\mu_0^2$, therefore we can use the end of preceeding section to obtain the theory around the correct ground state, $v = \sqrt{\mu_0^2/\lambda}$. Therefore, the shifted action reads

$$S(\varphi) = \frac{1}{2} \int_0^\beta \int \left[\varphi(x, \tau) \left(-\frac{\partial^2}{\partial\tau^2} - \Delta + m_0^2 \right) \varphi(x, \tau) - \rho_0 \varphi^3 + \frac{\lambda}{2} \varphi^4(x, \tau) \right] dx d\tau. \quad (5.28)$$

where $\rho_0 = 2\lambda v$, $m_0^2 = 3\lambda v^2 - \mu_0^2$, and $\varphi = \phi - v$.

As we have seen, this introduces a new interacting contribution to the action. Applying the same structure constructed in the last chapter (see Sec. 4.3.1), this new interaction generates a new vertex in the Feynman diagrams, given by

$$\text{---} \text{---} \text{---} \text{---} = \rho_0, \quad (5.29)$$

then, the correlation functions of the theory include the contribution of this new vertex. Diagrammatically, at one loop level, the mass of the theory is given by

$$G^{(2)}(p^2 = -m^2) = m_R^2 = \text{---} + \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---}. \quad (5.30)$$

Instead of using the dimensional regularization in these diagrams, we use the analytic regularization, introduced in Sec. 3.2.1 and also applied in Sec. 4.2.1. For that, let us write

$$m_R^2(\beta) = m_0^2 + \delta m_0^2 + 6 \Delta m_1^2(\beta) + 18 \Delta m_2^2(\beta), \quad (5.31)$$

where we denote $\Delta m_1^2(\beta)$ and $\Delta m_2^2(\beta)$ as the contributions of the tadpole and the self-energy diagram of Eq. (5.30), 6 and 18 are symmetry factors, and δm_0^2 is a d -dependent mass counterterm. We define $d = D - 1$ and omit the d -dependence in the $\Delta m(\beta)$ functions to simplify the notation. Let us first discuss the tadpole contribution.

We note that now one of the dimensions is periodic due to the KMS condition; therefore, the spectrum in this dimension will be discrete. This discrete spectrum is called **Matsubara frequencies**. Different procedures are used in the literature to evaluate the Matsubara sum of the tadpole. One can use a method where the Matsubara frequency sum separates into temperature-independent and temperature-dependent parts. An alternative procedure is to use a mix of dimensional and analytic regularization [74, 128–130]. Here we will use an analytic regularization procedure, where the number of dimensions of the space is not treated as a complex continuous variable [131]. A detailed study comparing an analytic regularization procedure and a cut-off method in the Casimir effect can be found in Refs. [47, 132–134]. The analytic regularization procedure aims to replace divergent integrals with analytic functions of certain regularization parameters.

We denote the thermal contribution from the tadpole, after analytic continuation, by $\Delta m_1^2(\beta, \mu, s)|_{s=1}$. By performing the angular part of the integral over the continuous momenta of the non-compact d -dimensional space, for $s \in \mathbb{C}$, the quantity $\Delta m_1^2(\beta)$ can be written as $\Delta m_1^2(\beta, \mu, s)$, where

$$\Delta m_1^2(\beta, \mu, s) = \frac{\lambda(\mu, s) \beta}{2^{d+1} \pi^{\frac{d}{2}+1} \Gamma(\frac{d}{2})} \int_0^\infty dp p^{d-1} \sum_{n \in \mathbb{Z}} \left[\pi n^2 + \frac{\beta^2}{4\pi} (p^2 + m_0^2) \right]^{-s} \quad (5.32)$$

with $\lambda(\mu, s) = \lambda_0(\mu^2)^{s-1}$, where μ has mass dimension. The function $\Delta m_1^2(\beta, \mu, s)$ is defined in the region where the above integral converges, $\Re(s) > s_0$.

The self-energy contribution to the mass, $\Delta m_2^2(\beta)$, can be obtained from the tadpole as:

$$\Delta m_2^2(\beta) = \left[-\frac{\rho^2(\mu, s)}{\lambda(\mu, s)} \Delta m_1^2(\beta, \mu, s) \right]_{s=2}, \quad (5.33)$$

where $\rho(\mu, s) = \rho_0(\mu^2)^{s-2}$. Therefore, one can focus on the $\Delta m_1^2(\beta, \mu, s)$ function.

After a Mellin transform and reordering of some quantities, we can write $\Delta m_1^2(\beta, \mu, s)$ as:

$$\Delta m_1^2(\beta, \mu, s) = \frac{\lambda(\mu, s)}{2\pi\Gamma(\frac{d}{2})\Gamma(s)} \left(\frac{1}{\beta} \right)^{d-1} \int_0^\infty \left[r^{d-1} \int_0^\infty t^{s-1} \sum_{n \in \mathbb{Z}} e^{-(\pi n^2 + r^2 + m_0^2 \beta^2 / 4\pi)t} dt \right] dr, \quad (5.34)$$

where we made the change of variable $r^2 = \beta^2 p^2 / 4\pi$. The integral over r is straightforward. Using the Θ -function defined on Eq. (3.79), we can split the t -integral into two

$$\Delta m_1^2(\beta, \mu, s) = C_d(\beta, \mu, s) \left[\int_0^1 t^{s-\frac{d}{2}-1} e^{-m_0^2 \beta^2 t / 4\pi} \Theta(t) dt + \int_1^\infty t^{s-\frac{d}{2}-1} e^{-m_0^2 \beta^2 t / 4\pi} \Theta(t) dt \right] \quad (5.35)$$

with $C_d(\beta, \mu, s)$ defined as

$$C_d(\beta, \mu, s) = \frac{\lambda(\mu, s)}{4\pi\Gamma(s)} \left(\frac{1}{\beta} \right)^{d-1}. \quad (5.36)$$

Next, by making a change of variable $t \rightarrow 1/t$ in the first integral and using the modular property of the Θ -function, one can write $\Delta m_1^2(\beta, \mu, s)$ as a sum of four integrals:

$$\Delta m_1^2(\beta, \mu, s) = C_d(\beta, \mu, s) \left[2I_d^{(1)}(\beta, s) + 2I_d^{(2)}(\beta, s) + I_d^{(3)}(\beta, s) + I_d^{(4)}(\beta, s) \right], \quad (5.37)$$

where

$$I_d^{(1)}(\beta, s) = \int_1^\infty t^{s-\frac{d}{2}-1} e^{-m_0^2 \beta^2 t / 4\pi} \psi(t) dt, \quad (5.38)$$

$$I_d^{(2)}(\beta, s) = \int_1^\infty t^{-s+\frac{d}{2}-\frac{1}{2}} e^{-m_0^2 \beta^2 / 4\pi t} \psi(t) dt, \quad (5.39)$$

$$I_d^{(3)}(\beta, s) = \int_1^\infty t^{s-\frac{d}{2}-1} e^{-m_0^2 \beta^2 t / 4\pi} dt, \quad (5.40)$$

$$I_d^{(4)}(\beta, s) = \int_1^\infty t^{-s+\frac{d}{2}-\frac{1}{2}} e^{-m_0^2 \beta^2 / 4\pi t} dt, \quad (5.41)$$

in which $\psi(v)$ is given by Eq. (3.78).

Now we can use the standard result that a function that is analytic on a domain $\Omega \subset \mathbb{C}$ has a unique extension to a function defined in $\mathbb{C}$, except for a discrete set of points. Using the fact that $\psi(t) = O(e^{-\pi t})$ as $t \rightarrow \infty$, the integrals $I_d^{(1)}(s, \beta)$ and $I_d^{(2)}(s, \beta)$ represent everywhere regular functions of s for $m_0^2 \beta^2 \in \mathbb{R}_+$. The upper bound ensures uniform convergence of the integrals on every bounded domain in $\mathbb{C}$. On the other hand, at low temperatures, the integrals $I_d^{(3)}(s, \beta)$ and $I_d^{(4)}(s, \beta)$ are finite too. Therefore, one can take the limit $s \rightarrow 1$ to obtain the tadpole contribution to the thermal correction to the mass. Note that the thermal correction from the self-energy contribution is also finite; recall that to obtain this contribution we have to evaluate the four integrals for $s = 2$. We stress that these results are valid only in the low-temperature situation.

We note that we are left with an ultraviolet divergence that needs to be normalized. The divergence comes from the integral $I_d^{(4)}(\beta, s)$. The renormalization is done by introducing a mass counterterm of the form $-\delta m_0^2 = C_d(\beta, \mu, s) I_d^{(4)}$. This is a temperature-dependent counterterm coming from the subtraction at zero momentum of the self-energy diagram. Going beyond one-loop approximation, one can show that the counterterms of a finite temperature field theory are the same as those of the zero temperature theory. The final result is then:

$$\Delta m_1^2(\beta) = C_d(\beta, 1) \left[2I_d^{(1)}(\beta, 1) + 2I_d^{(2)}(\beta, 1) + I_d^{(3)}(\beta, 1) + I_d^{(4)}(\beta, 1) \right], \quad (5.42)$$

$$\Delta m_2^2(\beta) = -C_d(\beta, 2) \frac{\rho_0^2}{\mu^2 \lambda_0} \left[2I_d^{(1)}(\beta, 2) + 2I_d^{(2)}(\beta, 2) + I_d^{(3)}(\beta, 2) + I_d^{(4)}(\beta, 2) \right], \quad (5.43)$$

Finally, the critical temperature of this pure system is given by the value of β for which the renormalized mass squared vanishes. Fig. 5.2 presents the results for renormalized squared mass $m_R^2(\beta)$ for $d = 3$ as a function of m_0 and selected values of λ_0 .

Therefore we have that, in the context of the Ising model, the magnetization becomes zero smoothly as we increase the temperature. This is what we expected in the context of a second order phase transition.

5.2 Quenched Disorder

As we said before, most real systems have some kind of impurities that may or may not affect the physical properties of the system. These impurities can be modeled in many ways. Here we are interested in the impurities that can be

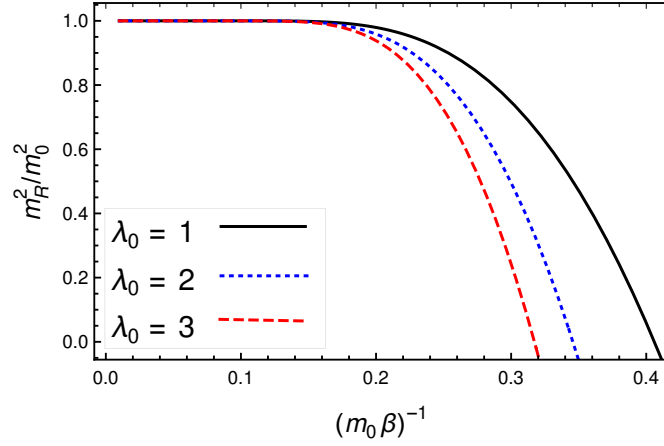


Figure 5.2: The renormalized squared mass as a function of $(m_0\beta)^{-1}$, for different values of the coupling constant λ_0 for $d = 3$. We set $\mu^2 = m_0^2$.

modeled by disorder, that is, some additional degree of freedom that we have not added in our description of the system.

Disordered systems are characterized by some random function, $h(x)$. The function $h(x)$ can model different situations, such as impurities in the lattice and inhomogeneities in the crystal. The usual way to choose the random function $h(x)$ is to take a function with mean zero and a non-vanishing covariance. Therefore, this information must be taken into the partition function, and we may write

$$Z = \text{Tr} e^{-\beta S(\phi, h)}, \quad (5.44)$$

where $S(\phi, h)$ is the action of the degrees of freedom and the disorder. If the disorder of the system is in thermal equilibrium with the other degrees of freedom, we can take the disorder average before summing up all the degrees of freedom, that is, we can write

$$e^{-\beta S_{\text{eff}}(\phi)} = \text{Tr}_h e^{-\beta S(\phi, h)} = \mathbb{E} \left[e^{-\beta S(\phi, h)} \right], \quad (5.45)$$

where Tr_h denotes the trace over $h(x)$. Therefore, we can define the free energy and obtain the thermodynamic properties of the system. When we can proceed in the preceding way, that is, when the disorder is in equilibrium with the whole system, we say that we have a **annealed disorder**.

Now, if the disorder is not in equilibrium with the other degrees of freedom, or the probability distribution is independent of the other degrees of freedom, we cannot take the total trace as in Eq. (5.44). Instead, we have a partition function for each realization of the disorder, that is

$$Z[h] = \text{Tr}_\phi e^{-\beta S(\phi, h)}. \quad (5.46)$$

Therefore, we have a free energy for each realization of the disorder

$$W[h] = -\ln Z[h]. \quad (5.47)$$

In order to obtain the physical properties of the system, we need to take the average of the free energy with respect to the disorder; then it follows that

$$F = \mathbb{E}[W[h]] = -\mathbb{E}[\ln Z[h]]. \quad (5.48)$$

This kind of disorder is called **quenched disorder** or static disorder, and it is the case that we are interested in in this thesis. Static disorder, for instance, manifests in many condensed-matter systems, such as disordered metals, impure semiconductors, and classical or quantum spin systems [3, 121, 135, 136]. The effects of random couplings on second-order phase transitions in d -dimensional systems, driven by thermal and disorder fluctuations, are controlled by the Harris criterion [137]. Under coarse-graining of fluctuations, which is the usual approach in the treatment of disordered systems, one can identify two distinct behaviors of the system's criticality under disorder. Namely, if the correlation length exponent of the pure system ν satisfies the inequality $\nu \geq \frac{2}{d}$, the effects of disorder may be disregarded in the physics of large length scales. Otherwise, for $\nu < \frac{2}{d}$ the disorder-induced fluctuations modify the critical behavior. In the latter case, the critical exponents must change under the coarse-graining procedure, that is, when one integrates over the disorder. There are two dimensions of particular relevance in pure and quenched disordered models. The first one is the lower critical dimension d_c^- , which is the lowest spatial dimension at which there is no long-range order. The second one is the upper critical dimension d_c^+ , which is the dimension above which the model is Gaussian in the infrared.

As we know, the logarithm diverges at the origin; such a divergence is not algebraic and introduces difficulties in the computation of averages. These complications have been known since the 70's [138] and, over the years, many proposals have been used to compute this average. As a matter of fact, we have the replica trick [138, 139], the dynamic [140, 141] and supersymmetric approaches [4]. Another way to find the quenched free energy is the distributional zeta-function method [142, 143], which is the one we use in this thesis.

The disorder can be coupled in different ways to our degrees of freedom; mainly, there are two cases that are most common in the literature: additive and multiplicative disorder. The additive disorder is intended to model randomness in the structure or internal degrees of freedom that we did not take into account in the pure Hamiltonian. The multiplicative disorder can be viewed as an external random effect acting on the system, like a force.

One of the principal models of disordered systems is the so-called **Edwards-**

Anderson model, given by

$$H = - \sum_{i,j} s_i J_{ij} s_j - \sum_i h_i s_i, \quad (5.49)$$

where J_{ij} is now a random variable with mean zero and non-vanishing covariance. Note that, apart from the random nature of J_{ij} , it is the Ising model. If h_i is random and **not** J_{ij} , we have a model with additive disorder called the **Random Field Ising Model**. The Edwards-Anderson model was the first to attempt to explain the spin-glass phase of some materials.

The spin-glass phase appears when a system is not able to satisfy the conditions that minimize the energy at every site. For example, take the Ising model on a triangular lattice; if we fix $J_{ij} < 0$, the state of minimum energy is to anti-align the spins. However, due to the nature of the triangular lattice, this cannot be satisfied at every site of the lattice simultaneously; this effect is called **frustration**. This leads to clusters of frustrated states in a spin-glass phase.

The Edwards-Anderson model cannot be solved exactly; however, its long-range version called the **Sherrington-Kirkpatrick model** [144], was solved using the replica trick, and most of its results can be found in Ref. [3].

The soft/continuous version of the Sherrington-Kirkpatrick model can be obtained in the same way as given in Sec. 5.1, and it reads

$$S(\phi, h) = \int \left[\frac{1}{2} \phi(x) (-\Delta + m_0^2) \phi(x) - h(x) \phi^2(x) + \frac{\lambda_0}{2} \phi^4(x) \right] dx, \quad (5.50)$$

where $h(x)$ is a random function; note that we keep the notation $d^D x = dx$ from the last chapter. In this thesis, we refer to the preceding action as the **random mass model**. For the random field Ising model, or simply **random field model**, we have the continuous action given by

$$S(\phi, h) = \int \left[\frac{1}{2} \phi(x) (-\Delta + m_0^2) \phi(x) - h(x) \phi(x) + \frac{\lambda_0}{2} \phi^4(x) \right] dx. \quad (5.51)$$

In Ref. [145] the following two results were presented for the RFIM, which is dominated by disorder fluctuations. Using Peierls' arguments [146], these authors proved that $d_c^- = 2$. Using renormalization group techniques, they also proved that $d_c^+ = 6$. The first result was discussed by Imbrie [147] and the latter was confirmed by Aizenman and Wehr [148, 149]. Concerning the existence of the phase transition, in Refs. [150, 151] it was proved that there is an ordered phase for $d \geq 3$. See also Ref. [152]. Other important results discussing the behavior of the pure and the disordered models were obtained by many authors. It was proved that the critical exponents of the system with quenched disorder are identical to the critical exponents of the pure system in $(d - 2)$ dimensions [153–

[158]. While this dimensional reduction breaks down at low dimensions ($d < 5$), recent high-precision numerical studies [159] have demonstrated that it holds with remarkable accuracy at $d = 5$. This suggests that the dimensional reduction becomes valid above a critical dimension, where non-perturbative effects associated with multiple energy minima become less relevant [158].

In this thesis we investigate the application of the distributional zeta-function method to the previous two actions, mostly in the case of the random field, where we have most of our original results.

5.2.1 Distributional zeta-function method

As we have stressed, it is not trivial to calculate the average of the logarithm. Let us assume that we have an action $S(\phi, h)$ where h is a random function coupled, in some way, to the variable ϕ .

Now take a measure space $(x, \mathcal{X}, \mu)$ (see after definition A.15), and $f : X \rightarrow (0, \infty)$ any integrable function. Then we define the *generalized zeta function* as

$$\zeta_{\mu, f}(s) = \int_{\Omega} f^{-s}(x) d\mu(x), \quad (5.52)$$

for any $s \in \mathbb{C}$. We have that $f^{-s} = e^{-s \ln f}$, by the principal branch of the logarithm. If we set $f(x) = x$, $X = \mathbb{N}$, and μ as the counting measure, we obtain the Riemann zeta function, defined in Eq. (3.82). Now if $f(x) = x$, $X = \mathbb{R}$, and μ counts the eigenvalues of an operator, with the respective multiplicity, we obtain the spectral zeta function of Eq. (3.104).

In our case, let us define $f(x) = Z[h]$, where $Z[h]$ is the partition function of $S(\phi, h)$ for one realization of the disorder (see Eq. (5.46)), and $d\mu = [dh]P(h)$, that is, the probability distribution of the disorder field. In this case we write the **distributional zeta-function** (or **DZF**) as

$$\Phi(s) = \int \frac{1}{Z^s[h]} P(h) [dh] = \mathbb{E} \left[\frac{1}{Z^s[h]} \right]. \quad (5.53)$$

Noticing that $Z[h] = (Z[h] + Z[-h])/2$, we have

$$Z[h] = \int \cosh \left[\int h(x) \phi^n(x) dx \right] e^{-S(\phi, 0)} [d\phi], \quad (5.54)$$

therefore it follows that $Z[h] \geq Z[0]$ and

$$\int \left| \frac{1}{Z^s[h]} \right| P(h) [dh] \leq \frac{1}{Z^{\Re(s)}[0]} < \infty, \quad (5.55)$$

for $\Re(s) \geq 0$. Thus the integral in Eq. (5.53) converges in the upper half-complex plane $\Re(s) \geq 0$; we notice that this means that there is no need to perform an analytical continuation over $\Phi(s)$.

It is direct to compute that

$$-\lim_{s \rightarrow 0^+} \frac{Z^{-s}[h] - 1}{s} = -\frac{d}{ds} Z^{-s}[h] \Big|_{s=0^+} = \ln Z[h], \quad (5.56)$$

then, using Eq. (5.48), it follows

$$F = - \int -\frac{d}{ds} Z^{-s}[h] \Big|_{s=0^+} P(h)[dh]. \quad (5.57)$$

We notice that we can interpret $P(h)[dh] = [dP(h)]$ in the sense of a Radon-Nikodym derivative (see theorem A.35), that is, $P(h) = \frac{[dP(h)]}{[dh]}$. Since $Z[h] \geq Z[0]$, we can use the Lebesgue dominated convergence theorem (theorem A.32) to write

$$F = \frac{d}{ds} \Phi(s) \Big|_{s=0^+}. \quad (5.58)$$

Then we have that the quenched free energy is given by the derivative of the distributional zeta function evaluated at $s = 0$, similar to the case of the spectral zeta function that gives Eq. (4.37). To obtain a more practical expression, we must choose a representation of the distributional zeta function; for that, let us take a Mellin transform

$$\frac{1}{Z^s[h]} = \frac{1}{\Gamma(s)} \int_0^\infty e^{-Z[h]t} t^{s-1} dt. \quad (5.59)$$

Therefore it follows

$$\Phi(s) = \frac{1}{\Gamma(s)} \int \left[\int_0^\infty e^{-Z[h]t} t^{s-1} dt \right] P(h)[dh], \quad (5.60)$$

now we choose some positive real number a and split the distributional zeta function as $\Phi = \Phi_1 + \Phi_2$, where

$$\Phi_1(s) = \frac{1}{\Gamma(s)} \int \left[\int_0^a e^{-Z[h]t} t^{s-1} dt \right] P(h)[dh], \quad (5.61)$$

$$\Phi_2(s) = \frac{1}{\Gamma(s)} \int \left[\int_a^\infty e^{-Z[h]t} t^{s-1} dt \right] P(h)[dh]. \quad (5.62)$$

The function Φ_2 is entire¹. For the function Φ_1 , we can use a series representation of the exponential to write

$$\Phi_1(s) = \frac{1}{\Gamma(s)} \int \left[\int_0^a t^{s-1} \sum_{k=0}^\infty \frac{(-1)^k}{k!} [Z[h]t]^k dt \right] P(h)[dh], \quad (5.63)$$

¹Holomorphic in the whole complex plane.

and once the series converges, we can write

$$\begin{aligned}
\Phi_1(s) &= \frac{1}{\Gamma(s)} \int \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} [Z[h]]^k P(h)[dh] \int_0^a t^{k+s-1} dt \\
&= \frac{1}{\Gamma(s)} \int \sum_{k=0}^{\infty} \frac{(-1)^k a^{k+s}}{k!(k+s)} Z^k[h] P(h)[dh] \\
&= \frac{1}{\Gamma(s)} \sum_{k=0}^{\infty} \frac{(-1)^k a^{k+s}}{k!(k+s)} \mathbb{E} [Z^k[h]].
\end{aligned} \tag{5.64}$$

For $k = 0$, we have a singularity at $s = 0$; however, using $s\Gamma(s) = \Gamma(s+1)$, we can write

$$\Phi_1(s) = \frac{a^s}{\Gamma(s+1)} + \frac{1}{\Gamma(s)} \sum_{k=1}^{\infty} \frac{(-1)^k a^{k+s}}{k!(k+s)} \mathbb{E} [Z^k[h]], \tag{5.65}$$

which is finite for all $\Re(s) \geq 0$. Now we can compute the derivative of Φ_1

$$\left. \frac{d}{ds} \Phi_1(s) \right|_{s=0^+} = (\ln a + \gamma_E) + \sum_{k=1}^{\infty} \frac{(-1)^k a^{k+s}}{k!k} \mathbb{E} [Z^k[h]], \tag{5.66}$$

where we use the fact that $\Gamma(s)$ has a pole of order one at $s = 0$ and γ_E is the Euler-Mascheroni constant.

For Φ_2 , we have

$$\left. \frac{d}{ds} \Phi_2(s) \right|_{s=0^+} = \int \left[\int_a^{\infty} \frac{1}{t} e^{-Z[h]t} dt \right] P(h)[dh] = R(a), \tag{5.67}$$

and using, again, $Z[h] \geq Z[0]$, we obtain

$$|R(a)| \leq \int \left[\int_a^{\infty} \frac{1}{t} e^{-Z[0]t} dt \right] P(h)[dh] \leq \frac{1}{Z(0)a} e^{-Z(0)a}, \tag{5.68}$$

therefore, $R(a) \rightarrow 0$ as a increases.

Reuniting all these results, we have the following representation of the quenched free energy

$$F = \sum_{k=1}^{\infty} \frac{(-1)^k a^{k+s}}{k!k} \mathbb{E} [Z^k[h]] - (\ln a + \gamma_E) + R(a). \tag{5.69}$$

Once the thermodynamic properties are derivatives of the free energy and we can take a large enough, the last three contributions can be neglected and we can write

$$F = \sum_{k=1}^{\infty} \frac{(-1)^k a^{k+s}}{k!k} \mathbb{E}[Z^k[h]]. \quad (5.70)$$

The set of these last results was first derived in Ref. [142], where N. F. Svaiter and B. F. Svaiter introduced the **DZF** method. Since its derivation, the distributional zeta function has been used to recover the known results obtained by the replica trick [160–164], without relying on dubious mathematical manipulations, and to further our understanding of disordered systems.

The quantity $\mathbb{E}[Z^k[h]]$ can be directly computed once the probability distribution of the disorder is fixed; it is given by

$$\mathbb{E}[Z^k(j, h)] = \int Z^k(j, h) P(h) [dh] = \int \prod_{i=1}^k e^{-S_{\text{eff}}(\phi_i^k)} [d\phi_i^k], \quad (5.71)$$

where $S_{\text{eff}}(\phi_i^k)$ denotes the effective action, which is obtained through the coarse graining over the disordered variable $h(x)$.

5.3 Applications of the DFZ method

In this section, we apply the distributional zeta function to different scenarios of the random mass model (Eq. (5.50)) and the random field model (Eq. (5.51)) to obtain both novel results and confirmations of the distributional zeta function method.

5.3.1 Random Mass Model

To introduce key terminology related to the distributional zeta function, we first present the random mass model described by Eq. (5.50). To obtain practical results, we fix a disorder probability distribution. For simplicity, we consider a Gaussian distribution, given by

$$P(h) = p_0 \exp \left[-\frac{1}{2\varrho^2} \int (h(x))^2 dx \right], \quad (5.72)$$

where ϱ is a positive parameter and p_0 is a normalization constant. In this case, we have a delta-correlated disorder:

$$\mathbb{E}[h(x)h(y)] = \varrho^2 \delta(x - y). \quad (5.73)$$

The explicit form of the effective action can be written as

$$S_{\text{eff}}(\phi^k) = \int \left\{ \frac{1}{2} \sum_{i=1}^k \phi_i^k(x) (-\Delta + m_0^2) \phi_i^k(x) + \frac{1}{2} \sum_{i,j=1}^k g_{ij} [\phi_i^k(x) \phi_j^k(x)]^2 \right\} dx, \quad (5.74)$$

where $g_{ij} \equiv \lambda_0 \delta_{ij} - \varrho^2$. One can notice that such an action is invariant under the exchange of indices $i \leftrightarrow j$. To proceed from this action, we have two main approaches: the *replica symmetric* method and the *overlap matrix* method. First, we show that in the replica symmetric approach, we recover the free-energy landscape of a glass phase. Subsequently, we demonstrate that the overlap matrix approach allows us to obtain the partition function as an average over random matrices. Within this approach, one can employ the method known as the Parisi ansatz.

Diagonal Ansatz and Glass Phase

From Eq. (5.74), we observe that there is a value of k for which the interaction has a negative sign. This would lead to an instability in the free energy. However, revisiting the expansion of $\ln \cosh x$ (Eq. (5.11)), we note that we can select a term of order x^6 . This allows us to write

$$S_{\text{eff}}(\phi_i^k) = \int \sum_{i=1}^k \left[\frac{1}{2} \phi_i^k(x) (-\Delta + m_0^2) \phi_i^k(x) \right. \quad (5.75)$$

$$\left. + \frac{1}{4} \sum_{j=1}^k g_{ij} (\phi_i^k(x))^2 (\phi_j^k(x))^2 + \frac{\rho}{6} (\phi_i^k(x))^6 \right] dx, \quad (5.76)$$

which ensures the boundedness from below of the free energy. Now, we assume that $\phi_i = \phi_j$, meaning that all fields are equal. This approach is called the replica symmetric or *diagonal ansatz*. This leads to the following action:

$$S_{\text{eff}}(\phi_i^k) = \int \sum_{i=1}^k \left[\frac{1}{2} \phi_i^k(x) (-\Delta + m_0^2) \phi_i^k(x) + \frac{1}{4} (\lambda - k\varrho^2) (\phi_i^k(x))^4 + \frac{\rho}{6} (\phi_i^k(x))^6 \right] dx. \quad (5.77)$$

Using the preceding action, we observe that the potential of the theory exhibits multiple minima. Ref. [162] proves that the free energy possesses many ground states, a characteristic feature of glass-like phases.

Within the replica trick, this replica symmetric ansatz leads to negative entropy and does not exhibit a glass-like phase. To obtain the glass phase in the

replica trick, the artificial construction known as replica symmetry breaking is necessary.

However, one may argue that our diagonal ansatz is also artificial, as there is no fundamental reason to impose such an assumption. In the next application, we explore the overlap matrix approach.

Overlap Matrix Approach

We begin by analyzing the interacting contribution of the effective action given in Eq. (5.74). First, we have

$$\sum_{i,j=1}^k g_{ij} [\phi_i^k(x) \phi_j^k(x)]^2 = \sum_{\langle i,j \rangle=1}^k g_{ij} [\phi_i^k(x) \phi_j^k(x)]^2 + \sum_{i=1}^k g_{ii} [\phi_i^k(x) \phi_i^k(x)]^2, \quad (5.78)$$

where the symbol $\langle i, j \rangle$ denotes the sum over all $i \neq j$. At this point, we note a significant difference between discrete and continuous systems. In the discrete case, apart from a summation over all sites and a pre-factor, we essentially deal with the product of two Ising spins (or even Heisenberg spins). Since Ising spins take values ± 1 , the square of two of them is always unity, while the product of two spins in different “replicas” is referred to as an overlap. A more general approach that retains this property states that *the self-overlap does not depend on the state* [3].

In this framework, we can rewrite the interaction contribution as follows:

$$\sum_{i,j=1}^k g_{ij} [\phi_i^k(x) \phi_j^k(x)]^2 = -\varrho^2 \sum_{\langle i,j \rangle=1}^k [\phi_i^k(x) \phi_j^k(x)]^2 + k(\lambda_0 - \varrho) [\phi_1^k(x)]^4, \quad (5.79)$$

where we have used the fact that $\phi_i^k(x) \phi_i^k(x) \equiv [\phi_1^k(x)]^2 \forall i$, and the explicit form of the matrix g_{ij} . To simplify the notation, let us define $\phi_1^k(x) \equiv \phi(x)$; also, the limits of the sums will be omitted from now on.

As can be explicitly seen, the interaction action of the theory is decomposed into two different contributions. First, the sum of the squares of all self-overlaps, which takes the form of a self-interacting field theory. Second, the sum of the remaining squared overlaps between two “replicas”. Using the fact that the action will appear in the argument of the exponential, we can make use of the Hubbard-Stratonovich identity,

$$e^{\frac{a}{2}s^2} = \frac{1}{\sqrt{2\pi a}} \int d\alpha e^{-\frac{\alpha^2}{2a} + \alpha s}, \quad (5.80)$$

to introduce an auxiliary variable. Using a suitable change of variables², we can write

$$e^{\frac{g^2}{2} \sum_{\langle i,j \rangle} [\phi_i^k(x) \phi_j^k(x)]^2} = \int e^{-\frac{1}{2} \sum_{\langle i,j \rangle} (Q_{ij}(x))^2 + \sum_{\langle i,j \rangle} Q_{ij}(x) \phi_i(x) \phi_j(x)} \prod_{\langle i,j \rangle=1}^k \frac{[dQ_{ij}]}{\sqrt{2\pi}}, \quad (5.81)$$

In this scenario, the effective action can be written as

$$S_{\text{eff}}(\phi_i^k, Q_{ij}) = \int \left\{ \frac{1}{2} \sum_{i,j} \phi_i^k(x) [-\Delta + m_0^2 - 2Q_{ij}(x)] \phi_j^k(x) + \frac{k}{2} (\lambda_0 - \varrho) \phi^4(x) - \frac{1}{2} \sum_{\langle i,j \rangle} (Q_{ij}(x))^2 \right\} dx. \quad (5.82)$$

A saddle point of S_{eff} with respect to Q_{ij} shows us that

$$\frac{\delta S_{\text{eff}}(\phi_i^k, Q_{ij})}{\delta Q_{ij}(x)} = 0 \Rightarrow Q_{ij} = \frac{1}{2} \sum_{\langle i,j \rangle} \phi_i(x) \phi_j(x), \quad (5.83)$$

which means that $Q_{ij} = Q_{ji}$ and $Q_{ii} = 0$, so the matrix $\mathbf{Q}$, whose components are Q_{ij} , must have zeros on all diagonal elements and be symmetric.

In the replica trick, it is customary to apply the replica ansatz over the matrix $\mathbf{Q}$.

In the overlap interpretation, one can define such a matrix as follows:

$$\mathbf{Q} = \Phi \otimes \Phi - \text{diag} [\Phi \otimes \Phi], \quad (5.84)$$

where Φ denotes the vector with components ϕ_i^k and $\text{diag}[A]$ is the diagonal matrix formed from the diagonal elements of the matrix A . Thus, the sum over $\langle i, j \rangle$ acting on Q_{ij} can be replaced by the sum over i, j with the condition that $Q_{ii} = 0$.

To simplify the final form of the partition function, further manipulations can be performed on the last term of Eq. (5.82):

$$\sum_{\langle i,j \rangle} (Q_{ij}(x))^2 = \sum_{i,j} Q_{ij}(x) Q_{ij}(x) = \sum_i \left[\sum_j Q_{ij}(x) Q_{ji}(x) \right] = \text{tr}_{(i)} [\mathbf{Q}^2], \quad (5.85)$$

²It is natural to understand that the strength of the disorder can influence the overlap. Thus, we can absorb ϱ into the new variables, which will later be identified as components of the overlap matrix.

where $\text{tr}_{(i)}$ denotes the trace over the indices i . If we define the matrix $\mathbf{G}$ as the matrix with components given by $\frac{1}{2}(-\Delta + m_0^2)\delta_{ij}$, we can write the effective action entirely in terms of matrices:

$$\begin{aligned} S_{\text{eff}}(\Phi, \mathbf{Q}) &= \int \left\{ \Phi(x) [\mathbf{G} + \mathbf{Q}] \Phi(x) + \frac{1}{2}(\lambda_0 - \varrho)\phi^4(x)\text{tr}_{(i)} [\mathbb{1}_{k \times k}] - \frac{1}{2}\text{tr}_{(i)} [\mathbf{Q}^2] \right\} dx \\ &= S_0(\Phi, \mathbf{Q}) + S_I(\phi) + S_{\mathbf{Q}}(\mathbf{Q}). \end{aligned} \quad (5.86)$$

Now we are able to write the partition function:

$$\mathbb{E}[Z^k(j, h)] = \int e^{-S_{\text{eff}}(\Phi, \mathbf{Q}, J)} \prod_{i=1}^k [d\phi_i^k] \prod_{\langle i, j \rangle=1}^k \frac{[dQ_{ij}]}{\sqrt{2\pi}}, \quad (5.87)$$

where J is the vector with components given by the source $j_i^k(x)$. Now we have two different and **independent** variables in the partition function: the field variables, which are components of the vector Φ , and the overlap variables, which are the components of the matrix $\mathbf{Q}$. Since there is no interaction term combining both variables, we can proceed with the usual perturbation theory developed in Sec. 4.3. We have:

$$\mathbb{E}[Z^k(j, h)] = \int \left[e^{-S_{\mathbf{Q}}(\mathbf{Q})} e^{-P_4\left(\frac{\delta}{\delta J}\right)} \int e^{-S_0(\Phi, \mathbf{Q}, J)} \prod_{i=1}^k [d\phi_i^k] \right] \prod_{\langle i, j \rangle=1}^k \frac{[dQ_{ij}]}{\sqrt{2\pi}}, \quad (5.88)$$

where we defined $P_4\left(\frac{\delta}{\delta J}\right) = \frac{1}{2}(\lambda_0 - \varrho)\left(\frac{\delta}{\delta J(x)}\right)^4$.

To make the calculations more explicit, let us focus only on the last integral:

$$\int e^{-S_0(\Phi, \mathbf{Q}, J)} \prod_{i=1}^k [d\phi_i^k] = \int \exp \left\{ - \int [\Phi(x) (\mathbf{G} + \mathbf{Q}) \Phi(x) + J(x)\Phi(x)] dx \right\} \prod_{i=1}^k [d\phi_i^k]. \quad (5.89)$$

It is a Gaussian functional integral over the variables ϕ_i^k . Such integrals can be performed, and the result is:

$$\int e^{-S_0(\Phi, \mathbf{Q}, J)} \prod_{i=1}^k [d\phi_i^k] = e^{-\frac{1}{2}\text{Tr}[\ln(\mathbf{G} + \mathbf{Q})]} \exp \left[\frac{1}{2} \int J(x)(\mathbf{G} + \mathbf{Q})^{-1} J(x) dx \right]. \quad (5.90)$$

Due to the nature of $\mathbf{Q}$, the operator in the last equation is non-diagonal in the $\mathbb{R}^k$ space. However, as previously shown, the $\mathbf{Q}$ must be a symmetric matrix, and an ansatz over the non-diagonal elements can be taken. The literature has been

investigating such ansätze. The two most popular are the Replica Symmetric ansatz and the Parisi ansatz, both of which give a matrix $\mathbf{Q}$ that is symmetric (by definition) and real. Due to the Spectral Theorem of linear algebra, we know that a symmetric and real matrix can be diagonalized by an orthogonal transformation. Let S be the orthogonal transformation that diagonalizes $(\mathbf{G} + \mathbf{Q})^{-1}$, then choose the source to be $J(x) = J'(x)S$:

$$J(x)(\mathbf{G} + \mathbf{Q})^{-1}J(x) = J'(x)S(\mathbf{G} + \mathbf{Q})^{-1}S^T J'(x) = J'(x)\mathbf{D}^{(\mathbf{Q})}J'(x), \quad (5.91)$$

where $\mathbf{D}^{(\mathbf{Q})}$ denotes the matrix of eigenvalues of $(\mathbf{G} + \mathbf{Q})^{-1}$. To exemplify, take the replica symmetric ansatz, where $Q_{ij} = (1 - \delta_{ij})q$. We have

$$\mathbf{D}^{(\text{RS})} = \begin{bmatrix} \left[\frac{1}{2}(-\Delta + m_0^2) - kq\right]^{-1} & 0 & \dots & 0 \\ 0 & \left[\frac{1}{2}(-\Delta + m_0^2) - q\right]^{-1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \left[\frac{1}{2}(-\Delta + m_0^2) - q\right]^{-1} \end{bmatrix}_{k \times k} \quad (5.92)$$

It is important to keep in mind that the matrix $\mathbf{D}^{(\mathbf{Q})}$ depends on the ansatz of $\mathbf{Q}$. However, Eq. (5.91) is satisfied for any ansatz of $\mathbf{Q}$ over $\mathbb{R}$.

Using the previous results and the identity $\text{Tr}[\ln A] = \ln[\det A]$, we can rewrite the k -th moment of the partition function as

$$\begin{aligned} \mathbb{E}[Z^k(J', h)] &= \int \left\{ e^{-\frac{1}{2}\text{Tr}[\ln \mathbf{D}^{(\mathbf{Q})}]} + \int dx \text{tr}_{(i)} \mathbf{Q}^2 \right. \\ &\quad \times e^{-P_4\left(\frac{\delta}{\delta J(x)}\right)} \exp\left[\frac{1}{2} \int J'(x)\mathbf{D}^{(\mathbf{Q})}J'(x) dx\right] \left. \right\} \prod_{\langle i,j \rangle=1}^k \frac{[dQ_{ij}]}{\sqrt{2\pi}} \\ &= \left\langle e^{-P_4\left(\frac{\delta}{\delta J(x)}\right)} \exp\left[\frac{1}{2} \int J'(x)\mathbf{D}^{(\mathbf{Q})}J'(x) dx\right] \right\rangle_{\mathbf{Q}}, \end{aligned} \quad (5.93)$$

which means that the local quantities obtained by the evaluation of $\mathbb{E}[Z^k(J', h)]$ are obtained after averaging over the overlaps configurations, given by the ansatz of $\mathbf{Q}$. We note that if one does not wish to make any ansatz over the matrix $\mathbf{Q}$, one could perform the average in the sense of random matrices.

Now let us explore the Parisi ansatz and the so-called "Replica Symmetry Breaking" (RSB). RSB will be called any ansatz in which two off-diagonal non-symmetric elements of the matrix $\mathbf{Q}$ cannot be permuted in the **series** in which the mean of the logarithm is represented, Eq. (5.74).

To clarify what this means, let us particularize a simple ansatz for the $k \times k$ -dimensional $\mathbf{Q}$ matrix:

$$Q_{ij} = \begin{cases} q_1 & \text{if } \left\lfloor \frac{i}{k} \right\rfloor = \left\lfloor \frac{j}{k} \right\rfloor \text{ and } i \neq j \\ q_0 & \text{if } \left\lfloor \frac{i}{k} \right\rfloor \neq \left\lfloor \frac{j}{k} \right\rfloor \text{ and } i \neq j \end{cases}, \quad (5.94)$$

always with $Q_{ii} = 0$, where $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x . This is a RSB ansatz. In such a situation, we have

$$\mathbf{Q}_{2 \times 2} = \begin{bmatrix} 0 & q_0 \\ q_0 & 0 \end{bmatrix}, \quad \mathbf{Q}_{3 \times 3} = \begin{bmatrix} 0 & q_1 & q_0 \\ q_1 & 0 & q_0 \\ q_0 & q_0 & 0 \end{bmatrix}, \quad (5.95)$$

$$\mathbf{Q}_{k \times k} = \begin{bmatrix} 0 & q_1 & q_1 & \cdots & q_1 & q_0 \\ q_1 & 0 & q_1 & \cdots & q_1 & q_0 \\ \vdots & & \ddots & & & \vdots \\ q_1 & & \cdots & & & q_0 \\ q_0 & & \cdots & & q_0 & 0 \end{bmatrix}. \quad (5.96)$$

With the additional imposition that q_0, q_1 are real-valued functions, all the preceding constructions can be applied to every term in the series of the DZF (see Eq. (5.70)). As one can see, all non-diagonal elements are equal except those in the last row and column. The choice made in Eq.(5.94) is a simple one; however, when we analyze the action of Eq. (5.74), we can notice that the components of the matrix $\mathbf{Q}$ in the second term of the series ($k = 2$) are completely different from those in the third contribution of the series ($k = 3$). Specifically, $Q_{12} = q_0$ for $k = 2$, while $Q_{12} = q_1$ for $k = 3$. Therefore, RSB means that we do not have, necessarily, a symmetry **between two terms** of the sum; however, the intrinsic symmetry $Q_{ij} = Q_{ji}$ is **preserved term by term**.

With the precise meaning of RSB established, aside from the misleading nomenclature, we can go further and implement the so-called “one-step Parisi ansatz” [3, 121]. First, let us break the series over the average of the logarithm of the partition function into two contributions:

$$\mathbb{E}[\ln Z[h, j]] = \sum_{k=1}^m c_k \mathbb{E}[(Z(j, h))^k] + \sum_{k=m+1}^{\infty} c_k \mathbb{E}[(Z(j, h))^k] \equiv s_m + s_{\infty}. \quad (5.97)$$

Each $\mathbb{E}[(Z(j, h))^k]$ is given by Eq. (5.87). Now, assume the following ansatz for $\mathbf{Q}$:

$$Q_{ij} = \begin{cases} q_1 & \text{if } \left\lfloor \frac{i}{m} \right\rfloor = \left\lfloor \frac{j}{m} \right\rfloor \text{ and } i \neq j, \\ q_0 & \text{if } \left\lfloor \frac{i}{m} \right\rfloor \neq \left\lfloor \frac{j}{m} \right\rfloor \text{ and } i \neq j, \end{cases} \quad (5.98)$$

where $[x]$ denotes the smallest integer greater than or equal to x [3]. Evidently, each term in s_m has the following matrix for $\mathbf{Q}$:

$$\mathbf{Q}_{a \times a} = \mathbf{Q}_{a \times a}^{(RS)} = \begin{bmatrix} 0 & q_1 & \cdots & q_1 \\ q_1 & 0 & \cdots & q_1 \\ \vdots & & \ddots & \vdots \\ q_1 & \cdots & q_1 & 0 \end{bmatrix}, \quad (5.99)$$

where $a = 1, 2, \dots, m$. A component description of such a matrix is:

$$Q_{ab} = (1 - \delta_{ab})q_1; \quad a, b = 1, 2, \dots, m, \quad (5.100)$$

which is the RS ansatz in the s_m contribution. Assuming that q_1 is a real-valued function, the diagonalization previously discussed is the same as presented in Eq. (5.91). For a term $k = m+1, m+2, \dots$ in $\mathbb{E}[\ln Z[h, j]]$, we have the matrix $\mathbf{Q}$ given by:

$$\mathbf{Q}_{k \times k} = \begin{bmatrix} 0 & q_1 & \cdots & q_1 & q_0 & \cdots & q_0 \\ q_1 & 0 & \cdots & q_1 & q_0 & \cdots & q_0 \\ \vdots & & \ddots & \vdots & q_0 & \cdots & q_0 \\ q_1 & \cdots & q_1 & 0 & q_0 & \cdots & q_0 \\ q_0 & \cdots & & q_0 & 0 & q_1 & \cdots & q_1 \\ q_0 & \cdots & & q_0 & q_1 & 0 & \cdots & q_1 \\ q_0 & \cdots & & q_0 & \vdots & & \ddots & \vdots \\ q_0 & \cdots & & q_0 & q_1 & \cdots & q_1 & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_{m \times m}^{(RS)} & \mathbf{Q}_{m \times n}^{(0)} \\ \mathbf{Q}_{n \times m}^{(0)} & \mathbf{Q}_{n \times n}^{(RS)} \end{bmatrix}, \quad (5.101)$$

where $\mathbf{Q}_{m \times n}^{(0)}$ is the $m \times n$ matrix with every entry equal to q_0 , and $n \equiv k - m$. The other component of the action is the trace over the squared matrix $\mathbf{Q}$. In the s_m contribution, this quantity is given by:

$$\text{tr}_{(i)} [\mathbf{Q}_{a \times a}^2] = a(a-1)q_1^2, \quad (5.102)$$

while in each term of s_∞ , we have:

$$\begin{aligned} \text{tr}_{(i)} [\mathbf{Q}_{k \times k}^2] &= [m(m-1) + n(n-1)] q_1^2 + 2mnq_0^2 \\ &= [(m-k)^2 + m^2 - k^2] q_1^2 + 2m(k-m)q_0^2. \end{aligned} \quad (5.103)$$

To be clear, let us analyze the integral over the components of the matrix $\mathbf{Q}$. Such integrals are ansatz-dependent, as each ansatz has a different number of independent entries in the matrix. For now, denote the entire Q -dependent function in $\mathbb{E}[\ln Z[h, j]]$ by $f(Q_{ij})$. Roughly speaking, we have:

$$\mathbb{E}[(Z(j, h))^k] = \int \prod_{\langle i, j \rangle=1}^k [dQ_{ij}] f(Q_{ij}), \quad (5.104)$$

If not all components of the matrix $\mathbf{Q}$ are independent, we will get a (divergent) factor due to the volume of the functional space where such functions are defined³. For example, take the case $k = 2$. Since $Q_{12} = Q_{21} \equiv q_1(x)$ and $Q_{11} = Q_{22} = 0$, we get:

$$\begin{aligned} \mathbb{E}[(Z(j, h))^k] &= \int [dQ_{12}] [dQ_{21}] f(Q_{12}) \\ &= \int [dq_1] [dq_1] f(q_1) \\ &= \langle f(q_1) \rangle_{q_1} \int [dq_1] = N_\infty \langle f(q_1) \rangle_{q_1}. \end{aligned} \quad (5.105)$$

Such (divergent) volume factors are not new in the functional integral approach, and they can be easily dropped out if we “normalize” the functional integral, which is strictly necessary for a probabilistic interpretation of such quantities. Even if we keep all Q_{ij} different and independent, we will have, due to the intrinsic symmetry of Q_{ij} , at least $k(k-1)/2$ volume factors in a $k \times k$ matrix $\mathbf{Q}$, and this number increases with the ansatz choice. Thus, for now, we will keep in mind this normalization and disregard the pure volume contribution of the functional space.

In this scenario, it is easy to see that in the one-step ansatz, Eq. (5.98), we have at most two different entries in the matrix $\mathbf{Q}$, namely, $q_1(x)$ and $q_0(x)$. Depending on the region in the series, all terms in s_m only involve the integral over $q_1(x)$, while terms in s_∞ involve an extra integral over $q_0(x)$. Therefore, apart from the normalization, all contributions in s_m are the averages taken with respect to the function $q_1(x)$, while the contributions in s_∞ are the averages over both $q_1(x)$ and $q_0(x)$.

The so-called “Parisi ansatz” is obtained by successive applications of the first step (second step, third step, etc.). In our context, the next steps are immediately obtained: take some $\tilde{m} < m$, split the series of the average of the logarithm into $s_{\tilde{m}}$, s_m , and s_∞ , and fix $Q_{ij} = q_2(x)$ if $\left\lceil \frac{i}{\tilde{m}} \right\rceil = \left\lceil \frac{j}{\tilde{m}} \right\rceil$. Continue in this manner to obtain an infinite tower of matrices $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \dots$. Each step breaks the series of the distributional zeta-function into more contributions, starting with the replica symmetric ansatz and introducing additional averages.

The generalization of this procedure leads us again to the notion of averaging over an ensemble of random matrices.

³It is important to note that, from the beginning, we are omitting the x -dependence of Q_{ij} . This has been focused in the internal space. However, such dependence is evident in the saddle point for Q , Eq. (5.83), and the fact that we denote the measure over Q_{ij} in the same way as a functional measure.

5.3.2 Random field model

Now we will look for some results obtained in the random field model, Eq. (5.51). Assuming again a δ -correlation, i.e., Eq. (5.73), we obtain the following effective action:

$$S_{\text{eff}}(\phi) = \int \left\{ \frac{1}{2} \sum_{i=1}^k \phi_i^k(x) (-\Delta + m_0^2) \phi_i^k(x) - \varrho^2 \sum_{i,j=1}^k \phi_i^k(x) \phi_j^k(x) + \frac{\lambda_0}{2} \sum_{i=1}^k [\phi_i^k(x) \phi_i^k(x)]^2 \right\} dx. \quad (5.106)$$

Through simple inspection, one can notice that, unlike the random mass, the modification due to the disorder does not directly affect the interaction part; instead, it affects the Gaussian part of the action functional. This can be understood as a modification in the differential operator.

A prototype model that can be studied as a continuous field in the presence of a random field is the binary fluid in a porous medium [165]. When the binary-fluid correlation length is smaller than the porous radius, one has a system for studying finite-size effects in the presence of a surface field. When the binary fluid correlation length is much larger than the porous radius, the random porous medium can exert a random field effect. Even in this situation, one can introduce boundaries, obtaining a Casimir-like effect [166], known as the statistical or critical Casimir effect [167–169].

Similarly to the random mass case, we explore the random field model in two cases: the diagonal ansatz and the *diagonalization approach*. We present the results of the diagonal ansatz when the disorder is kept at low temperatures. For the diagonalization approach, we explore some novel results.

Diagonal ansatz in the critical Casimir effect

As we have shown explicitly, the zero-point energy of a massless system has an associated Casimir effect, which is characterized by the induced force between classical surfaces due to quantum effects. The physical reason behind the Casimir effect can be traced to the presence of massless excitations and the change in the thermodynamic equilibrium of the vacuum (state with zero number occupation) due to the presence of boundaries that change the fluctuating spectrum of the theory [21].

Given the physical interpretation of Casimir forces, one can expect that a similar effect occurs for critical systems with infinite correlation lengths in the presence of boundaries. Such a situation was first discussed in fluids by Fisher

and de Gennes [167]. As a matter of fact, thermal fluctuations can induce Casimir-like long-ranged forces in any correlated medium, with a critical system being one such example. In such a situation, the massless excitations are not associated with photons but with some other quasi-particles, *e.g.*, phonons or Goldstone bosons. This effect is referred to as the critical or statistical Casimir effect. So far, the critical Casimir effect has been reviewed only a few times, *e.g.*, in Refs. [168–172].

The quantum Nyquist theorem [173] allows one to identify regimes where thermal fluctuations dominate over those of quantum origin, with the possibility of systems becoming critical. Such situations are the subject of statistical field theory. When a system reaches the critical regime, correlations become long-ranged, and critical Casimir forces appear. In addition to thermal fluctuations, disorder fluctuations can also drive a system to criticality [174].

Therefore, the simplest application of the random field model of Eq. (5.106) is to study when the system reaches criticality due to the disorder effects. The application of the distributional zeta function method in this scenario first appears in Ref. [175]. Analyzing Eq. (5.106), we notice that the ϕ^4 term is necessary to stabilize the ground state of the system since the disorder average introduces a negative contribution, quadratic in the fields.

Here, we assume the diagonal ansatz $\phi_i^k(x) = \phi_j^k(x)$ for the function space; in which case the effective action becomes:

$$S_{\text{eff}}(\phi_i^k) = \int \sum_{i=1}^k \left[\frac{1}{2} \phi_i^k(x) (-\Delta + m_0^2 - k\rho^2) \phi_i^k(x) + \frac{\lambda}{4} \sum_{i=1}^k (\phi_i^k(x))^4 \right] dx. \quad (5.107)$$

One can see in Eq. (5.107) that there exists a combination of m_0^2 , k and ρ for which $m_0^2 - k\rho^2 < 0$, signaling the spontaneous breaking of the discrete symmetry $\phi_i^k \rightarrow -\phi_j^k$. As usual, one can move from the “false” vacuum to the “true” vacuum by an appropriate shift of the fields, as presented at the end of Sec. 5.1, and identify the mass in the Gaussian contribution to the action.

$$m_\rho^2 \equiv 2(k\rho^2 - m_0^2) > 0. \quad (5.108)$$

To discuss the Casimir energy, it is sufficient to consider the Gaussian contribution. This is because, as shown by several studies within quantum field theory scenarios [176–179], radiative corrections are always subleading compared to the free-field contribution. Since the critical Casimir effect studied here is formally identical to the quantum scalar case, as discussed in Secs. 3.2–4.2.1, the scenario is the same. Therefore, we drop the non-Gaussian terms in the action.

Now, compactifying one dimension and assuming Dirichlet boundary conditions, we can recast the mean over the k -th moment, Eq. (5.71), as

$$\mathbb{E}[Z^k(h)] = \left[\det(-\Delta + m_\rho^2)_{\Omega_L} \right]^{-\frac{k}{2}}. \quad (5.109)$$

From now on, we consider the situation where $m_\rho^2 > 0$. Using the spectral zeta-function regularization, Sec. 4.2.1, we can write the functional determinant as:

$$\mathbb{E} [Z^k(h)] = \exp \left[\frac{k}{2} \frac{d}{ds} \zeta_\rho(s) \Big|_{s=0} \right]. \quad (5.110)$$

The $\zeta_\rho(s)$ can be constructed as

$$\zeta_\rho(s) = \frac{A_{d-1}}{(2\pi)^{d-1}} \int d^{d-1}p \sum_{n=1}^{\infty} \left[p^2 + m_\rho^2 + \left(\frac{\pi n}{L} \right)^2 \right]^{-s}. \quad (5.111)$$

Following the same steps as those between Eqs. (4.39) and (4.51), but for a nonzero mass, we obtain:

$$\frac{d\zeta_\rho(s)}{ds} \Big|_{s=0} = \frac{1}{2} \frac{dC_d(L, s)}{ds} \Big|_{s=0} \left[2I_{1,d}^\rho(0) + I_{2,d}^\rho(0) - I_{3,d}^\rho(0) \right], \quad (5.112)$$

with

$$I_{1,d}^\rho(s) = \int_0^\infty dt \, t^{\frac{d}{2}-s-1} e^{\frac{-L^2 m_\rho^2}{\pi t}} \psi(t), \quad (5.113)$$

$$I_{2,d}^\rho(s) = \int_0^\infty dt \, t^{\frac{d}{2}-s-1} e^{\frac{-L^2 m_\rho^2}{\pi t}}, \quad (5.114)$$

$$I_{3,d}^\rho(s) = \int_0^\infty dt \, t^{\frac{d}{2}-s-\frac{3}{2}} e^{\frac{-tL^2 m_\rho^2}{\pi}}. \quad (5.115)$$

Since we now have a nonzero mass, all integrals are convergent. Some care must be taken to define the energy of the system. First of all, we recall that at zero temperature, the quenched free energy can be written as

$$\begin{aligned} F_q(L) &= E_q(L) = -\mathbb{E} [W(j, h)] \\ &= \sum_{k=1}^{\infty} \frac{(-1)^k a^k}{kk!} \mathbb{E} [(Z(j, h))^k]. \end{aligned} \quad (5.116)$$

Using the previous results and exponentiating the a^k , we obtain the Casimir energy in the presence of quenched disorder. From now on, we will refer to this quantity as the *quenched Casimir* energy:

$$E_q(L) = \sum_{k=k_c}^{\infty} \frac{(-1)^k}{kk!} \exp \left[k \ln a + \frac{k}{2} \frac{d}{ds} \zeta_\rho(s) \Big|_{s=0} \right], \quad (5.117)$$

with k_c defined as

$$k_c \equiv \left\lfloor \frac{m_0^2}{\rho^2} \right\rfloor, \quad (5.118)$$

where $\lfloor x \rfloor$ is the greatest integer less than or equal to x .

Analyzing the behavior of the integrals in Eq. (5.113)-(5.115), it is immediate to see that for each $k > k_c$, the exponential damping makes their contributions subleading. Therefore, the main contribution in the expression for the Casimir energy will be

$$E_q(L) = \frac{(-1)^{k_c}}{k_c k_c!} \exp \left[k_c \ln a + \frac{k_c}{2} \frac{d}{ds} \zeta_\rho(s) \Big|_{s=0} \right]. \quad (5.119)$$

Clearly, from the last equation, we can see the connection between a and the thermodynamic limit: since $\zeta_\rho(s)$ is an extensive quantity, a must be chosen to maximize the exponential. Therefore, the Casimir force is given by:

$$f_d(L) \equiv -\frac{\partial E_q(L)}{\partial L} = \frac{(-1)^{k_c+1}}{2k_c!} \frac{\partial}{\partial L} \frac{d}{ds} \zeta_\rho(s) \Big|_{s=0}. \quad (5.120)$$

With the results obtained so far, we have that

$$f_d(L) = \frac{A_{d-1}}{2^{d+1}} \frac{(-1)^{k_c+1}}{k_c!} \left\{ -\frac{1}{L^d} [2I_{1,d}^\rho(0) + I_{2,d}^\rho(0) - I_{3,d}^\rho(0)] \right. \\ \left. + \frac{L^{1-d}}{d-1} \frac{\partial}{\partial L} [2I_{1,d}^\rho(0) + I_{2,d}^\rho(0) - I_{3,d}^\rho(0)] \right\}. \quad (5.121)$$

The derivative of $I_{i,d}^\rho$ deserves closer attention. All of these integrals have an exponential that depends on L^2 , and thanks to the exponential and the $\psi(t)$ term, their derivatives with respect to $L/2$ do not change their convergence properties. In a power series expansion in $L/2$, the contribution of the second term of Eq. (5.121) has a global contribution proportional to $-L^{2-d}$, which ensures that this contribution is the leading one in powers of $L/2$. Now, defining the quenched Casimir pressure as the quenched Casimir force per unit area (or $d-1$ volume), we can write

$$p_d(L) = \frac{(-1)^{k_c}}{2^{d+1} k_c! L^d} \left[\frac{L^2}{d-1} B_d(0) + D_d(0) \right], \quad (5.122)$$

where $B_d(0)$ and $D_d(0)$ are defined by

$$B_d(0) = -\frac{1}{L} \frac{\partial}{\partial L} [2I_{1,d}^\rho(0) + I_{2,d}^\rho(0) - I_{3,d}^\rho(0)], \quad (5.123)$$

$$D_d(0) = 2I_{1,d}^\rho(0) + I_{2,d}^\rho(0) - I_{3,d}^\rho(0), \quad (5.124)$$

which are positive constants. Clearly, for $m_\rho^2 = 0$, the $B_d(0)$ term vanishes, and the well-known behavior is recovered. The most interesting feature of Eqs. (5.120) and (5.122) is the fact that the factor of $(-1)^{k_c}$ can change the force or pressure from repulsive to attractive depending on the values of m_0^2 and ρ^2 .

Diagonal ansatz in the low temperature case

Here we present the results and calculations of Ref. [180].

Recent experimental and theoretical advances have driven increased interest in low-temperature physics and quantum phase transitions [125, 126, 181–183]. The intersection of these two areas of research—the physics of systems with quenched disorder and low temperatures—leads to the following questions [184–187]: 1) What is the effect of randomness in models at low temperatures in the broken symmetry phases? 2) How is the link between nonlocality (anisotropy) and the appearance of generic scale invariance⁴ in systems with continuous and discrete symmetry? It is well known that models with continuous symmetry can exhibit generic scale invariance due to the Goldstone theorem [188]. Nevertheless, even in the case of discrete symmetry, the presence of quenched disorder also leads to generic scale invariance. This behavior agrees with Garrido *et al.* [189], who claim that a necessary, but not sufficient, condition for generic scale invariance is an anisotropic system. Later on, Vespignani and Zapperi [190] showed that the breakdown of locality is essential to the emergence of generic scale invariance. A well-known fact is that low temperatures in quenched disordered systems introduce spatial non-locality. Thus, one can merge the previous questions into a single one: how is the link between low temperatures and generic scale invariance in such systems?

As we have seen in Sec. 5.1.1, a finite-temperature quantum field theory is similar to a field theory defined over $\mathbb{R}^d \times S^1$. As a matter of fact, in Euclidean scalar quantum field theories, finite temperature effects and periodic boundary conditions in one of the spatial dimensions are on the same footing. That is, the scalar theory defined on a $\mathbb{R}^d \times S^1$ space is formally equivalent to the thermal scalar field theory since the momentum variable associated with one of the spatial coordinates runs over discrete values, multiples of $2\pi/L$, where L is the length of one of the compactified spatial dimensions, which is similar to the Matsubara frequencies when one replaces L with β .

The behavior of a system in which quantum and disorder fluctuations dominate can be described either by a d -dimensional Euclidean quantum field theory (with $\beta \rightarrow \infty$) or a statistical field theory in $(d + 1)$ dimensions. Here, we use this

⁴A system presents generic scale invariance when its 2-point correlation function is algebraically decaying.

equivalence to avoid misunderstandings, since we will use stochastic differential equations with Markov time. In addition, we assume that the disorder field is strongly correlated in the compactified dimension (imaginary time). This assumption implies a spatially non-uniform disorder field in the $(d+1)$ -dimensional classical Euclidean field theory, which we assume to be delta-correlated:

$$\mathbb{E}[h(z, \mathbf{x})h(z', \mathbf{y})] = \varrho^2 \delta^d(\mathbf{x} - \mathbf{y}). \quad (5.125)$$

In this case, we get a $(d+1)$ Euclidean space with fields obeying periodic boundary conditions in one spatial coordinate and already on the true ground state⁵. As in the finite-temperature case, the series representation of the quenched free energy leads to an effective action for each moment of the partition function, namely:

$$\begin{aligned} S_{\text{eff}}(\varphi_i^k, j_i^k) = & \frac{1}{2} \int_0^L \left\{ \int \left[\sum_{i=1}^k \left(\varphi_i^k(z, x) \left(-\frac{\partial^2}{\partial z^2} - \Delta + m_0^2 \right) \varphi_i^k(z, x) + \rho_0(\varphi_i^k(z, x)) \right)^3 \right. \right. \\ & \left. \left. + \frac{\lambda_0}{2} (\varphi_i^{(k)}(z, x))^4 \right] dx \right\} dz - \frac{1}{2} \int_0^L \left[\int \sum_{r,s=1}^k \varphi_r^k(z, x) j_s^k(z, \mathbf{x}) dx \right] dz \\ & - \frac{\varrho^2}{2L^2} \int_0^L \int_0^L \left[\int \sum_{r,s=1}^k \varphi_r^k(z, x) \varphi_s^k(z', x) dx \right] dz' dz, \end{aligned} \quad (5.126)$$

with $\varphi_i^{(k)}(0, \mathbf{x}) = \varphi_i^{(k)}(L, x)$ and $j_i^{(k)}(0, x) = j_i^{(k)}(L, x)$. One sees that the last term in this expression is spatially non-local. Such a non-local contribution also appears in other models. For example, using renormalization group techniques and the replica trick in a random mass model, Refs. [191, 192] find non-isotropic scaling behavior. In our approach, because the disorder is anisotropic, we find similarly that the critical behavior of the system is different for the compactified and non-compactified directions.

In order to avoid unnecessary complications, once we already have a non-local action, and for practical purposes, we assume the diagonal ansatz over the fields: $\varphi_i^k(z, x) = \varphi_j^k(z, x)$ in the function space and also $j_i^k(z, x) = j_l^k(z, x) \forall i, j$. For simplicity, we redefine $\varphi_i'^k(z, x) = \frac{1}{\sqrt{k}} \varphi_i^k(z, x)$ and $\lambda'_0 = \lambda_0 k$. All the terms of the series have the same structure, and one minimizes each term of the series one by one.

Instead of computing correlation functions directly from the functional integral for the effective action in Eq. (5.126), we sample the corresponding field configurations with a linear, nonlocal stochastic partial differential equation with

⁵Just apply the technique of Sec. 5.1.1 in the action of Eq. (5.106).

additive noise. This generalizes the commonly used stochastic equations in equilibrium Landau-Ginzburg theories [193–196] to this spatially anisotropic non-equilibrium case, allowing us to discuss the temporal behavior of the system; see, for example, Ref. [197]. Specifically, we assume that $\xi_i(t, z, x)$ is genuine Gaussian-Markovian noise:

$$\langle \xi_i^k(t, z, x) \xi_j^k(t', z', x') \rangle = 2Y \delta_{ij} \delta(t - t') \delta(z - z') \delta^d(x - x'), \quad (5.127)$$

where $\langle \dots \rangle$ denotes an average over all possible realizations of the noise. The corresponding stochastic equation sampling the field configurations $\varphi_i^k(t, z, x)$ with weight $S_{\text{eff}}(\varphi_i^k, j_i^k)$ is then given by the generalized Langevin equation:

$$\frac{\partial}{\partial t} \varphi_i^k(t, z, x) = -Y \frac{\delta S_{\text{eff}}(\varphi_i^k, j_i^k)}{\delta \varphi_i^k(z, \mathbf{x})} \bigg|_{\varphi_i^k(z, \mathbf{x}) = \varphi_i^k(t, z, \mathbf{x})} + \xi_i^k(t, z, \mathbf{x}). \quad (5.128)$$

This equation is similar to the one that, after a coarse-grained procedure, describes the relaxational dynamics of classical non-equilibrium systems. In our case, $Y = 1$. Performing the functional derivatives, the generalized Langevin equation can be written as:

$$\begin{aligned} \frac{\partial}{\partial t} \varphi_i^k(t, z, x) + \left(-\frac{\partial^2}{\partial z^2} - \Delta + m_0^2 \right) \varphi_i^k(t, z, x) - \frac{Q^2}{L^2} \sum_{s=1}^k \int_0^L \varphi_s^k(t, v', x) dv' \\ = \xi_i^k(t, z, x) + j_i^k(t, z, x). \end{aligned} \quad (5.129)$$

To deal with the nonlocal term, we employ a fractional derivative formalism, similar to the one used in studies of anomalous diffusion in transport processes through a disordered medium [198]. Specifically, we use the Riemann-Liouville fractional integrodifferential operator of order α , D_a^α [199]. Let $f \in \mathcal{L}^1[a, b]$ and $0 < \alpha < 1$; then $D_a^\alpha f$ exists almost everywhere in $[a, b]$, with $D_a^\alpha f$ defined by [199]:

$$D_a^\alpha f(v) = \frac{1}{\Gamma(\alpha)} \int_a^v f(s) (v - s)^{\alpha-1} ds. \quad (5.130)$$

Therefore, the nonlinear term is given in terms of D_a^α as:

$$D_0^\alpha \left(\varphi_i^k(t, z, x) + \sum_{s=1, s \neq i}^k \varphi_s^k(t, z, x) \right). \quad (5.131)$$

The operator $D_a^\alpha f \equiv \frac{d^\alpha f(x)}{d|x|^\alpha}$ possesses a well-defined Fourier transform, namely

$$\mathcal{F} \left[\frac{d^\alpha f(x)}{d|x|^\alpha} \right] = -|k|^\alpha f(k), \quad \text{for } 1 \leq \mu < 2. \quad (5.132)$$

We define the Fourier transform on the time and spatial coordinates of a generic function $g(t, z, x)$ by $\tilde{g}(\omega, q_z, q_\perp) = \mathcal{F}_{t,z,x}[g(t, z, x)]$, where $q_z = q_z(n) = n\pi/L$, $n \in \mathbb{Z}$. The Langevin equation in terms of the Fourier-transformed functions is then given by:

$$\left[-i\omega + \left(\mathbf{q}_\perp^2 + q_z^2 + m_0^2 + k\varrho^2|q_z| \right) \right] \tilde{\phi}_i^k(\omega, q_z, q_\perp) = \tilde{\xi}_i^k(\omega, q_z, q_\perp) + \tilde{j}_i^k(\omega, q_z, q_\perp), \quad (5.133)$$

in which we again assume the diagonal ansatz, $\phi_i^k(x) = \phi_j^k(x)$ and $j_i^k(x) = j_j^k(x)$. From this, one can compute the dynamic susceptibility $\chi_0^k(\omega, q_z, q_\perp)$, which is given by the response propagator $G_0^k(\omega, q_z, q_\perp)$:

$$G_0^k(\omega, q_z, q_\perp) = \frac{1}{-i\omega + (q_\perp^2 + q_z^2 + m_0^2 + k\varrho^2|q_z|)}. \quad (5.134)$$

Near criticality in the pure system, i.e., for $\varrho = 0$, three critical exponents of the Gaussian model can be obtained: the two static exponents $\nu = \frac{1}{2}$ and $\eta = 0$, and the dynamical exponent $z = 2$. Using the principle of causality, for the $G_0^k(t, q_z, q_\perp) = \mathcal{F}_t^{-1}G_0^k(\omega, q_z, q_\perp)$, contour integration leads to:

$$\begin{aligned} G_0^k(t, q_z, q_\perp) &= \mathcal{F}_t^{-1}G_0^k(\omega, q_z, q_\perp) \\ &= \theta(t) e^{-\left(q_\perp^2 + q_z^2 + m_0^2 + k\varrho^2|q_z| \right)t}, \end{aligned} \quad (5.135)$$

where $\theta(t)$ is the Heaviside theta function. Clearly, the function $G_0^k(t, q_z, q_\perp)$ decays exponentially to zero as $t \rightarrow \infty$.

The next step is to find the Gaussian dynamic correlation function. Using the noise correlator in Fourier space for large L , we get

$$\begin{aligned} \langle \tilde{\phi}^{(k)}(\omega, q_z, q_\perp) \tilde{\phi}^{(k)}(\omega', q'_z, q'_\perp) \rangle &= (2\pi)^{d+1} \delta(\omega + \omega') \delta(q_z + q'_z) \delta(q_\perp + q'_\perp) \\ &\quad \times C_0^{(k)}(\omega, q_z, q_\perp), \end{aligned} \quad (5.136)$$

where

$$C_0^{(k)}(\omega, q_z, q_\perp) = 2(G_0^{(k)}(\omega, q_z, q_\perp))^2 \quad (5.137)$$

is called the dynamical structure factor. The temporal correlation decays exponentially, with a modified relaxation rate due to the disorder. An experimentally accessible quantity is the static structure factor $C_0^{(k)}(q_z, q_\perp)$, defined as

$$C_0^{(k)}(q_z, q_\perp) = \frac{1}{2\pi} \int_{-\infty}^{\infty} C_0^{(k)}(\omega, q_z, q_\perp) d\omega, \quad (5.138)$$

from which one can find the correlation lengths in the model. Since the disorder is anisotropic, the behavior of the system is different for distinct directions. In the Gaussian approximation in four-dimensional space, using a Fourier representation for $G_0^{(k)}(z - z', x - y)$, one can show that

$$G_0^{(k)}(z - z', x - y) = \frac{1}{(2\pi)^2} \frac{1}{|x - y|} \int_0^\infty e^{-|x-y|\sqrt{q_z^2 + m_0^2 + k\rho^2}q_z} \cos(q_z(z - z')) dq_z. \quad (5.139)$$

Defining the quantity $\varsigma = \rho^2/2m_0$, we can write

$$G_0^{(k)}(z - z', x - y) = \frac{1}{(2\pi)^2} \frac{m_0}{|x - y|} e^{-m_0|x-y|} \int_0^\infty e^{\sqrt{u^2 + 2k\varsigma u + 1}} \cos(m_0 u(z - z')) du. \quad (5.140)$$

It is not possible to express this integral in terms of known functions, but we can circumvent this difficulty in the following way. We recall that the contribution of the terms of the series representation for the quenched free energy is given by

$$\mathbb{E}[W(j, h)] = \sum_{k=1}^\infty c(k) \mathbb{E}[(Z(j, h))^k], \quad (5.141)$$

where $c(k) = \frac{(-1)^{k+1}}{kk!}$ ⁶. For small k such that $k\varsigma \rightarrow 0$, we can write, for large $(|x - y|^2 + |z - z'|^2)$, that the correlation function in a specific moment is given by

$$G_0^{(k)}(z - z', \mathbf{x} - \mathbf{y}) = \frac{1}{\sqrt{8\pi^5}} \frac{\sqrt{m_0} e^{-m_0\sqrt{|z-z'|^2 + |\mathbf{x}-\mathbf{y}|^2}}}{(|z - z'|^2 + |x - y|^2)^{\frac{3}{4}}}. \quad (5.142)$$

The contributions of these terms are the usual ones, for which the bulk correlation length $\xi = m_0^{-1}$ can be defined. However, since $m_0^2 > 0$, there is no long-range order. Nevertheless, the existence of long-range order can be obtained from the series representation of the quenched free energy.

For any real number κ , let $[\kappa]$ denote the largest integer $\leq \kappa$, that is, the integer r for which $r \leq \kappa < r + 1$. We are interested in the critical moment of the partition function, which is the $k_c = \lfloor \frac{2m_0}{\rho^2} \rfloor$ moment. For this k_c -th moment, the two-point correlation function has the form

$$G_0^{(k_c)}(z - z', x - y) = \frac{1}{(2\pi)^2} \frac{e^{-m_0|x-y|}}{|z - z'|^2 + |x - y|^2}. \quad (5.143)$$

⁶Note that a is assumed large enough, therefore we absorb it in the normalization.

This expression reflects the spatial anisotropy due to disorder. In the k_c -th moment, it is an explicit manifestation of generic scale invariance.

A direct question that this result raises is: what is the effect of the generic scale invariance over the mass (2-point correlation function) in perturbation theory? Using the static ($\omega = 0$) propagator obtained in Eq. (5.134), we try to answer such a question at the one-loop level. Once we have the system in the ordered phase (with persistent magnetization), the loop contributions here are the same as in Sec. 5.1.1, that is, we must compute the diagrams of Eq. (5.30) with the propagator of Eq. (5.134), algebraically:

$$m_R^2(L, \varrho, k) = m_0^2 + \delta m_0^2 + 6 \Delta m_1^2(L, \varrho, k) + 18 \Delta m_2^2(L, \varrho, k), \quad (5.144)$$

where 6 and 18 are symmetry factors, and again a mass counterterm δm_0^2 was introduced. Let us first discuss the contribution from the tadpole diagram $\Delta m_1^2(L, \varrho, k)$ using the analytic regularization procedure discussed in Sec. 5.1.1. For $s \in \mathbb{C}$, $\Delta m_1^2(L, \varrho, k)$ can be obtained by the analytic continuation of $\Delta m_1^2(L, \varrho, k, \mu, s)|_{s=1}$, with

$$\Delta m_1^2(L, \varrho, k, \mu, s) = \frac{\lambda(\mu, s)L}{2^{d+1}\pi^{\frac{d}{2}+1}\Gamma(\frac{d}{2})} \int_0^\infty p^{d-1} \sum_{n \in \mathbb{Z}} \left[\pi n^2 + \frac{L}{2} k \varrho^2 |n| + \frac{L^2}{4\pi} (p^2 + m_0^2) \right]^{-s} dp, \quad (5.145)$$

where a trivial angular part of the integral was performed, and $\lambda(\mu, s) = \lambda_0(\mu^2)^{s-1}$, where μ has the dimension of mass. As in the case $\varrho = 0$, this function is defined in the region where the above integral converges, $\Re(s) > s_0$. Comparing the previous equation with Eq. (5.32), one can notice that the anisotropic disorder introduces a contribution proportional to $|n|$ into the correlation function. Then the formalism discussed in Sec. 5.1.1 must be adapted. Again, the contribution from the bubble diagram (self-energy) can be obtained from the tadpole:

$$\Delta m_2^2(L, \varrho, k) = \left[-\frac{\rho^2(\mu, s)}{\lambda(\mu, s)} \Delta m_1^2(L, \varrho, k, \mu, s) \right]_{s=2}, \quad (5.146)$$

where $\rho(\mu, s) = \rho_0(\mu^2)^{s-2}$.

After a Mellin transform and performing the p integral, Eq.(5.144) can be written as:

$$\Delta m_1^2(L, \varrho, k, \mu, s) = \frac{\lambda(\mu, s)}{4\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \int_0^\infty t^{s-\frac{d}{2}-1} \sum_{n \in \mathbb{Z}} e^{-\left(\pi n^2 + \frac{L}{2} k \varrho^2 |n| + m_0^2 L^2 / 4\pi\right)t} dt. \quad (5.147)$$

Next, we split the summation into the $n = 0$ and $n \neq 0$ contributions. For simplicity, we write $\Delta m_1^2(L, \varrho, k, \mu, s)|_{n=0} = \Delta m_1^2(L, \mu, s)|_{n=0}$:

$$\Delta m_1^2(L, \mu, s)|_{n=0} = \frac{\lambda(\mu, s)}{4\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} A(s, d), \quad (5.148)$$

where

$$A(s, d) = \int_0^\infty t^{s-\frac{d}{2}-1} e^{-m_0^2 L^2 t/4\pi} dt. \quad (5.149)$$

For some d and s , this integral has infrared divergence. Different methods for infrared regularization have been discussed in the literature; see, for example, Ref. [200]. Here we implement another approach to deal with this infrared divergence [34]. The integral $A(s, d)$ is defined for $\Re(s) > \frac{d}{2}$, and can be analytically continued to $\Re(s) > \frac{d}{2} - 1$ for $s \neq \frac{d}{2}$. We write a regularized quantity $A_R(s, d)$ as

$$A_R(s, d) = \int_0^1 t^{s-\frac{d}{2}-1} \left(e^{-m_0^2 L^2 t/4\pi} - 1 \right) dt + \int_1^\infty t^{s-\frac{d}{2}-1} e^{-m_0^2 L^2 t/4\pi} + \frac{1}{(s - \frac{d}{2})} dt, \quad (5.150)$$

which is valid for $\Re(s) > \frac{d}{2}$. For $\Re(s) > \frac{d}{2} - 1$ and $s \neq \frac{d}{2}$, the right-hand side exists and defines a regularization of the original integral. The contribution $\Delta m_1^2(L, \varrho, k, \mu, s)|_{n \neq 0}$ is written as

$$\Delta m_1^2(L, \varrho, k, \mu, s)|_{n \neq 0} = \frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \int_0^\infty t^{s-\frac{d}{2}-1} \sum_{n=1}^\infty e^{-\pi(n^2 + kL\varrho^2 n/2\pi + m_0^2 L^2/4\pi^2)t} dt. \quad (5.151)$$

As we can expect, this integral cannot be directly evaluated, however, there are some values of k which dominate this integral. To obtain such values, we write

$$\Delta m_1^2(L, \varrho, k, \mu, s)|_{n \neq 0} = \frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \int_0^\infty \left[t^{s-\frac{d}{2}-1} e^{-t(m_0^2 - k^2 \varrho^4/4)L^2/4\pi} \times \sum_{n=1}^\infty e^{-\pi t(n + Lk\varrho^2/4\pi)^2} \right] dt. \quad (5.152)$$

This can be split into three contributions:

$$\Delta m_1^2(L, \varrho, k, \mu, s)|_{n \neq 0} = -\frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \sum_{i=1}^3 I_i(L, \varrho, k, \mu, s). \quad (5.153)$$

where

$$I_1(L, \varrho, k, \mu, s) = \int_0^\infty t^{s-\frac{d}{2}-1} e^{-t(m_0^2 L^2/4\pi)} dt, \quad (5.154)$$

$$I_2(L, \varrho, k, \mu, s) = \int_0^\infty t^{s-\frac{d}{2}-1} e^{-t(m_0^2 - k^2 \varrho^2/4)L^2/4\pi} \sum_{n=1}^\infty e^{-\pi t(n - Lk\varrho^2/4\pi)^2} dt, \quad (5.155)$$

$$I_3(L, \varrho, k, \mu, s) = \int_0^\infty t^{s-\frac{d}{2}-1} \Theta\left(t, \frac{Lk\varrho^2}{4\pi}\right) e^{-t(m_0^2 - k^2 \varrho^2/4)L^2/4\pi} dt. \quad (5.156)$$

We used the *theta-series* (or *Jacobi theta*) defined by

$$\Theta(t; \alpha) = \sum_{n=-\infty}^\infty e^{-\pi t(n+\alpha)^2}. \quad (5.157)$$

for any $\alpha, t \in \mathbb{C}$ with $\Re(t) > 0$. Note that the Θ -function defined at Eq. (3.79) is a particular case for $\alpha = 0$. It is clear that $\Theta(t; \alpha) = \Theta(t; \alpha + 1)$, and by the Poisson summation formula, we have

$$\begin{aligned} \Theta\left(\frac{1}{t}; \alpha\right) &= \sqrt{t} \sum_{n=-\infty}^\infty e^{-\pi n^2 t + 2\pi i n \alpha} \\ &= \sqrt{t} e^{-\pi \alpha^2/t} \Theta(t; -i\alpha/t). \end{aligned} \quad (5.158)$$

Let us split the integral $I_3(L, \varrho, k, \mu, s)$ into two regions. Since the theta-series $\Theta(t; \alpha)$ is holomorphic in the half-plane $\Re(t) > 0$, the $I_3(L, \varrho, k, \mu, s)$ contribution must be written as

$$I_3(L, \varrho, k, \mu, s) = I_3^{(1)}(L, \varrho, k, \mu, s) + I_3^{(2)}(L, \varrho, k, \mu, s), \quad (5.159)$$

where $I_3^{(1)}(L, \varrho, k, \mu, s)$ is given by

$$I_3^{(1)}(L, \varrho, k, \mu, s) = \int_1^\infty t^{\frac{d}{2}-s-\frac{1}{2}} e^{-(m_0^2 - k^2 \varrho^2/4)L^2/(4\pi t)} \sum_{n=-\infty}^\infty e^{-\pi n^2 t + i k L \varrho^2 n/2} dt, \quad (5.160)$$

$$I_3^{(2)}(L, \varrho, k, \mu, s) = \int_1^\infty t^{s-\frac{d}{2}-1} \Theta\left(t, \frac{Lk\varrho^2}{4\pi}\right) e^{-t(m_0^2 - k^2 \varrho^2/4)L^2/4\pi} dt. \quad (5.161)$$

The integral $I_3^{(2)}(L, \varrho, k, \mu, s)$ converges absolutely for any s and converges uniformly with respect to s in any bounded part of the plane. Hence, the integral represents an everywhere regular function of s . Concerning the integral $I_3^{(1)}(L, \varrho, k, \mu, s)$, to guarantee the convergence we must choose $k_{(q)} = \lfloor (\frac{2\pi q}{L}) \frac{2}{\varrho^2} \rfloor$,

where q is a natural number. Therefore, in the series representation for the free energy with $k = 1, 2, \dots$ we have that for the moments of the partition function such that $k_{(q)} = \lfloor (\frac{2\pi q}{L}) \frac{2}{\varrho^2} \rfloor$, where $(\frac{2\pi q}{L})$ are the positive Matsubara frequencies ω_q , the system is critical. This is an interesting result: there is a critical set of moments in the series representation for the free energy, after averaging over the quenched disorder, instead of only one as in the case of an isotropic disorder. A more general proof using generalized Hurwitz-zeta functions is based on the fact that zeta function regularization with a meromorphic extension to the whole complex plane needs an eligible sequence of numbers [201].

This result is similar to the one obtained in the Dicke model, where there is a quantum phase transition when the couplings between the raising and lowering off-diagonal operators and the bosonic mode, the energy gap between the energy eigenstates of the two-level atoms, and the frequency of the bosonic mode satisfy a specific constraint [202–206]. Once we are interested in the critical behavior, we will focus on the set of the critical moments. Substituting the above-discussed result in Eq. (5.151), one gets that

$$\Delta m_1^2(L, q, \mu, s)|_{n \neq 0} = \frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \int_0^\infty t^{s-\frac{d}{2}-1} e^{-\pi(m_0^2 L^2 / 4\pi^2 - q^2)t} \sum_{n=1}^\infty e^{-\pi(n+q)^2 t} dt. \quad (5.162)$$

Finally, let us show that $\Delta m_1^2(L, q, \mu, s)|_{n \neq 0}$ and also $\Delta m_2^2(L, q, \mu, s)|_{n \neq 0}$ are written in terms of the Hurwitz-zeta function, see Eq. (3.140). A simple calculation shows that choosing q such that $q_0 = \lfloor \frac{m_0 L}{2\pi} \rfloor$, the quantity $\Delta m_1^2(L, q, \mu, s)|_{n \neq 0}$ is given by

$$\Delta m_1^2(L, q_0, \mu, s)|_{n \neq 0} = \frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \int_0^\infty t^{s-\frac{d}{2}-1} \sum_{n=1}^\infty e^{-\pi(n+q_0)^2 t} dt. \quad (5.163)$$

With the special choice $q_0 = \lfloor \frac{m_0 L}{2\pi} \rfloor$, we obtain the critical value of k_c , which was used to obtain Eq. (5.143). We interpret this result in the following way: in the infinite number of moments that define the free energy, we obtain a subset of critical moments. In this subset, there is a particular set, for a specific value of q , that generates the tree-level behavior. Going back to the above integral, this simplification allows one to write $\Delta m_1^2(L, q_0, \mu, s)|_{n \neq 0}$ as

$$\Delta m_1^2(L, q_0, \mu, s)|_{n \neq 0} = \frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \left[\int_0^\infty t^{s-\frac{d}{2}-1} \sum_{n=0}^\infty e^{-\pi(n+q_0)^2 t} dt - A_R(s, d) \right]. \quad (5.164)$$

Let us analyze the quantity $F_d(L, , q_0, \mu, s)$, defined by

$$F_d(L, q_0, \mu, s) = \Delta m_1^2(L, q_0, \mu, s)|_{n \neq 0} + \frac{\lambda(\mu, s)}{2\pi\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} A_R(s, d). \quad (5.165)$$

Using an inverse Mellin transform, we can write $F_d(L, q_0, \mu, s)$ as:

$$F_d(L, q_0, \mu, s) = \lambda(\mu, s) \left(\frac{1}{L}\right)^{d-1} \frac{\Gamma(s - \frac{d}{2}) \pi^{\frac{d}{2}-s-1}}{2\Gamma(s)} \zeta_H(2s - d, q_0), \quad (5.166)$$

where the $\zeta_H(z, a)$ is the Hurwitz-zeta function defined in Eq. (3.140). For $d = 3$, the contribution from the tadpole is finite, but the contribution from the self-energy is divergent. An important formula that must be used in the renormalization procedure is

$$\lim_{z \rightarrow 1} \left[\zeta_H(z, a) - \frac{1}{z-1} \right] = -\psi(a), \quad (5.167)$$

where $\psi(a)$ is the digamma function defined as $\psi(z) = \frac{d}{dz} [\ln \Gamma(z)]$. Using the Hurwitz-zeta function and the integral $A_R(s, d)$, we can write:

$$\Delta m_1^2(L, q_0, \mu, s)|_{n \neq 0} = \frac{\lambda(\mu, s)}{2\Gamma(s)} \left(\frac{1}{L}\right)^{d-1} \left[\pi^{\frac{d}{2}-s-1} \Gamma\left(s - \frac{d}{2}\right) \zeta_H(2s - d, q_0) - \frac{1}{\pi} A_R(s, d) \right]. \quad (5.168)$$

Next, we prove that for a fixed value of q_0 the renormalized squared mass vanishes for a family of L 's. In low-temperature field theory we get the same result, i.e, there are critical temperatures where the renormalized squared mass vanishes, namely:

$$m_R^2(L, q_0) = m_0^2 + \delta m_0^2 + 6 \Delta m_1^2(L, 1)|_{n=0} + 18 \Delta m_2^2(L, 2)|_{n=0} + 6 \Delta m_1^2(L, q, 1)|_{n \neq 0} + 18 \Delta m_2^2(L, q, 2)|_{n \neq 0}. \quad (5.169)$$

Defining the dimensionless quantities $b = m_0 L$, $\lambda_1 = 6\lambda_0$, and $\rho_2 = \rho_0 \sqrt{18}$, we can write the latter equation as:

$$\begin{aligned} \frac{b^{d-1}}{m_0^{d-3}} - \frac{\lambda_1}{4\pi} A_R(1, d) + \frac{\rho_2^2}{4\pi\mu^2} A_R(2, d) + \delta m_0^2 + \frac{\lambda_1 \pi^{\frac{d}{2}-2}}{2} \Gamma\left(1 - \frac{d}{2}\right) \zeta_H\left(2 - d, \frac{b}{2\pi}\right) \\ - \frac{\rho_2^2 \pi^{\frac{d}{2}-3}}{2\mu^2} \Gamma\left(2 - \frac{d}{2}\right) \zeta_H\left(4 - d, \frac{b}{2\pi}\right) = 0. \end{aligned} \quad (5.170)$$

Let us discuss the case $d = 3$, in which case Eq. (5.170) becomes:

$$b^2 - \frac{\lambda_1}{4\pi} A_R(1, 3) + \frac{\rho_2^2}{4\pi\mu^2} A_R(2, 3) - \lambda_1 \zeta_H\left(-1, \frac{b}{2\pi}\right) - \frac{\rho_2^2}{2\pi\mu^2} \lim_{d \rightarrow 3} \zeta_H\left(4-d, \frac{b}{2\pi}\right) + \delta m_0^2 = 0. \quad (5.171)$$

The contribution coming from $A_R(s, d)$ is irrelevant for large $m_0 L$, as one can verify in Eq. (5.150). Using the identity $(n+1)\zeta_H(-n, a) = -B_{n+1}(a)$, where the $B_{n+1}(a)$ are the Bernoulli polynomials, we rewrite the Hurwitz-zeta function as

$$\zeta_H\left(-1, \frac{b}{2\pi}\right) = -\left(\frac{b^2}{8\pi^2} - \frac{b}{4\pi} + \frac{1}{12}\right). \quad (5.172)$$

We use the Eq. (5.167) we fix the counterterm contribution in the renormalization procedure. Then, we have that Eq. (5.171) becomes:

$$b^2 + \lambda_1 \left(\frac{b^2}{8\pi^2} - \frac{b}{4\pi} + \frac{1}{12}\right) + \frac{\rho_2^2}{2\pi\mu^2} \psi\left(\frac{b}{2\pi}\right) = 0. \quad (5.173)$$

Since $q_0 = \lfloor \frac{b}{2\pi} \rfloor$, we can write the digamma function as

$$\psi(q_0 + \sigma) = \psi(\sigma) + \sum_{q=1}^{q_0} \frac{1}{\sigma + q}, \quad (5.174)$$

where σ is the non-integer part of $\frac{b}{2\pi}$. With $\sigma < 1$ we can use a Taylor's series and write Eq. (5.173) as:

$$b^2 + \lambda_1 \left(\frac{b^2}{8\pi^2} - \frac{b}{4\pi} + \frac{1}{12}\right) + \frac{\rho_2^2}{2\pi\mu^2} \left(-\frac{1}{\sigma} - \gamma + \frac{\pi^2}{6}\sigma + H_{q_0}(1) + \sigma H_{q_0}(2)\right) = 0, \quad (5.175)$$

where $H_{q_0}(1)$ and $H_{q_0}(2)$ are the generalized harmonic numbers, defined in Eq. (3.133). The Eq. (5.175) has zeros for different values of L as showed in Fig. 5.3.

In one-loop approximation we proved that in the set of moments that defines the quenched free energy there is a denumerable collection of moments that can develop critical behavior. With the bulk in the ordered phase, in these moments temperature or finite size effects lead the moments from the ordered to a disordered phase. Also, in the set of moments, there appears a large number of critical temperatures.

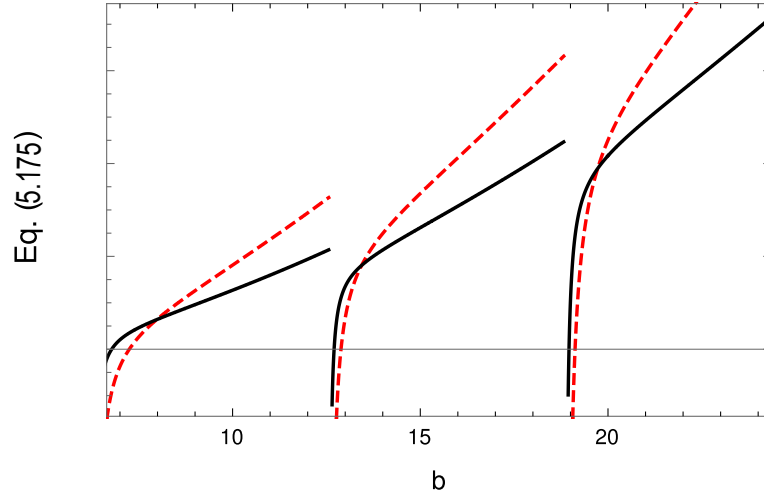


Figure 5.3: Plot of Eq. (5.175) as a function of $b = m_0 L$ for two different values of λ_0 (once $\rho_0^2 = 2m_0^2 \lambda_0$): $\lambda_0 = 1$ (continuous black) and $\lambda_0 = 3$ (dashed red). We set $\mu^2 = m_0^2$.

In the study of complex spatial patterns and structure in nature there appears the idea of self-organized criticality [207, 208]. The authors of these references suggest fractal structures and $1/f$ -noise are common characteristics of irreversible dynamics of a critical state, without a fine tuning of external parameters. The algebraic decay of the correlation function in space and time for generic parameters is called generic scale invariance. Our Eqs. (5.143), (5.175) and Fig. 5.3 are a manifestation of generic scale invariance in an equilibrium system.

As showed in Ref. [209] the presense of Goldstone modes does not change the behavior of this system. Therefore, in a system with a continuous symmetry, we have both, the direct scale invariance (due the Goldstone modes) and the indirect scale invariance, due the disorder in low temperatures.

Diagonalization procedure and bounds in the partiton functions

Here we present the calculations and results of Ref. [210]

Let us recast the coarse-grained action of the random field model, Eq. (5.106), as the following:

$$S_{\text{eff}}(\phi) = \int \left\{ \sum_{i,j=1}^k \phi_j^k(x) \left[\frac{1}{2} (-\Delta + m_0^2) \delta_{ij} - \varrho^2 \right] \phi_i^k(x) + \frac{\lambda_0}{2} \sum_{i=1}^k [\phi_i^k(x)]^4 \right\} dx. \quad (5.176)$$

Such an action has a non-diagonal propagator. The literature has some different approaches to deal with it, as in some of the minimal supersymmetric standard model extensions [211, 212], or one can use a Hubbard-Stratonovich identity as

in the Bose-Hubbard model [213]. Still, another way is to use the ansatz $\phi_i^k = \phi_j^k$, as discussed previously. Although such an ansatz leads to consistent results, it is an unnecessary simplification, as one can use the spectral theorem of linear algebra to formally diagonalize the propagator.

Let us focus only on the quadratic part of the effective action, that is:

$$\sum_{i,j=1}^k S_0(\phi_i, \phi_j) = \frac{1}{2} \sum_{i,j=1}^k \int \phi_i(x) (G_{ij}^0 - \sigma^2) \phi_j(x) dx, \quad (5.177)$$

where $G_{ij}^0 = (-\Delta + m_0^2) \delta_{ij}$. Such an action can be equivalently represented by:

$$\sum_{i,j=1}^k S_0(\phi_i, \phi_j) = \frac{1}{2} \int d^d x (\Phi, G\Phi), \quad (5.178)$$

where G is the $k \times k$ full matrix with components $G_{ij}^0 - \sigma^2$, $\Phi(x)$ is the vector with components $\phi_i(x)$, and $(\cdot, \cdot)$ is the natural inner product in $\mathbb{R}^k$. Now noticing that G is real and symmetric, one can find its diagonalization by an orthogonal matrix O :

$$D = (O, GO) = \begin{bmatrix} G_{11}^0 - k\sigma^2 & 0 & \cdots & 0 \\ 0 & G_{22}^0 & \cdots & 0 \\ \vdots & \cdots & \ddots & \vdots \\ 0 & \cdots & & G_{kk}^0 \end{bmatrix}_{k \times k}. \quad (5.179)$$

Foremost, we should notice that, from the start, in $\mathbb{R}^k$, which appears as a result of the average, does not have any special properties. Besides the usual vector space properties, Eq. (5.176) does not impose any other qualities in this space. Then, to keep the formulation as general as possible, we shall assume minimal properties over $\mathbb{R}^k$. Now, defining that $\tilde{\Phi}(x) = O\Phi(x)$ is the vector with components $\tilde{\Phi} = (\varphi, \varphi_1, \dots, \varphi_{k-1})$, we are able to present a third expression of the free effective action:

$$\sum_{i,j=1}^k S_0(\phi_i) = \frac{1}{2} \int \varphi(x) (-\Delta + m_0^2 - k\sigma^2) \varphi(x) dx + \frac{1}{2} \sum_{a=1}^{k-1} \int \varphi_a(x) (-\Delta + m_0^2) \varphi_a(x) dx, \quad (5.180)$$

which is clearly the sum of k free actions with two distinct differential operators.

As we have seen, there is no problem in the application of the diagonalization approach, Eq. (5.176), for the free effective action. The functional measure is also well-behaved under the diagonalization, since the matrix which performs the transformation is orthogonal and the absolute value of the Jacobian will be

unity. The source j_i , introduced to generate the correlation functions, can always be chosen in such a way that it transforms with the inverse transformation of the vector Φ , and it is also well-behaved. From now on, we discuss the source-free case. So, for free actions, the diagonalization approach is able to describe the system without any ansatz over functional space. A problem emerges once we turn on the interaction.

From Eq. (5.179), there is always a set of $k - 1$ degenerate eigenvalues, which means that one needs to orthogonalize the respective eigenvectors, which are columns of O . This feature of the matrix O introduces difficulties in the interacting part. As one can see from Eq. (5.176), after the disorder average, the effective interaction is not symmetric under rotations in $\mathbb{R}^k$. Such an interaction is known in the literature as cubic anisotropic interaction [214–216].

Technical difficulties arise when k increases. Such a feature can be directly related to the non-perturbative behavior of the RFIM. However, here the non-perturbative behavior is of a different kind than the usual one that appears in field theories. It is non-perturbative due to the impossibility of writing explicitly the interaction for any value of k after taking the quenched average. This situation is similar to the case of the Bose-Hubbard model [217].

Nevertheless, we show that the effective action given by Eq. (5.176) has an upper and a lower bound, which are rotationally symmetric. We will construct two effective actions in which the diagonalization procedure does not affect the interacting part, and such actions will establish an upper and a lower bound for the partition function of RFIM.

Once the free case has been treated and presents no problems, let us focus on the cubic anisotropic interaction:

$$S_{\text{CA}}^{(k)}(\phi_i) = \frac{\lambda_0}{4!} \int \sum_{i=1}^k (\phi_i(x))^4 dx. \quad (5.181)$$

We adopt the notation $\|\bullet\|_p$ for the p -norm in $\mathbb{R}^k$, so that $\|\Phi(x)\|_p = [\sum_i |\phi_i(x)|^p]^{1/p}$ for any $x \in \mathbb{R}^d$; hence, the interaction can be recast as:

$$S_{\text{CA}}^{(k)}(\Phi) = \frac{\lambda_0}{4!} \int \|\Phi(x)\|_4^4 dx. \quad (5.182)$$

With that in mind, we can go further. Observe that for any $a \in \mathbb{R}^k$,

$$\|a\|_1 \leq \sqrt{k} \|a\|_2, \quad \|a\|_2 \leq \|a\|_1. \quad (5.183)$$

The first inequality above can be proved by writing $\|a\| = (a, s)$ with $s_i = 1$ if $a_i \geq 0$, $s_i = -1$ otherwise, and applying the Cauchy-Schwarz inequality, corollary A.55.

The second inequality can be verified by direct computation of $\|a\|_1^2 - \|a\|_2^2$. Fix $x \in \mathbb{R}^d$ and set $a_i = \varphi_i(x)^2$ for $i = 1, \dots, k$ and $a = (a_1, \dots, a_k)$. Since $\|a\|_1 = \|\Phi(x)\|_2^2$ and $\|a\|_2 = \|\Phi(x)\|_4^2$, it follows from the above inequalities that

$$\frac{\|\Phi(x)\|_2^2}{\sqrt{k}} \leq \|\Phi(x)\|_4^2 \leq \|\Phi(x)\|_2^2. \quad (5.184)$$

This inequality can be used to obtain a bound for the cubic anisotropic interaction:

$$\frac{1}{k} S_{\mathcal{O}(k)}(\Phi) \leq S_{\text{CA}}^{(k)}(\Phi) \leq S_{\mathcal{O}(k)}(\Phi), \quad (5.185)$$

where we have defined the interaction action

$$S_{\mathcal{O}(k)}(\Phi) = \frac{\lambda_0}{4!} \int \|\Phi(x)\|_2^4 dx. \quad (5.186)$$

Such a result is useful since, for all $x \in \mathbb{R}^d$, the norm $\|\cdot\|_2$ is invariant under orthogonal transformations in $\mathbb{R}^k$:

$$\begin{aligned} \|\Phi(x)\|_2 &= \sqrt{(\Phi(x), \Phi(x))} = \sqrt{(O^T \tilde{\Phi}(x), O^T \tilde{\Phi}(x))} \\ &= \sqrt{(\tilde{\Phi}(x), O O^T \tilde{\Phi}(x))} = \sqrt{(\tilde{\Phi}(x), \tilde{\Phi}(x))} = \|\tilde{\Phi}(x)\|_2, \end{aligned} \quad (5.187)$$

for any orthogonal matrix O , that is, $O^T O = I$, with O^T denoting the transpose of O . Now it is clear why the label $\mathcal{O}(k)$ is chosen in Eq. (5.186). This denotes that the interaction is invariant under the orthogonal transformations $\mathcal{O}(k)$. From this, one can use the actions given by Eqs. (5.178) and (5.186) to construct the following actions:

$$S_{\text{U}}^{(k)}(\Phi) = \frac{1}{2} \int (\Phi(x), G\Phi(x)) dx + \frac{\lambda_0}{4!} \int \|\Phi(x)\|_2^4 dx, \quad (5.188)$$

$$S_{\text{L}}^{(k)}(\Phi) = \frac{1}{2} \int (\Phi(x), G\Phi(x)) dx + \frac{\lambda_0}{4!k} \int \|\Phi(x)\|_2^4 dx, \quad (5.189)$$

These actions are natural upper and lower limits for the effective action given by Eq. (5.176), that is,

$$S_{\text{L}}^{(k)}(\Phi) \leq S_{\text{eff}}^{(k)}(\Phi) \leq S_{\text{U}}^{(k)}(\Phi), \quad (5.190)$$

and also, due to the property of the norm $\|\cdot\|_2$, both actions exhibit nicer orthogonal transformations in $\mathbb{R}^k$.

Using the same orthogonal matrix that was used to diagonalize G , Eq. (5.179), we can write the diagonalized action in terms of the components of $\tilde{\Phi}$ as

$$S_{\#}^{(k)}(\phi, \phi_a) = \int \left[\frac{1}{2} \phi(x) (-\Delta + m_0^2 - k\sigma^2) \phi(x) + \frac{1}{2} \sum_{a=1}^{k-1} \phi_a(x) (-\Delta + m_0^2) \phi_a(x) + \frac{\lambda_{\#}}{4!} \left(\phi^2(x) + \sum_{a=1}^{k-1} \phi_a^2(x) \right)^2 \right] dx, \quad (5.191)$$

with $S_{\#}^{(k)} = S_U^{(k)}$, and $S_L^{(k)}$, adopting $\lambda_{\#} = \lambda_0$, and λ_0/k , respectively. Analyzing such an action, we can verify that it represents the action for two different kinds of scalar fields, with different masses. The underlying symmetry of this action is $\mathbb{Z}_2 \times \mathcal{O}(k-1)$. In different contexts, such actions have been studied [126, 218]. One interesting feature is that, considering any phase transitions, this action intrinsically preserves the no-go theorems of Mermin-Wagner, Hohenberg, and Coleman [219–221].

Now we can construct the partition function for each of these actions. Due to the monotonicity of the exponential, we get that

$$Z_L^{(k)} \leq \mathbb{E} [Z^k(j, h)] \leq Z_U^{(k)}, \quad (5.192)$$

where

$$Z_L^{(k)} = \int \prod_{i=1}^k [d\varphi_i] \exp \left(-S_U^{(k)}(\Phi) \right), \quad (5.193)$$

$$Z_U^{(k)} = \int \prod_{i=1}^k [d\varphi_i] \exp \left(-S_L^{(k)}(\Phi) \right). \quad (5.194)$$

That is, without any ad hoc choice of subsets in $\mathbb{R}^k$, we are able to obtain partition functions that are bounds in each term of the series of Eq. (5.70).

The fundamental question that can be answered with these results is the nature of the phase transition of the continuous RFIM. This problem can be examined using the concepts of the lower critical dimension of the RFIM and no-go theorems. The model is bounded by two theories $\mathbb{Z}_2 \times \mathcal{O}(k-1)$. In these theories, there are two different phase transitions: (i) $\mathbb{Z}_2 \times \mathcal{O}(k-1) \rightarrow \mathcal{O}(k-1)$, and (ii) $\mathbb{Z}_2 \times \mathcal{O}(k-1) \rightarrow \mathcal{O}(k-2)$ [126]. Since the lower critical dimension for the RFIM is two, case (i) cannot represent a phase transition due to disorder. We have thus obtained a new result. The phase transition of the continuous RFIM can be restricted by a $\mathbb{Z}_2 \times \mathcal{O}(k-1) \rightarrow \mathcal{O}(k-2)$ phase transition. The situation

is similar to that of the cubic anisotropic model, which is confined between the Ising model and the Heisenberg model. A question that can be answered by this method is whether the nature of the phase transition depends on the particular choice of the probability distribution for the random field [159, 222]. In the case of a different probability distribution, the symmetry of the bounds can shed some light on such a question. Also, it is possible to elucidate the nature of the phase transition in the continuous RFIM by connecting the bounds established in the distributional zeta-function approach using the interpolation method similar to the one pioneered by Guerra [223]. An interpolation between the diagonal ansatz and the bounds can be made as follows. Noting that the interaction in the diagonal approximation resembles the self-interaction of the field variable $\phi(x)$ in Eq. (5.191), we may define a new field variable $\tilde{\psi}(x) = A\tilde{\Phi}(x)$, with $A_{11} = 1$, $A_{ab} = \sqrt{t}\delta_{ab}$, $A_{1a} = A_{a1} = 0$ for $a, b \in \{2, \dots, k\}$, and $t \in [0, 1]$, so that the new action interpolates between the bounds and the diagonal ansatz.

Critical Casimir effect via diagonalization approach

Here we present the calculations and results of Ref. [224].

Here we revisit the Casimir effect in disordered systems, now considering a continuous symmetry. More specifically, we consider continuous fields that model order parameters possessing a continuous symmetry in scenarios where the disorder fluctuations dominate over the thermal fluctuations. Examples of systems realizing such a scenario include a binary fluid in the presence of an external random field in the critical regime, superfluids, and liquid crystals. In such a situation, when the criticality is reached, one has to take into account the soft modes (Goldstone bosons) due to the symmetry breaking [108, 225]. Another difference from the previous approach is that now we use the *diagonalization procedure*, previously presented. Our primary aim is to answer whether the soft modes associated with the Goldstone boson favor or suppress the Casimir force and whether they affect the sign of the force. The result that we obtain for such a question is that the soft modes do not affect the change of the sign of the force. However, an interesting effect due to the disorder arises. In the regime of strong disorder, where we only have the Casimir effect due to the presence of the soft mode, the Goldstone mode contribution may change from attractive to repulsive. In other words, the presence of disorder may change the sign of the “universal amplitude” due to the Goldstone modes.

To start, let us consider the action

$$S(\phi, \phi^*) = \frac{1}{2} \int [\phi^*(x) (-\Delta + m_0^2) \phi(x) + \lambda V(\phi, \phi^*) + h^*(x)\phi(x) + h(x)\phi^*(x)] dx; \quad (5.195)$$

as before, m_0^2 is the bare mass, λ is a strictly positive constant, and $V(\phi, \phi^*)$ is a polynomial in the field variables. Here we would like to point out that in the case of interacting field theories confined in compact domains, it is necessary to introduce surface counterterms [226–230]. The main difference here is that $h(x)$ is now a complex random field [100, 209, 231], with a probability distribution $P(h, h^*)$. Again, to simplify the problem, we consider a Gaussian distribution,

$$P(h, h^*) \equiv p_0 e^{-\frac{1}{\rho^2} \int |h(x)|^2 dx}. \quad (5.196)$$

The k -th moment in the series, Eq. (5.70), with $j(x) = 0$, generalizes to:

$$\mathbb{E} [Z^k(h)] = \int \prod_{i,j=1}^k [d\phi_i^k][d\phi_j^{k*}] e^{-S_{\text{eff}}(\phi_i^k, \phi_j^{k*})}, \quad (5.197)$$

with

$$S_{\text{eff}}(\phi_i^k, \phi_j^{k*}) = \sum_{i,j} [S_0(\phi_i^k, \phi_j^{k*}) + \lambda S_I(\phi_i^k, \phi_j^{k*})]. \quad (5.198)$$

Here, $S_0(\phi_i^k, \phi_j^{k*})$ is the quadratic action:

$$S_0(\phi_i^k, \phi_j^{k*}) = \frac{1}{2} \int \phi_i^{k*}(x) (G_{ij}^0 - \rho^2) \phi_j^k(x) dx, \quad (5.199)$$

in which, for later convenience, we defined

$$G_{ij}^0 \equiv (-\Delta + m_0^2) \delta_{ij}, \quad (5.200)$$

and $S_I(\phi_i, \phi_j^*)$ is the interaction action corresponding to $V(\phi, \phi^*)$. The propagator corresponding to $S_0(\phi_i, \phi_j^*)$ is not diagonal in $\mathbb{R}^k$. To circumvent this nagging feature, we use the diagonalization procedure. Defining the vector $\Phi(x)$ as the vector which has components $\phi_i(x)$, we can rewrite the sum of the quadratic actions as

$$\begin{aligned} \sum_{i,j=1}^k S_0(\phi_i, \phi_j^*) &= \frac{1}{2} \int (\Phi(x), G\Phi^*(x)) dx \\ &= \frac{1}{2} \int (\tilde{\Phi}(x), D\tilde{\Phi}^*(x)) dx \end{aligned} \quad (5.201)$$

where $\tilde{\Phi}(x) = O\Phi(x)$, O is the matrix that diagonalizes G , and D is the diagonal matrix given by Eq. (5.179). Let $\varphi_i(x)$ denote the components of $\tilde{\Phi}(x)$. Using the

component notation, one can write the diagonal form of the quadratic action in Eq. (5.201) as

$$\begin{aligned} \sum_{i,j=1}^k S_0(\phi_i, \phi_j^*) &= \frac{1}{2} \int \varphi^*(x)(-\Delta + m_0^2 - k\rho^2)\varphi(x)dx \\ &+ \frac{1}{2} \sum_{a=1}^{k-1} \int \varphi_a^*(x)(-\Delta + m_0^2)\varphi_a(x)dx, \end{aligned} \quad (5.202)$$

where, to simplify the notation henceforth, we defined $\varphi_1(x) \equiv \varphi(x)$ and also changed the dummy index in the second line. Since O is an orthogonal matrix, one has that

$$\prod_{i,j=1}^k [d\phi_i][d\phi_j^*] = [d\varphi][d\varphi^*] \prod_{a,b=1}^{k-1} [d\varphi_a][d\varphi_b^*]. \quad (5.203)$$

Therefore, using Eqs. (5.202) and (5.203) in Eq. (5.197), we obtain:

$$\mathbb{E}[Z^k(h)] = \int e^{-S_\rho(\varphi, \varphi^*) - \sum_a S_O(\varphi_a, \varphi_a^*) - \lambda S_I(\varphi_a, \varphi_a^*)} [d\varphi][d\varphi^*] \prod_{a,b=1}^{k-1} [d\varphi_a][d\varphi_b^*], \quad (5.204)$$

where $S_\rho(\varphi, \varphi^*)$ is the action carrying the information on the strength ρ of the disorder,

$$S_\rho(\varphi, \varphi^*) = \frac{1}{2} \int \varphi^*(x)(-\Delta + m_0^2 - k\rho^2)\varphi(x)dx, \quad (5.205)$$

and $S_O(\varphi_a, \varphi_a^*)$ is a $O(k-1)$ -symmetric action, independent of the strength of the disorder, given by:

$$S_O(\varphi_a, \varphi_a^*) = \frac{1}{2} \int \varphi_a^*(x)(-\Delta + m_0^2)\varphi_a(x)dx. \quad (5.206)$$

The action $S_I(\varphi_a, \varphi_a^*)$ will not be needed in our study of the Casimir effect, but its presence with a $\lambda > 0$ is required to guarantee the action's boundness.

We proceed recalling that each moment of the partition function contributes to the total quenched free energy, Eq. (5.70). To obtain the Casimir energy we compactify one of the dimensions, $\mathbb{R}^d \rightarrow \mathbb{R}^{d-1} \times [0, L]$, and impose some boundary conditions. As can be seen in Eq. (5.205), there is a combination of k, m_0^2 and ρ for which the effective mass $m_0^2 - k\rho^2$ becomes negative, indicating the symmetry breaking $U(1) \rightarrow \mathbb{Z}_2$, giving rise to a Goldstone (soft) mode. Of course, the Casimir force is present even for those terms in the sum with a positive effective mass, as the condition for its presence is that the correlation length becomes of the order of the system's compactified size L . That is, the total energy receives

contributions from symmetry-preserving and symmetry-breaking terms. Our interest in this application of the distributional zeta-function method is to study the interplay between the contributions to the energy of the symmetry-breaking soft mode and the critical mode, both induced by the disorder. Therefore, we neglect the symmetry-preserving modes. We assess this interplay by first performing a shift in the field $\varphi(x)$ to expose the symmetry breaking, then neglect all non-Gaussian terms, and finally, take the large L limit.

We perform the symmetry-breaking field shift for the situation with $m_0^2 - k\rho^2 < 0$ in Eq. (5.205), proceeding analogous to the procedure at the end of Sec. 5.1 and Sec. 5.1.1. In the Cartesian representation of the fields $\varphi(x)$ and $\varphi^*(x)$, we have that

$$\varphi(x) = \frac{1}{\sqrt{2}} [\psi_1(x) + i\psi_2(x)], \quad (5.207)$$

$$\varphi^*(x) = \frac{1}{\sqrt{2}} [\psi_1(x) - i\psi_2(x)]. \quad (5.208)$$

The minima of the action lie on the circle

$$\psi_1^2 + \psi_2^2 = \frac{2(k\rho^2 - m_0^2)}{\lambda} \equiv v^2. \quad (5.209)$$

Defining the shifted fields $\chi = \psi_1 - v$ and $\psi = \psi_2$, the Gaussian part of the action becomes

$$S_\rho(\chi, \psi) = \frac{1}{2} \int d^d x [\chi(x)(-\Delta + m_\rho^2)\chi(x) + \psi(x)(-\Delta)\psi(x)], \quad (5.210)$$

where we defined $m_\rho^2 = 2(k\rho^2 - m_0^2)$. In the new variables, after dropping all non-Gaussian terms, Eq. (5.204) assumes the following enlightening form:

$$\mathbb{E}[Z^k(h)] = Z_\rho Z_G [Z_O]^{k-1}, \quad (5.211)$$

where

$$Z_\rho = \int [d\chi] e^{-\frac{1}{2} \int d^d x \chi(x)(-\Delta + m_\rho^2)\chi(x)}, \quad (5.212)$$

$$Z_G = \int [d\psi] e^{-\frac{1}{2} \int d^d x \psi(x)(-\Delta)\psi(x)}, \quad (5.213)$$

$$Z_O = \int [d\varphi][d\varphi^*] e^{-\frac{1}{2} \int d^d x \varphi^*(x)(-\Delta + m_0^2)\varphi(x)}, \quad (5.214)$$

are the partition functions corresponding to the contributions of the disorder, the Goldstone mode, and a $O(k-1)$ symmetric model, respectively.

Now, we take a slab geometry with one compactified dimension, $\Omega_L = \mathbb{R}^{d-1} \times [0, L]$, and impose Dirichlet boundary conditions on all fields

$$A_\alpha(x_1, \dots, x_{d-1}, 0) = A_\alpha(x_1, \dots, x_{d-1}, L) = 0, \quad (5.215)$$

with $\alpha = \{\rho, G, O\}$ and $\{A_\rho, A_G, A_O\} = \{\chi, \psi, \phi\}$, respectively. Using the result in Eq. (4.34) for each of the partition functions in Eqs. (5.212), (5.213), and (5.214), we obtain for the k -th moment of the partition function, Eq. (5.211), the following expression:

$$\mathbb{E} [Z^k(h)] = \left[\det(-\Delta + m_\rho^2)_{\Omega_L} \right]^{-\frac{1}{2}} \left[\det(-\Delta)_{\Omega_L} \right]^{-\frac{1}{2}} \left[\det(-\Delta + m_0^2)_{\Omega_L} \right]^{-\frac{k-1}{2}}. \quad (5.216)$$

The last term contributes neither to the critical nor to the soft Goldstone modes. As such, it can be dropped by redefining the energy.

The relevant contributions to the Casimir energy can be regularized using the spectral zeta regularization

$$\mathbb{E} [Z^k(h)] = \exp \left\{ \frac{1}{2} \frac{d}{ds} \left[\zeta_\rho(s) + \zeta_G(s) \right] \Big|_{s=0} \right\}. \quad (5.217)$$

By the same arguments used to obtain Eq. (5.119), one concludes that the main contribution to the total quenched Casimir energy is given by

$$E_c^T = \frac{(-1)^{k_c}}{k_c k_c!} \exp \left\{ k_c \ln a + \frac{1}{2} \frac{d}{ds} \left[\zeta_\rho(s) + \zeta_G(s) \right] \Big|_{s=0} \right\}. \quad (5.218)$$

We define the following zeta function

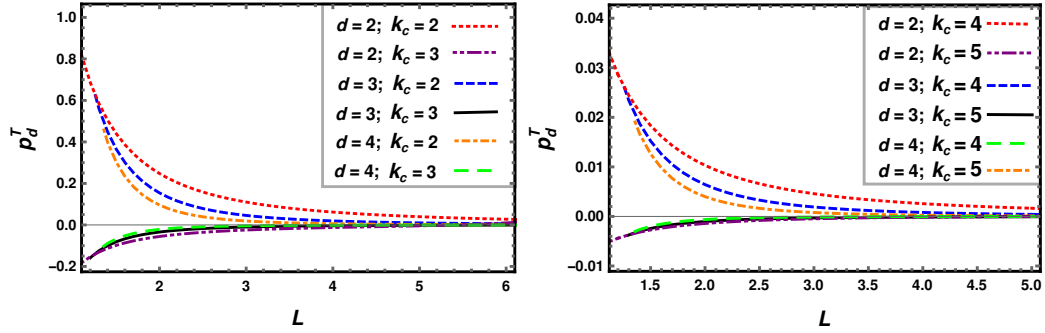
$$\zeta_\alpha(s) = \frac{A_{d-1}}{(2\pi)^{d-1}} \int \sum_{n=1} \left[p^2 + m_\alpha^2 + \left(\frac{\pi n}{L} \right)^2 \right]^{-s} dp, \quad (5.219)$$

with $\alpha = \{\rho, G\}$ and $m_G^2 = 0$. Using the same definitions and arguments in Sec. 4.2.1, one can rewrite $\zeta_\alpha(s)$ as

$$\zeta_\alpha(s) = C_d(L, s) \int_0^\infty t^{s-\frac{1}{2}(d+1)} e^{-\frac{tL^2}{\pi} m_\alpha^2} \psi(t) dt. \quad (5.220)$$

Following the same steps taken between Eqs. (4.44) and (4.47), it is straightforward to obtain that

$$\zeta_\alpha(s) = C_d(L, s) \left[2I_{1,d}^\alpha(s) + I_{2,d}^\alpha(s) - I_{3,d}^\alpha(s) \right], \quad (5.221)$$



(a) Plot of the quenched Casimir pressure, Eq. (5.225), for dimensions 2, 3, and 4 and $k_c = 2$, and 3.

(b) Plot of the quenched Casimir pressure, Eq. (5.225), for dimensions 2, 3, and 4 and $k_c = 4$, and 5.

Figure 5.4: Critical Casimir force for different parameters.

where

$$I_{1,d}^\alpha(s) = \int_0^\infty t^{\frac{d}{2}-s-1} e^{\frac{-L^2}{\pi t} m_\alpha^2} \psi(t) dt, \quad (5.222)$$

$$I_{2,d}^\alpha(s) = \int_0^\infty t^{\frac{d}{2}-s-1} e^{\frac{-L^2}{\pi t} m_\alpha^2} dt, \quad (5.223)$$

$$I_{3,d}^\alpha(s) = \int_0^\infty t^{\frac{d}{2}-s-\frac{3}{2}} e^{\frac{-tL^2}{\pi} m_\alpha^2} dt, \quad (5.224)$$

and $C_d(L, s)$ is given in Eq. (4.45).

One obtains the quenched Casimir force analogously to Eq. (5.121). Such a force receives contributions from the spectral zeta functions of soft and critical modes. In the case of $\alpha = G$, we have the same situation of Sec. 4.2.1 for $m_0 = 0$, *i.e.*, the contribution of the soft modes to the Casimir force is given by Eq. (4.52). For $\alpha = \rho$, we have the calculation of our first application of the distributional zeta-function and the corresponding contribution is given by Eq. (5.112). Putting all together, we obtain for the total quenched Casimir pressure of the system the following expression:

$$p_d^T(L) = \frac{(-1)^{k_c}}{k_c k_c! 2^{d-1} L^d} \left[\frac{L^2}{d-1} B_d(0) + D_d(0) + \frac{\zeta(d)}{2\pi} \right]. \quad (5.225)$$

Such a result can be plotted as a function of L for different dimensions and values of k_c . Figs. 5.4a and 5.4b display $p_d^T(L)$ for dimensions 2, 3, and 4 for different values of k_c . Note the different scales in the axes of the two figures.

This result has some interesting features. First of all, if we ignore the Goldstone mode contributions, the resulting equation differs from Eq. (5.122) by a multiplicative factor, $4/k_c$. This factor comes from the exact diagonalization of the quadratic actions; when one uses the ansatz $\phi_i^k(x) = \phi_j^k(x) \forall i, j$, as used previously, the multiplicative factor does not appear. Of course, such a difference is irrelevant to gathering qualitative understanding. However, the qualitative similarity between the results holds only when one can neglect the contribution from the partition function Z_O , Eq. (5.214). This is the case whenever the corresponding action does not reach criticality, a situation that can occur due to nonzero temperature or finite-size effects. Another feature of Eq. (5.225) is that the critical and the soft mode effects are noncompetitive; they are of the same sign. Still another interesting feature is that, when $k_c \rho \gg m_0^2$, one can neglect the contribution of Z_ρ , Eq. (5.212), to the Casimir energy; in practice, one can set $B_d(0) = D_d(0) = 0$ in Eq. (5.225). This is interesting because then only soft modes contribute, but with a factor proportional to $(-1)^{k_c}$, which means that a change of sign may occur. In other words, there is a universal constant due to the soft modes, given by $\zeta(3)/16\pi$, with an overall sign that can be either negative (as usual) or positive, depending on the value of k_c .

Analog model for Euclidean Wormholes

Here, we present the main calculations and results of Refs. [232, 233].

The program of describing the gravitational field using quantum theory faces many conceptual difficulties, mainly related to causality and locality. Quantum field theory, formulated on a classical gravitational background spacetime, is an intermediate step toward such a program [234–236]. A problem that permeates this approach is the absence of a specific vacuum state associated with matter fields in a generic spacetime. However, in globally hyperbolic spacetimes, this issue is circumvented by the use of Hadamard states. To go further, one can discuss the effects of the fluctuations of the metric fields on the quantum matter fields. It has been shown that a bath of gravitons in a squeezed state induces fluctuations of light cones [237–239]. Ref. [240] proposed an analog model for fluctuating light cones induced by quantum gravity effects. The model builds on the fact that acoustic waves in a disordered medium propagate with a random speed of sound. Further studies discussing analog models can be found in Refs. [241–244]. Here, we build on similar ideas to propose an analog model for Euclidean wormhole effects on a real scalar field.

In recent years, there has been a growing perception [245] that long-distance physics issues are as important in quantum gravity as the most-discussed short-distance physics issues. A central, open question in this respect is: How does the nonlocality of quantum gravity affect the expectation value of a measurable

observable? Returning to local quantum field theory, one can define Schwinger functions from the expectation values of operator products in Minkowski space-time. These are the corresponding analytically continued vacuum expectation values in Euclidean space, as we have seen in Chaps. 3-4.

In the functional integral formalism [246] in Euclidean space, the Schwinger functions are moments of a measure in the functional space of classical fields. In such a functional integral scenario, one can discuss topology fluctuations and wormholes [247–250], which are quantum gravity features particularly relevant to the issue of quantum coherence loss in Hawking black hole evaporation.

The basic feature of wormholes in Euclidean field theory is the existence of nonlocal physics in a connected manifold or geometry that connects disconnected boundaries. The contribution to the free energy from these connected topologies was discussed in Ref. [251] using the replica trick. The replica trick provides a convenient way to compute averages of the free energy (the log of the partition function) [138]. In a related study, Ref. [252] proposes an integral representation of $\ln x$ to compute the free energy of spacetime D -branes. The author of that reference argues that the bulk gravity picture of such an integral representation involves wormholes connecting multiple asymptotic boundaries. Replica wormholes also play a role in the computation of the von Neumann entropy of Hawking radiation [253].

Two of the most fundamental questions facing Euclidean quantum gravity are the following: 1) What is the empirical support for the mathematical formalism of Euclidean quantum gravity? 2) What are the physical effects of topological fluctuations on the Euclidean quantum fields? In the absence of cosmological experiments, we propose a condensed matter analog model that might provide insight into these questions. We propose an analog model for topological fluctuations in Euclidean fields based on external disordered fields described by a statistical field theory.

As we have seen previously, low temperatures or anisotropic disorder induce nonlocal terms in the resulting effective action (see Eq. (5.126)).

We briefly discuss matter fields in a generic Riemannian manifold. Suppose a compact manifold with Riemannian signature $\mathcal{M}$. The space of fields is the space $C^\infty(\mathcal{M}, \mathbb{R})$ of smooth functions defined on $\mathcal{M}$. Let $S : C^\infty(\mathcal{M}, \mathbb{R}) \rightarrow \mathbb{R}$ be an action functional of the gravitational g and matter ϕ fields. Using a functional measure for the gravitational and matter fields, the partition function is given by:

$$Z = \int [dg][d\phi] e^{-S(g)-S(\phi)} \quad (5.226)$$

where $S(g)$ and $S(\phi)$ are the gravitational field and matter field actions, respectively. For simplicity, we take a single scalar field to represent the matter degrees

of freedom. The gravitational field action is given by:

$$S(g) = -\frac{1}{16\pi G} \int_{\mathcal{M}} d^d x \sqrt{g} (R - 2\Lambda) - \frac{1}{8\pi G} \int_{\partial\mathcal{M}} K d^{d-1}\Sigma + C. \quad (5.227)$$

As usual, $g = \det(g_{ij})$, G is Newton's constant, R is the Ricci-scalar, Λ is the cosmological constant, K is the trace of the second fundamental form on the boundary, and C is a constant that can be tuned to achieve a convenient on-shell configuration, e.g., in flat space $S(g) = 0$. For the matter field action, we take:

$$S(\phi) = \frac{1}{2} \int d^d x \sqrt{g} \phi(x) (-\Delta + m^2) \phi(x) + \frac{\lambda_0}{4} \int d^d x \sqrt{g} \phi^4(x). \quad (5.228)$$

Many authors [248–250, 254] have emphasized that the effects of wormholes and topology fluctuations are encoded in a nonlocal matter-field contribution to the Euclidean partition function, namely

$$Z = \int [dg][d\phi] \exp \left[-S(\phi, g) + \frac{1}{2} \int d^d x \int d^d y \sum_{i,j} \phi_i(x) C_{ij}(x, y) \phi_j(y) \right], \quad (5.229)$$

in which $C_{ij}(x, y)$ encodes the space nonlocality, with each pair i, j representing a wormhole. In the next section, we show that such a nonlocal term arises naturally in a matter system in the presence of disorder.

As mentioned above, in a Euclidean quantum gravity scenario, many authors have stressed the necessity of performing the average of the free energy or the generating functional of connected correlation functions of the system [251, 252].

Here, our main assumption is that the topology fluctuations in the Euclidean path integral in Eq. (5.227) can be effectively modeled by coupling a quenched disorder field to the matter field ϕ . In practice, one removes the functional measure of the metric from the functional integral and takes the disorder average of the corresponding free energy over ensembles of disorder realizations. Proceeding in this way, the Euclidean wormholes' effective action is readily identified. The topology fluctuation information is then effectively accounted for by the quenched disorder field.

Let us suppose that we have the random field action, Eq. (5.51), with the probability distribution of the disorder given by

$$P(h) = p_0 \exp \left\{ -\frac{1}{2\varrho^2} \int d^d x \int d^d y h(x) F^{-1}(x - y) h(y) \right\}, \quad (5.230)$$

where ϱ is a positive parameter associated with the strength of the disorder, p_0 is a normalization constant, and $F(x - y)$ defines the disorder correlation $E[h(x)h(y)] = \varrho^2(x - y)$.

For the random field case, the effective actions S_{eff} defining the k -th moment of the partition function in Eq. (5.71) are given by:

$$S_{\text{eff}}(\phi_i^k) = \int d^d x \int d^d y \sum_{i,j=1}^k \frac{1}{2} \phi_i^k(x) [G^{-1}(k)]_{ij}(x-y) \phi_j^k(y), \quad (5.231)$$

where $[G^{-1}(k)]_{ij}(x-y)$ is the inverse of the two-point correlation function

$$[G^{-1}(k)]_{ij}(x-y) = \left[(-\Delta + m^2) \delta^{(d)}(x-y) \delta_{ij} - \varrho^2 F_{ij}(x-y) \right], \quad (5.232)$$

where $F_{ij}(x-y)$ is the matrix with all entries equal to $F(x-y)$. The term proportional to ϱ^2 comes from averaging over the random field h and contains a nonlocal contribution when $F(x-y)$ is not δ -correlated in (x, y) . The nonlocal contribution is analogous to the nonlocal term in Eq. (5.229). The first term in this last equation gives the bare contribution to the connected two-point correlation function even in the absence of disorder averaging, whereas the second term is normally a disconnected contribution but, due to the averaging, it becomes a connected contribution [121].

Proceeding with the diagonalization approach, we can write

$$\mathbb{E}[Z^k(h)] = \int \prod_{a=1}^{k-1} [d\phi_a^k] e^{-S_O(\phi_a^k)} \int [d\phi] e^{-S_\varrho^{(k)}(\phi)}, \quad (5.233)$$

with

$$S_O(\phi_a^k) = \int d^d x \sum_{a=1}^{k-1} \frac{1}{2} \phi_a^k(x) (-\Delta^2 + m^2) \phi_a^k(x), \quad (5.234)$$

$$S_\varrho^{(k)}(\phi) = \int d^d x \int d^d y \frac{1}{2} \phi(x) [G_0^{-1}(x-y) - k\varrho^2 F(x-y)] \phi(y). \quad (5.235)$$

How does this result relate to the original works about Euclidean wormholes? First, as already mentioned, the Gaussian disorder correlation leads to a probability distribution similar to that obtained in Coleman's work in Ref. [248]. Second, instead of calculating the mean value of the partition function with the wormhole contributions integrated out with non-Gaussian distributions for the topological fluctuations, as done by Preskill [250] and González-Díaz [255], here we are analyzing those effects on the disorder average of the free energy (the log of the partition function). As mentioned after Eq. (5.232), such an average leads to connected correlation functions that would be disconnected correlation functions in the absence of disorder. This feature leads to the interpretation that the quenched

field induces topology fluctuations, fluctuations that have “propagators” associated with them, in Preskill’s [250] sense. Said differently, the disorder average of the free energy in Eq. (5.233) is actually a superposition of the contributions given by (infinitely) many universes connected by Euclidean wormholes. This is the analog to the proposal by Klebanov, Susskind, and Banks [249] that our universe was in a thermal bath with many (possibly infinite) universes. Finally, a similar interpretation of the average of the free energy was presented in a recent work by Okuyama [252], in which a different method was used to compute the average free energy.

It is important to point out that a single term in the series does not define a brane (universe); rather, the brane interpretation applies only to the entire series. After the diagonalization and the redefinition of the fields in the functional space, a single term of the series has no direct interpretation at all. The entire series is needed to obtain physical quantities. Figure 5.5 provides a visualization of our result, in that all topology fluctuations are, in fact, Euclidean wormholes. As evinced by Eq. (5.235), we have two kinds of fluctuations: those that connect different branes (different universes), and those located on the same brane (same universe).

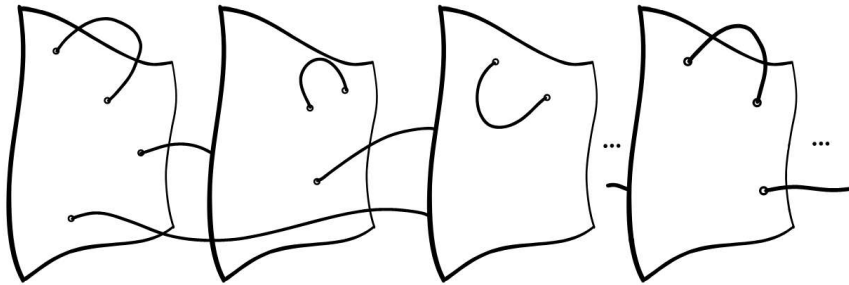


Figure 5.5: Visualization of the topology fluctuations obtained from the disorder-averaged free energy of the model.

A link with condensed matter physics is almost trivial. A disordered system at low temperatures, or for an anisotropic disorder, leads to a model with the same mathematical structure regarding the nonlocality induced by quantum gravity effects on matter fields. The series in Eq. (5.70) takes into account all possible configurations of the disorder. However, those configurations are not independent, since the disorder average is taken over the free energy, the generating functional of the connected correlation functions.

This concludes the formulation of the analog model. Physical quantities, such as the dynamic and static structure factors, can be readily computed by using a mean-field approximation to obtain the necessary matter-field correla-

tion functions. We recall that the static structure factor is proportional to the total intensity of light scattered by the fluid [256]. As such, the effects of the disorder-induced nonlocality should leave signals on the scattered light.

In summary, we have proposed an analog model for Euclidean wormholes and topological fluctuation effects in a Riemannian space. We aimed at modeling the effects of a quantum theory of gravitation on a matter field. The idea of modeling the internal degrees of freedom by a random field has logical appeal and historical background. Although we based our derivations using a scalar field, the formalism can be easily adapted to other fields, such as vector and spinor fields.

As a matter of fact, we know that, in a Bose-Einstein condensate (BEC), one has around 10% of the system as a non-condensed cloud of atomic gas surrounding the condensate [257, 258]. Such an atomic cloud affects the physical properties of the condensate.

Starting from the Hamiltonian of the condensate and the non-condensed cloud, one can construct the soft action as (for details, see Ref. [233])

$$S_0(\phi, \phi^*) + S_1 = \int \left[\phi^*(x) \left(-\frac{\Delta}{2m_\phi} + m_0^2(x) + \eta(x) \right) \phi(x) + g_\phi |\phi(x)|^4 + \phi(x)h^*(x) + \phi^*(x)h(x) + \phi^2(x)m^*(x) + \phi^{*2}(x)m(x) \right] dx, \quad (5.236)$$

where ϕ are the condensate field variables, while $\eta(r)$, $h(r)$, and $m(r)$ are related to the non-condensed cloud and are functions that only exist in the interface between the condensate and the non-condensed cloud.

Disregarding the second line of the action in Eq. (5.236) is equivalent to assuming the so-called Hartree-Fock-Bogoliubov-Popov approximation, which recovers the Gross-Pitaevskii action functional. Let us suppose that our system is in three dimensions and the condensate is confined in some semi-finite region. A bidimensional representation of the system is given in Fig. 5.6.

Then, it follows that the Gross-Pitaevskii action is given by

$$S(\phi, \phi^*, \eta) = \int \int_0^L \left\{ \phi^*(x, z) \left[-\frac{\Delta}{2m_\phi} + m_0^2(x, z) + \eta(x, z) \right] \phi(x, z) + g_\phi |\phi(x, z)|^4 \right\} dz dx. \quad (5.237)$$

We note that the interaction between the cloud and the BEC can be complex to model, since at the interface, we can have condensation of elements of the cloud and decondensation of part of the BEC. Therefore, we will model this interaction

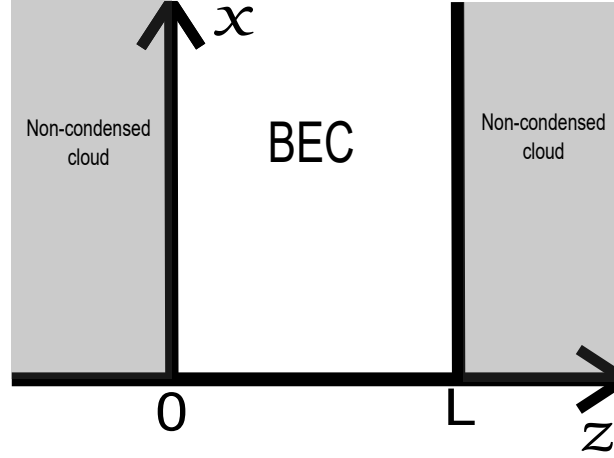


Figure 5.6: Bidimensional visualization of the BEC confined between non-condensed clouds.

by a quenched disorder. Take the probability distribution as

$$P(\eta) = p_0 \exp \left(-\frac{1}{2\rho^2} \int_0^L \int_0^L \int_0^L \eta(x, z) F^{-1}(x, z; x', z') \eta(x', z') dz dz' dx dx' \right) \quad (5.238)$$

where ρ is the strength of the multiplicative disorder $\eta(x, z)$ and $F(x, z; x', z')$ is the correlation function of the disorder. Therefore, the correlation of the disorder $\eta(x, z)$ is $\mathbb{E}[\eta(x, z)\eta(x', z')] = \rho^2 F(x, z; x', z')$. It follows that the effective action is given by

$$\begin{aligned} S_{\text{eff}}(\phi, \phi^*) &= \int_0^L \int_0^L \sum_{i=1}^k \phi_i^*(x, z) \left[-\frac{\Delta}{2m_\phi} + m_0^2(x, z) \right] \phi_i(x, z) dz dx \\ &+ \int_0^L \int_0^L \int_0^L \sum_{i,j=1}^k \left(\delta_{ij} g_\phi - \rho^2 F(x, z; x', z') \right) \phi_j^{*2}(x, z) \phi_i^2(x', z') dz' dz dx' dx. \end{aligned} \quad (5.239)$$

Such an action shares similarities with the effective action of Eq. (5.126) (just take $F(x, z; x', z') = \delta^2(x - x') [\delta(z) + \delta(z - L)]$), which is also non-local. This effective action is similar to the one that appears in the study of spin-glass systems at low temperatures and it is highly non-trivial [217]. However, this gives us that, in fact, the interaction between the non-condensed cloud can be interpreted as a quenched disorder in terms of known systems.

For simplicity, let us now disregard the non-linear couplings between the condensate and the non-condensate in Eq. (5.236) and the non-Gaussian contributions. That is, we disregard the contributions of η , m , and ϕ^4 and keep only

h. Supposing the covariance of $h(x, z)$ as $E[h^*(x, z)h(x', z')] = \sigma^2 F(x, z; x', z')$, where σ is the strength of the additive disorder, the effective action reads

$$S_{\text{eff}}(\varphi, \varphi^*) = \int \int_0^L \int_0^L \sum_{i,j=1}^k \phi_j^*(x, z) \left[\left(-\frac{\Delta}{2m_\varphi} + m_0^2(x, z) \right) \delta_{ij} \delta(x - x') \delta(z - z') - \sigma^2 F(x, z; x', z') \right] \phi_i(x', z') dz dz' dx dx', \quad (5.240)$$

If we define $G_{ij} = \left(-\frac{\Delta}{2m_\varphi} + m_0^2(x, z) \right) \delta_{ij} \delta(x - x') \delta(z - z') - \sigma^2 F(x, z; x', z')$, we obtain the same action as in Eq. (5.231), and therefore the same diagonalization procedure can be implemented to reproduce the Eqs. (5.234)-(5.235).

Therefore, we conclude that the system of a BEC and the non-condensed cloud can be a realization of the analog model for Euclidean wormholes. Objectively, a measurable quantity that can be obtained from this BEC model with dirty surfaces is the Casimir force, which will behaves like the the one plotted in Figure 5.4.

Generalized entropy of a Black Hole

Here we reproduce the main results of Ref. [259]. Details about quantum fields in curved space-time can be found in Refs. [21, 260, 261].

The limits of applicability of quantum field theory were tested through the formulation of quantum fields in curved spacetime, where problems of a different nature arise [262, 263]. After the introduction of the concept of black hole entropy by Bekenstein [264, 265], Hawking studied free quantum fields in a fixed curved background spacetime geometry. It was shown that a black hole of mass M_0 emits thermal radiation at a temperature β^{-1} , which is proportional to the surface gravity of the horizon (a null hypersurface generated by a congruence of null geodesics) [266, 267]. This effect, initially derived for a non-rotating neutral black hole, remains a topic of ongoing debate and continues to be a fertile ground for testing new ideas and techniques.

However, one can ask: In Euclidean quantum field theory, how do disorder fields affect the generalized entropy of a Schwarzschild black hole? Here, we include disorder fields in addition to the external matter and radiation fields. The microscopic degrees of freedom that are thought to contribute additional terms to a complete theory of black hole entropy have yet to be adequately identified [268]. Significant efforts have been made to explain the origin and behavior of these unknown contributions to entropy. Several common perspectives exist, including the statistical origin of Einstein's equations and the quantum properties

of the gravitational field. For example, in Ref. [269], it is argued that an accurate interpretation of entropy does not necessarily require additional degrees of freedom but arises solely from the quantum nature of gravity.

There are approaches that include the degrees of freedom of the black hole's interior [270]. These results, using the topological structure of replica wormholes, demonstrate why the black hole interior should be included in the computation of radiation entropy [271–274].

Based on Refs. [275–279], we define an effective model with disorder in Euclidean geometry. To account for the influence of disorder fields on matter fields and their contribution to generalized entropy, we study a self-interacting $\lambda\phi_d^4$ theory defined in a Euclidean section of the Schwarzschild manifold.

The Birkhoff theorem on manifolds ensures that any vacuum spherically symmetric solution of the Einstein equation is locally isometric to a region in Schwarzschild spacetime. Therefore, we start with the pseudo-Riemannian manifold that possesses the Schwarzschild metric in a d -dimensional spacetime [280]. The line element reads:

$$ds^2 = -\left(1 - \left(\frac{r_s}{r}\right)^{d-3}\right) dt^2 + \left(1 - \left(\frac{r_s}{r}\right)^{d-3}\right)^{-1} dr^2 + r^2 d\Omega_{d-2}^2. \quad (5.241)$$

The Schwarzschild radius r_s is proportional to the product of the d -dimensional Newton's constant and the black hole mass M_0 :

$$r_s^{d-3} = \frac{8\Gamma\left(\frac{d-1}{2}\right)}{(d-2)\pi^{\frac{d-3}{2}}} G^{(d)} M_0. \quad (5.242)$$

For simplicity, we use the notation $G^{(d)} M_0 = M$, so that in four dimensions, M has units of length.

After a Wick rotation, $t \rightarrow i\tau$, in the time coordinate, we obtain the d -dimensional Hawking instanton, i.e., a positive definite Euclidean metric for $r > r_s$:

$$ds_E^2 = \left(1 - \left(\frac{r_s}{r}\right)^{d-3}\right) d\tau^2 + \left(1 - \left(\frac{r_s}{r}\right)^{d-3}\right)^{-1} dr^2 + r^2 d\Omega_{d-2}^2. \quad (5.243)$$

This manifold has a conic singularity. The singularity at $r = r_s$ is removed by assuming that the imaginary time coordinate, τ , is periodic with period $4\pi r_s/(d-3)$. The bifurcate Killing horizon then becomes a rotation axis. This Euclidean section of the Schwarzschild solution, with compactified imaginary time, is homeomorphic to $\mathbb{R}^2 \times S^2$.

In this manifold, the Israel-Hawking-Hartle vacuum state is defined. Any quantum field defined in this manifold behaves as if it is held at a temperature

$\beta^{-1} = (d-3)/4\pi r_s$. In the Matsubara formalism, the periodicity in imaginary time corresponds to finite-temperature states, with the Euclidean space homeomorphic to $S^1 \times \mathbb{R}^3$ [281, 282]. Since, in principle, we do not have full mathematical control over expressions in the infinite volume limit, we must enclose the black hole within a finite-volume box and impose boundary conditions. From now on, we assume Dirichlet boundary conditions on the surface of the confining box. The total volume of the system is given by $\text{Vol}_d(\Omega) = \beta V_{d-1}$.

We also note that for Euclidean interacting field theories confined to compact domains, it is necessary to introduce surface counterterms to make the interacting field theory perturbatively renormalizable [227–230, 283].

In the following, we define operators on the Riemannian manifold. Since we are considering a scalar field, we need to define the Laplace-Beltrami operator. In any smooth connected d -dimensional Riemannian manifold, $\mathcal{M}^d$, the operator is defined by:

$$-\Delta_g = -\frac{1}{\sqrt{g}} \sum_{i,j=1}^d \frac{\partial}{\partial x^i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial x^j} \right), \quad (5.244)$$

where $(g^{ij}) = (g_{ij})^{-1}$, and $g = \det(g_{ij})$. We are working in a local arbitrary curvilinear coordinate system $x_v = (x_1, x_2, \dots, x_d)$. As usual, we define the Riemannian d -volume μ by $d\mu = \sqrt{g} dx_1 dx_2 \dots dx_d$. In general, we are interested in the Hilbert space of square-integrable functions defined on a compact domain, i.e., $\mathcal{H} = L^2(\Omega, d\mu)$, where $\Omega \subseteq \mathcal{M}^d$ is compact.

Using the fact that, in an interacting field theory, the black hole can remain in thermal equilibrium with a thermal bath [284], we consider a Euclidean self-interacting scalar model. The action functional for a single self-interacting scalar field is given by:

$$S(\phi) = \frac{1}{2} \int_{\beta} d\mu \left[\phi(x) (-\Delta_s + m_0^2) \phi(x) + \frac{\lambda_0}{12} \phi^4(x) \right], \quad (5.245)$$

where $-\Delta_s$ denotes the Laplace-Beltrami operator in the Euclidean section of the Schwarzschild manifold M_s^d , λ_0 is the bare coupling constant, and m_0^2 is the spectral parameter of the model. The notation $\int_{\beta}$ indicates that the imaginary time coordinate $x_1 = \tau$ is periodic, with $0 \leq x_1 \leq 4\pi r_s/(d-3)$, so $\phi(x_1, x_2, \dots, x_d) = \phi(x_1 + \beta, x_2, \dots, x_d)$. We define $x_2 = r$ as the radial coordinate. In this manifold, the Laplace-Beltrami operator is explicitly given by:

$$-\Delta_s \phi = \Delta_{\theta} \phi(x_3, \dots, x_d) + \left(1 - \left(\frac{r_s}{x_2} \right)^{d-3} \right)^{-1} \frac{\partial^2 \phi}{\partial x_1^2} + \frac{1}{x_2^{d-2}} \frac{\partial}{\partial x_2} \left(x_2^{d-2} \left(1 - \left(\frac{r_s}{x_2} \right)^{d-3} \right) \frac{\partial \phi}{\partial x_2} \right), \quad (5.246)$$

where Δ_θ denotes the Laplace-Beltrami operator on the $(d-2)$ -dimensional unit sphere S^{d-2} , corresponding to the contribution from the angular part. Finally, as previously mentioned, we assume Dirichlet boundary conditions, i.e., $\varphi(x)|_{\partial\mathcal{M}_s^d} = 0$, since we consider the entire system inside a reflecting wall. This procedure is necessary to ensure that the system has finite volume and that the spatially cut-off Schwinger function is well-defined.

By introducing an external source $j(x)$, we can proceed as in Sec. 4.2 to define the generating functional for all n -point correlation functions $Z(j)$ as:

$$Z(j) = \int \exp\left(-S(\phi) + \int_\beta j(x)\phi(x)d\mu\right) [d\phi], \quad (5.247)$$

where $[d\phi]$ is a functional measure, defined symbolically as $[d\phi] = \prod_{x \in S^1 \times \mathbb{R}^3} d\phi(x)$. By adding a random field h , coupled to the field variable, we can use the distributional zeta-function method, Eq. (5.70).

Once the average is taken, one must carefully choose the covariance of the disorder field. If one chooses a Gaussian disorder, all points on the Euclidean manifold will experience its effects uniformly. However, as discussed earlier, the disorder field attempts to represent degrees of freedom not included in this mesoscopic approach. Consequently, the disorder must encode information about fast-mode processes; in some sense, this information is captured by the disorder covariance. Since we know that Euclidean quantum field theory exhibits divergences near the boundary due to fast modes [226], we assume in this model that the disorder covariance also diverges near the boundary. Therefore, to preserve the system's symmetry, the disorder covariance increases as $x_2 \rightarrow 0$. For this reason, we choose the covariance of the disorder to be given by

$$\mathbb{E}[h(x)h(y)] = \frac{U(x_2)}{\sqrt{g}} \delta^d(x-y), \quad (5.248)$$

where we are assuming that the functional form of $U(x_2)$ is

$$U(x_2) = b^{\alpha-2}(x_2)^{-\alpha} \quad (5.249)$$

for positive definite α , and where b is a constant with units of length. Note that $x_2 = r$; hence, Eq. 5.249 exhibits spherical symmetry. This covariance leads us to the effective action given by

$$S_{\text{eff}}^{(k)}(\phi_i, j_i) = \int_\beta \left[\sum_{i=1}^k \left(\frac{1}{2} \phi_i(x) (-\Delta_s + m_0^2) \phi_i(x) + \frac{\lambda_0}{4!} (\phi_i(x))^4 \right) - \frac{U(x_2)}{2} \sum_{i,j=1}^k \phi_i(x) \phi_j(x) - \sum_{i=1}^k \phi_i(x) j_i(x) \right] d\mu. \quad (5.250)$$

Since we are interested solely in the thermodynamic properties of the model, we do not need to generate the correlation functions. Thus, we set $j_i(x) = 0$ for all i and omit the $j = 0$ argument in all quantities.

We now discuss the Gaussian contribution to the action given by Eq. (5.250), which suffices to capture the thermodynamic properties. The free part of the effective action can be recast as

$$S_0^{(k)}(\phi_i) = \frac{1}{2} \int_{\beta} d\mu \sum_{i,j=1}^k \phi_i(x) [(-\Delta_s + m_0^2) \delta_{ij} - U(x_2)] \phi_j(x), \quad (5.251)$$

therefore we can proceed with the diagonalization procedure. After diagonalization, it follows that

$$\mathbb{E}[Z^k(h)] = \int \exp(-S^{(k)}(\varphi)) [d\varphi] \int \exp(-S_0^{(k)}(\varphi_l)) \prod_{l=2}^k [d\varphi_l], \quad (5.252)$$

where we denote $\varphi_1 = \varphi$,

$$S^{(k)}(\varphi) = \frac{1}{2} \int_{\beta} \varphi(x) [-\Delta_s + m_0^2 - kU(x_2)] \varphi(x) d\mu, \quad (5.253)$$

and

$$S_0^{(k)}(\varphi_l) = \frac{1}{2} \int_{\beta} \sum_{l=2}^k \varphi_l(x) (-\Delta_s + m_0^2) \varphi_l(x) d\mu. \quad (5.254)$$

Performing all the Gaussian integrations, we can recast our quenched Gibbs free energy, Eq. (5.70), as

$$\mathbb{E}[W(h)] = \sum_{k=1}^{\infty} c_k [\det(-\Delta_s + m_0^2)]^{\frac{1-k}{2}} [\det(-\Delta_s + m_0^2 - kU(x_2))]^{-\frac{1}{2}}. \quad (5.255)$$

Notice that the first determinant is standard, as expected in the analysis of scalar fields on a Riemannian manifold. The regularity and self-adjointness of this operator follow from the properties of the Laplace-Beltrami operator. However, the second determinant describes a more complex situation, as it corresponds to a Schrödinger operator on a Riemannian manifold.

One must determine the self-adjointness and spectral properties of the Schrödinger operator on a Riemannian manifold within a Hilbert space. For $-\Delta$ in $L^2(\mathbb{R}^d)$, the Fourier transform establishes self-adjointness on the domain $D(-\Delta) = H^2(\mathbb{R}^d)$, which corresponds to a Sobolev space. If the Schrödinger operator is

not proven to be essentially self-adjoint, there may exist an infinite set of self-adjoint extensions, making it challenging to identify the physically correct one [285–287].

An important result was obtained by Oleinik [288]. The author proved that for non-bounded manifolds, in the absence of local singularities in the potential, the Schrödinger operator on a Riemannian manifold is essentially self-adjoint. In the case of bounded manifolds in $\mathbb{R}^d$, the result of Ref. [289] ensures that for potentials with algebraic divergences of order ≥ 2 , the Schrödinger operator is self-adjoint. Note that $U(x_2)$ is a real-valued function that is locally summable in L^2 and globally semi-bounded, i.e., $U(x_2) \geq -C$ for $x_2 \in M_s^d$, with a constant $C \in \mathbb{R}$. Therefore, we have a self-adjoint operator in the Hilbert space $L^2(M_s^d) = L^2(M_s^d, d\mu)$.

To preserve the universality of the second law of thermodynamics [290], Bekenstein conjectured that the total entropy of the system must satisfy the generalized second law

$$\Delta S_{gen} = \Delta S^{(1)} + \Delta S^{(2)} \geq 0, \quad (5.256)$$

where $S^{(1)}$ denotes the Bekenstein-Hawking entropy, which is proportional to the horizon area, and $S^{(2)}$ represents corrections from matter and radiation fields. We now proceed to discuss the contribution of $S^{(2)}$.

Since, in our case, we have a system with infinitely many degrees of freedom, we must use the concept of mean entropy, i.e., the entropy per unit $(d-1)$ -volume ($\beta^{-1} \text{Vol}_d(\Omega)$) [291],

$$s^{(2)} = \frac{\beta S^{(2)}}{\text{Vol}_d(\Omega)}. \quad (5.257)$$

Using the fact that $S = \ln Z + \beta E$, in Euclidean quantum field theory, we can derive the generalized entropy density from the Gibbs free energy. In the case of a compact Riemannian manifold, the contribution of the quantum fields to the generalized entropy in the absence of disorder is

$$s^{(2)} = \frac{1}{\text{Vol}_d(\Omega)} \left(\beta - \beta^2 \frac{\partial}{\partial \beta} \right) \ln Z(j) \Big|_{j=0}, \quad (5.258)$$

where $Z(j)|_{j=0}$ is the partition function. Here, we have the Gibbs entropy of a classical probability distribution.

In the presence of disorder, the contribution of external matter fields to the generalized entropy density $s^{(2)}$ is

$$s^{(2)} = \frac{1}{\text{Vol}_d(\Omega)} \left(\beta - \beta^2 \frac{\partial}{\partial \beta} \right) \mathbb{E}[W(h)]. \quad (5.259)$$

The form of Eq. 5.259 results from the assumption that the total volume and the temperature are not affected by the disorder. Using Eqs. (5.255) and (??), we obtain that

$$s^{(2)} = \sum_{k=1}^{\infty} \frac{c'_k}{\text{Vol}_d(\Omega)} \left(\beta - \beta^2 \frac{\partial}{\partial \beta} \right) [\det(-\Delta_s + m_0^2)]^{-\frac{k}{2}} \left[\frac{\det(-\Delta_s + m_0^2)}{\det(-\Delta_s + m_0^2 - kU(x_2))} \right]^{\frac{1}{2}}, \quad (5.260)$$

where $c'_k = \frac{(-1)^k}{kk!}$. Notice that a is assumed large enough due to its relation with the thermodynamic limit of disordered systems.

The entropy, on physical grounds, depends on the covariance of the disorder. It becomes necessary to specify $U(x_2)$ in order to obtain $s^{(2)}$. As we shall clarify below, we will obtain the values of the functional determinants using their eigenfunctions. One can verify in Eq. (5.246) that the operator Δ_s always contains the angular Laplace-Beltrami operator, $-\Delta_\theta$. Since $U(x_2)$ does not depend on the angular variables, we shall ignore such an angular operator. In practice, it is equivalent to work in $d = 2$. In the neighborhood of the event horizon, the effects of the internal degrees of freedom are expected to become more relevant. In such a region, where $x_2 = r \approx 2M$, we can define the radial coordinate $\rho = \sqrt{8M(r - 2M)}$, and the line element can be written as

$$ds^2 = \frac{\rho^2}{16M^2} d\tau^2 + d\rho^2, \quad (5.261)$$

where the horizon is located at $\rho = 0$. The equation of motion for the free field in the Euclidean Rindler space is given by

$$(-\Delta_R + m_0^2)\phi = \left(\frac{16M^2}{\rho^2} \frac{\partial^2}{\partial \tau^2} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + m_0^2 \right) \phi = 0, \quad (5.262)$$

where $-\Delta_R$ stands for the Laplace-Beltrami operator in the Rindler coordinates given by the line element (5.261). Therefore, we can observe that this operator is $-\Delta_s$ near the horizon after the angular part is disregarded.

In the near-horizon approximation, i.e., $\rho \approx 0$, the potential of the Schrödinger operator can be recast as

$$U(\rho, M) = \frac{a^{\alpha-2}}{(2M)^\alpha} \left(1 - \frac{\alpha \rho^2}{16M^2} \right). \quad (5.263)$$

Using the fact that the coordinate τ is periodic, the total entropy density will be a sum over all Matsubara modes:

$$s^{(2)} = \sum_{n=-\infty}^{\infty} s^{(2)}(n), \quad (5.264)$$

where $s^{(2)}(n)$ is given by Eq. (5.260) in the near-horizon approximation with the angular part disregarded.

Note that for small ρ , and defining $f(\alpha, M) = \frac{\alpha}{2^{4+\alpha}M^{2+\alpha}}$, the determinant that contains the potential can be written as

$$\det \left[-\Delta_R + ka^{\alpha-2} \rho^2 f(\alpha, M) + m_0^2 - \frac{ka^{\alpha-2}}{(2M)^\alpha} \right]. \quad (5.265)$$

We define an effective mass for each effective action as $m_{\text{eff}}^2(k, M) = m_0^2 - \frac{ka^{\alpha-2}}{(2M)^\alpha}$.

To continue, let us discuss the solution of the differential equation for each Matsubara mode. We have that $R_n(\rho)$ satisfies

$$\left[\rho^2 \frac{d^2}{d\rho^2} + \rho \frac{d}{d\rho} + m_{\text{eff}}^2 \rho^2 - n^2 \right] R_n(\rho) = 0. \quad (5.266)$$

Defining $w = m_{\text{eff}}^2 \rho^2$, the general solution of the above equation is written as

$$R_n(x) = AJ_n(w) + BY_n(w), \quad (5.267)$$

where $J_n(w)$ is the Bessel function of the first kind, and $Y_n(w)$ is the Bessel function of the second kind. Using the fact that the large n Matsubara modes give the main contribution to the generalized entropy [292], we can write an asymptotic expansion for $J_n(w)$ and $Y_n(w)$. Since $m_{\text{eff}}^2(k, M)$ can be negative for some k , we write $s^{(2)}(n)$ as

$$s^{(2)}(n) = s_{k < k_c}^{(2)}(n) + s_{k \geq k_c}^{(2)}(n). \quad (5.268)$$

Denoting by $[m]$ the largest integer less than or equal to m , we define a critical k given by $k_c = \lfloor \frac{(2M)^\alpha m_0^2}{a^{\alpha-2}} \rfloor$. Using $\beta = 8\pi M$, we have

$$s_{k < k_c}^{(2)}(n) = 8\pi \left(M - M^2 \frac{\partial}{\partial M} \right) \sum_{k=1}^{k_c-1} \frac{c'_k}{\text{Vol}_d(\Omega)} [\det(-\Delta_R + m_0^2)]^{\frac{-k}{2}} \left[\frac{\det(-\Delta_R + m_0^2)}{\det(-\Delta_R + m_{\text{eff}}^2)} \right]^{\frac{1}{2}}, \quad (5.269)$$

and

$$s_{k \geq k_c}^{(2)}(n) = 8\pi \left(M - M^2 \frac{\partial}{\partial M} \right) \sum_{k=k_c}^{\infty} \frac{c'_k}{\text{Vol}_d(\Omega)} [\det(-\Delta_R + m_0^2)]^{\frac{-k}{2}} \left[\frac{\det(-\Delta_R + m_0^2)}{\det(-\Delta_R + m_{\text{eff}}'^2)} \right]^{\frac{1}{2}}, \quad (5.270)$$

where $m_{\text{eff}}'^2 = -2m_{\text{eff}}^2$ is the shifted effective mass.

The spectrum of the Schrödinger operator is unknown. Therefore, we use an alternative procedure to calculate the above expression. It can be shown that the derivative of the spectral zeta function can be expressed in terms of the eigenfunctions as follows:

$$-\frac{d}{ds}\zeta(s)\Big|_{s=0} = \ln \left[\frac{R(0)}{R(-\infty)} \right], \quad (5.271)$$

where R denotes the respective eigenfunctions. This is known as the Gel'fand-Yaglom method, which involves manipulating the eigenfunctions instead of the eigenvalues. Using this procedure, it is possible to evaluate the generalized entropy density. We can see that an eigenfunction that is repeating in both limits will cancel out. This justifies the fact that we have disregarded the angular Laplace-Beltrami in Eq. (5.261). Since the eigenfunctions of such an operator are spherical harmonics, they are ρ -independent. For $\alpha = 2$, we obtain the following expression for the first contribution of Eq. 5.268:

$$s_{k < k_c}^{(2)}(n) = \sum_{k=1}^{k_c-1} \frac{c'_k}{\text{Vol}_d} \left[\frac{2\pi kn}{M m_{\text{eff}}^2} + 8\pi M \right]. \quad (5.272)$$

A similar result is obtained for the second contribution of Eq. 5.268:

$$s_{k \geq k_c}^{(2)}(n) = \sum_{k=k_c}^{\infty} \frac{c'_k}{\text{Vol}_d} \left[\frac{2\pi kn}{M m_{\text{eff}}'^2} + 8\pi M \right] \left(\frac{m_0}{m_{\text{eff}}'} \right)^n. \quad (5.273)$$

The generalized second law was introduced to ensure that the total entropy of the system also increases ($\Delta S^{(1)} + \Delta S^{(2)} \geq 0$). Starting from Eq. 5.268, we have that $S^{(2)}(n) = S_{k < k_c}^{(2)}(n) + S_{k \geq k_c}^{(2)}(n)$. Thus, the expressions for both contributions to the entropy are as follows:

$$S_{k < k_c}^{(2)}(n) = \sum_{k=1}^{k_c-1} c_k \left[\frac{kn}{4M^2 m_{\text{eff}}^2} + 1 \right] \left(\frac{m_0}{m_{\text{eff}}} \right)^n, \quad (5.274)$$

for $k \leq k_c$, and

$$S_{k \geq k_c}^{(2)}(n) = \sum_{k=k_c}^{\infty} c_k \left[\frac{kn}{4M^2 m_{\text{eff}}'^2} + 1 \right] \left(\frac{m_0}{m_{\text{eff}}'} \right)^n, \quad (5.275)$$

for $k \geq k_c$. If we consider the two angular variables that were disregarded, the result is preserved, as shown by Eq. (5.271). Further corrections must be analyzed. To determine the numerical validity of our results, we evaluate our expressions

under different scenarios. In Fig. 5.7, we plot the contributions for the sum of Eq. (5.274) and Eq. (5.275) for large Matsubara modes, which represent the main contribution to the entropy of the matter fields, as a function of the dimensionless parameter Mm_0 . We observe the entropy reaching a steady value, which is a trend followed by all large Matsubara modes. Since we have redefined the mass of the black hole as $M = G^{(d)}M_0$, we can conclude that, for a fixed scalar-field mass, the matter contribution agrees with the generalized second law, and the stable value is driven by the black hole mass. The approach to a constant value for the entropy contribution from the matter fields could be interpreted as a potential saturation of information on the black hole horizon [293–296]. The stabilization of entropy for large Matsubara modes suggests that high-energy modes contribute less significantly to the overall entropy, which is consistent with the ultraviolet cutoff often encountered in different field theory schemes [297, 298].

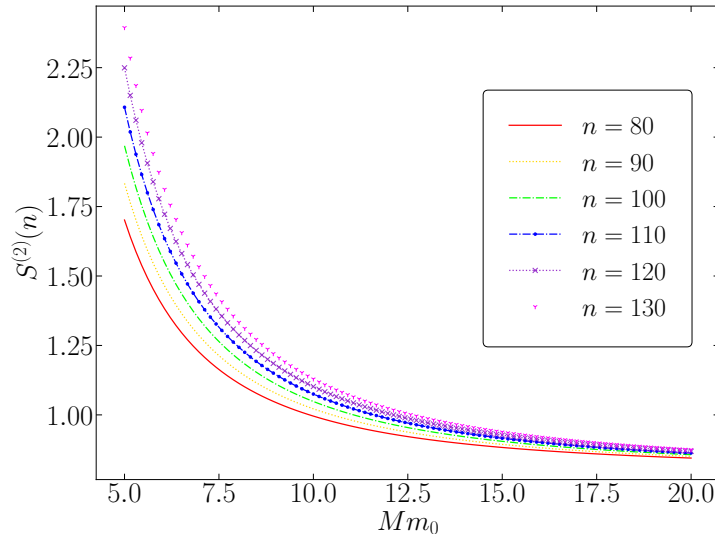


Figure 5.7: Behavior of the matter entropy as a function of the dimensionless parameter Mm_0 for different Matsubara modes n . We remark the redefinition of M as $M = G^{(d)}M_0$.

In Fig. 5.8, we examine the validity of the generalized second law of thermodynamics for different scalar fields, as expressed in Eq. (5.256), in black hole physics. In other words, we have added the Bekenstein-Hawking entropy to the matter fields' entropy described by Eq. (5.274) and Eq. (5.275), obtaining the expected results. The signature of black hole evaporation is the decrease of its mass, and we compare the total entropy of the system for different mass values. For a range of scalar-field mass values, our findings once again confirm the generalized second law, highlighting the robustness of our approach. This demonstrates

that the law holds not only for specific cases but across a broad spectrum of physical parameters. Furthermore, the interaction between the Bekenstein-Hawking entropy and the matter field entropy reveals the intricate balance between geometry and matter in determining the total entropy of the system [299, 300]. This balance is crucial for understanding the randomness of the degrees of freedom and the thermodynamic properties of black holes within a more comprehensive framework that incorporates both gravitational and quantum effects.

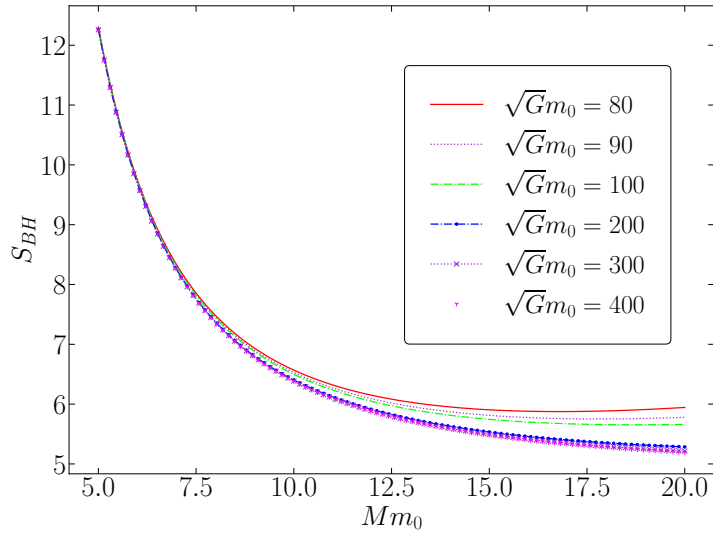


Figure 5.8: Behavior of the total black hole entropy S_{gen} as a function of the dimensionless parameter Mm_0 for different scaled field masses $\sqrt{G}m_0$. We remark the redefinition of M as $M = G^{(d)}M_0$.

This stabilization, influenced by the black hole mass, suggests a potential interpretation of information saturation. The addition of the Bekenstein-Hawking entropy to the matter field entropy confirms the generalized second law, where the model introduces a quenched disorder field.

Chapter 6

Conclusions

In this thesis, we have examined the fundamental principles and applications of quantum and statistical field theory. By exploring the mathematical structures underlying these theories, we have gained insight into how field-theoretic methods can be used to describe a wide range of physical phenomena.

Our discussion began with an overview of the mathematical foundations of the quantum field theory, highlighting its role in describing particle interactions and fundamental forces. We reviewed key concepts such as the Lagrangian formalism, path integrals, and Feynman diagrams, demonstrating how these tools enable precise calculations of scattering amplitudes and correlation functions.

We then turned our attention to statistical field theory, emphasizing its relevance in studying phase transitions, critical phenomena, and condensed matter systems. Using the partition function and correlation functions, we explored how statistical mechanics and quantum field theory are deeply interconnected, particularly through the renormalization group framework.

A significant portion of our study has been devoted to disordered systems and their impact on physical observables. Disorder plays a crucial role in various condensed matter systems, leading to intriguing phenomena such as Anderson localization, spin glass behavior, and quantum chaos. Traditional approaches such as replica symmetry breaking and supersymmetric techniques have been developed to address these challenges, but recent advancements in the distributional zeta function method offer a novel perspective.

The distributional zeta function method has proven to be a powerful analytical tool in extracting spectral properties of disordered operators. By analyzing the asymptotic properties of spectral densities, this method enables a deeper understanding of a wide range of phenomena and possesses a natural link with random matrix theory and applications. Its applications can be extended to fields such as topological physics, quantum chaos, and even aspects of quantum gravity, making it an essential tool in modern theoretical physics.

One of the key insights gained from our study is the power of field-theoretic methods in describing systems at different scales. The renormalization group, in particular, provides a systematic approach for understanding how physical theories change as one moves from microscopic to macroscopic scales. This idea has found applications in diverse areas, from condensed matter physics to high-energy particle physics and cosmology.

The study of disordered systems is also important in computational physics, where numerical methods such as Monte Carlo simulations and tensor network techniques are employed to investigate complex systems. The distributional zeta function method complements these numerical approaches by offering analytic insights into spectral properties and phase transitions.

Despite the significant progress made in the field, many open questions remain. The quest for a unified theory that incorporates gravity, the nature of dark matter, and the resolution of the hierarchy problem are among the pressing challenges in modern theoretical physics. Additionally, non-perturbative methods, such as lattice field theory, continue to be active areas of research, offering potential breakthroughs in our understanding of strongly interacting systems.

Future research directions in quantum and statistical field theory may involve further developments in computational techniques, new experimental insights, and the exploration of novel theoretical frameworks. The interplay between field theory and other disciplines, such as machine learning and complex systems, may also yield new perspectives and methodologies for tackling long-standing problems. Furthermore, extending the distributional zeta function method to broader classes of disordered systems and complex networks could unlock new possibilities in statistical physics and beyond.

In conclusion, the study of quantum and statistical field theory remains a vibrant and evolving field of research. The concepts and methods developed within these frameworks continue to shape our understanding of the fundamental forces of nature and the emergent properties of complex systems. As new discoveries unfold, field theory will undoubtedly remain a cornerstone of theoretical physics.

Appendices

Appendix A

Rudiments of Functional Analysis

Before starting with a bunch of definitions, lemmas, theorems, etc., it seems nice to mention that a reader with some previous knowledge in real analysis and set theory will be greatly favored in understanding this section. On top of that, we do not believe that such previous topics are strictly necessary to understand the underlying ideas that we are going to present here.

Of course, there is not enough room to cover the entire field of mathematics encapsulated by functional analysis. Because of that, we opt to present the main topics that we believe are most useful for our objectives. This means that we are going to present some of the most basic and general results of functional analysis. The topics that we would like to cover here are basic aspects of measure theory, Hilbert and Banach spaces, the spectral theorem for bounded operators, and also some aspects of the theory of generalized functions.

A.1 Measure Theory

While simple, measure theory is of fundamental importance for mathematics and physics. Such a construction provides us with useful generalizations and a robust framework for basic concepts that are used on a daily basis.

A self-contained presentation of measure theory would need to be presented with some developments of set theory. However, set theory is intrinsically entangled with the foundations of mathematics, and thinking too much about such a topic can be both entertaining and nerve-racking. To avoid the hard discussion, we just present some definitions, basic properties, and results of set theory. The basis of our analysis follows Refs. [301, 302].

After establishing what a set is, we can briefly discuss functions and metric spaces. After that, we are allowed to study measures, which are just a type of set function. Following this, we will define the integral in measure theory and some

special kinds of measures. It is important to note that our presentation is far from complete; we are focusing on the development of ideas that are of interest to us. A far more complete presentation can be found in the aforementioned bibliography.

Our main objective in this section is to construct the well-known Riemann integral and its generalization, while also presenting some fundamental results in measure theory.

Generically, we can say that a set E is a collection of elements x that satisfies some property P . Such a construction will be denoted by

$$E = \{x \mid x \text{ has property } P\}. \quad (\text{A.1})$$

If E has a small countable number of elements, we may write $E = \{x_1, x_2, x_3, x_4\}$. If a set contains a single element, e.g., $E = \{x\}$, we may denote the set E simply as $\{x\}$.

The set that contains no elements is called the *empty set* and can be defined as

$$\emptyset = \{x \mid x \neq x\}. \quad (\text{A.2})$$

Any affirmation about the empty set is both true and false at the same time. By these properties, $\emptyset$ belongs to any other set.

We use the double bar notation for the most usual sets, that is:

- $\mathbb{N}$ = set of natural numbers;
- $\mathbb{Z}$ = set of integer numbers;
- $\mathbb{R}$ = set of real numbers;
- $\mathbb{C}$ = set of complex numbers.

It is possible to define sets of sets, which we call *classes*, and also sets of classes, called *collections*. A set which is contained by another set is called a *subset*, and is usually denoted by $A \subset E$, where one reads “ A is a subset of E ” or “ E contains A ”. Two sets are equal if and only if $A \subset E$ **and** $E \subset A$. In such a situation, we may write $A = E$.

If we have at least two sets E_1, E_2 , we can define operations between sets. If we wish to pick elements that belong to E_1 **or** E_2 , we have a *union* of the sets E_1 and E_2 , such an operation is denoted by $E_1 \cup E_2$. Now, an operation that picks elements that belong to E_1 **and** E_2 is called *intersection* and denoted by $E_1 \cap E_2$. The elements of a set E that do not belong to E_1 are called the *complement* of E_1 , and are denoted by $(E - E_1)$. To represent the set of elements that are in E_1 but not in E_2 , we use $E_1 \setminus E_2$. The set of elements that are in one of E_1 or E_2 , but not in both, is given by the *symmetric difference* and denoted by $E_1 \Delta E_2 = (E_1 \setminus E_2) \cup (E_2 \setminus E_1)$.

The previous operations can be proved to satisfy the following known algebraic properties:

Proposition A.1. Take A , B , and C as any sets, then

- (i) $A \cup B = B \cup A$, $A \cap B = B \cap A$;
- (ii) $(A \cup B) \cup C = A \cup (B \cup C)$, $(A \cap B) \cap C = A \cap (B \cap C)$;
- (iii) $A \cap (B \cup C) = (A \cap B) \cup (A \cap C)$,
 $A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$;
- (iv) $A \cup \emptyset = A$, $A \cap \emptyset = \emptyset$;
- (v) if $A \subset X$, then $A \cap X = A$, $A \cup X = X$;
- (vi) $A \cup B = (A \Delta B) \Delta (A \cap B)$, $A \setminus B = A \Delta (A \cap B)$;

Denote every subset of a given class $\mathcal{E}$ by E . The union of the class, $\bigcup\{E \mid E \in \mathcal{E}\}$, is the set of elements that are in at least one set $E \in \mathcal{E}$. Its intersection, $\bigcap\{E \mid E \in \mathcal{E}\}$, is the set of elements that are in every set $E \in \mathcal{E}$. If we can index the class $\mathcal{E}$ such that $\mathcal{E} = \{E_\alpha \mid \alpha \in I\}$, we can use the notations $\bigcup_{\alpha \in I} E_\alpha$, $\bigcap_{\alpha \in I} E_\alpha$.

Now we can prove two useful results

Lemma A.2. (de Morgan's law) Suppose E_α , $\alpha \in I$ is a class of subsets of X , and E_1 is one set of the class, then

- (i) $\bigcap_{\alpha \in I} E_\alpha \subset E_1 \subset \bigcup_{\alpha \in I} E_\alpha$;
- (ii) $X - \bigcup_{\alpha \in I} E_\alpha = \bigcap_{\alpha \in I} (X - E_\alpha)$;
- (iii) $X - \bigcap_{\alpha \in I} E_\alpha = \bigcup_{\alpha \in I} (X - E_\alpha)$.

Proof. (i) follows from the definitions of union and intersection.

For (ii), take $x \in X - \bigcup_{\alpha \in I} E_\alpha$, then $x \in X$, $x \notin \bigcup_{\alpha \in I} E_\alpha \Rightarrow x \notin E_\alpha, \alpha \in I$. But, $x \in X - E_\alpha, \alpha \in I \Rightarrow x \in \bigcap_{\alpha \in I} (X - E_\alpha)$.

If $x \in \bigcap_{\alpha \in I} (X - E_\alpha)$, then, for all $\alpha \in I$, $x \in X$ and $x \notin E_\alpha$, so $x \notin \bigcup_{\alpha \in I} E_\alpha$. So, $x \in X - \bigcup_{\alpha \in I} E_\alpha$.

(iii) follows similarly to (ii). ■

Two sets that have no common elements are said *disjoint*, and naturally, if $A \cap B = \emptyset$ then A and B are disjoint. We can form a disjoint class by picking the set of disjoint sets, and the unions of disjoint classes can be called a *disjoint union*.

Lemma A.3. Given a finite or enumerable union of sets $\bigcup_{i=1}^p E_i$ (p can be infinite), there are subsets $F_i \subset E_i$ such that the sets F_i are disjoint and $\bigcup_{i=1}^p E_i = \bigcup_{i=1}^p F_i$.

Proof. We prove for p infinite; for p finite, only obvious changes are needed.

Assume $C = \bigcap_{i=1}^p E_i$ and define $F_1 = E_1$, and $F_n = E_n \setminus \bigcup_{i=1}^{n-1} E_i$ where $n = 1, 2, 3, \dots$. By our definition, we always have that $F_n \subset E_n$, and, if $i < j$, $F_i \cap E_j = \emptyset$. So, $F_i \cap F_j = \emptyset$.

Take $x \in C$ and n as the smallest integer such that $x \in E_n$, then $x \notin E_i$ if $i < n$. Thus, $x \in F_n$, and $x \in \bigcup_{i=1}^{\infty} F_i \Rightarrow C \subset \bigcup_{i=1}^{\infty} F_i$.

Now assume $x \in F_i$, then $x \in E_i$ and $x \notin E_{i-1}$. Thus, $x \in \bigcup_{i=1}^{\infty} E_i$ and $x \in \bigcup_{i=1}^{\infty} F_i \Rightarrow \bigcup_{i=1}^{\infty} F_i \subset C$. So, $C = \bigcup_{i=1}^{\infty} F_i$. ■

This last lemma allows us to say that any class that is enumerable can be represented as a disjoint union of sets.

To finish our discussion of set theory, let us define the convergence of a sequence of sets. Take a sequence of sets $\{E_i\} = E_1, E_2, \dots$, and define

$$\limsup E_i = \bigcap_{i=1}^{\infty} \left(\bigcup_{n=i}^{\infty} E_n \right), \quad \liminf E_i = \bigcup_{i=1}^{\infty} \left(\bigcap_{n=i}^{\infty} E_n \right), \quad (\text{A.3})$$

if $\limsup E_i = \liminf E_i = E$, it is said that the sequence converges to the set E . The interpretation of such objects for any sequence $\{E_i\}$ is the following: $\limsup E_i$ is the set of those elements which are in E_i for infinitely many E_i , and $\liminf E_i$ is the set of those elements which are in all but a finite number of sets E_i . If, for each n positive integer, $E_n \subset E_{n+1}$, the sequence is said *increasing*, if $E_n \supset E_{n+1}$, the sequence is said *decreasing*. Sequences that satisfy any of the previous cases are called *monotone* sequences.

Monotone sequences always converge. Take $\{E_i\}$ increasing, then $\bigcup_{i=n}^{\infty} E_i = \bigcup_{i=i}^{\infty} E_i$ and $\bigcap_{i=n}^{\infty} E_i = E_n$ for all n . So, $\limsup E_i = \liminf E_i = \bigcup_{i=1}^{\infty} E_i$. Now take $\{E_i\}$ decreasing, then $\bigcap_{i=n}^{\infty} E_i = \bigcap_{i=i}^{\infty} E_i$ and $\bigcup_{i=n}^{\infty} E_i = E_n$ for all n . Thus, $\limsup E_i = \liminf E_i = \bigcap_{i=1}^{\infty} E_i$.

Another important thing to understand in measure theory is to be able to define functions between elements of sets. Take two sets A and B , a mapping $f : A \rightarrow B$ establishes a relation between an element of A and an element of B . In such a map, A is called the *domain* of f , sometimes denoted as $D(f)$. The subset of B consisting of $f(x)$ for $x \in A$ is called the *range* of f , and is sometimes denoted by $\text{Ran}(f)$ or $f(A)$. If $f(A) = B$, f is a function from A *onto* B . One can also define the function $f^{-1} : \mathcal{B} \rightarrow \mathcal{A}$, where $\mathcal{A}$ and $\mathcal{B}$ are the classes of subsets of A and B . This function is defined as $f^{-1}(F) = \{x \in A \mid f(x) \in F\}$, for each $F \subset B$. $f(F)$ is called the *inverse image* of F under f . If $y \in B - f(A)$, then

$f^{-1}(\{y\}) = \emptyset$. If $f : A \rightarrow B$ is one-to-one, $y \in f(A)$, then $f^{-1}(\{y\})$ is a one-point set of A . Only in this last situation can we consider $f^{-1} : f(A) \rightarrow A$.

Let us assume that $f : A \rightarrow B$ uniquely determines an element of B for each $x \in A$. So, if $x_1, x_2 \in A$ and $x_1 \neq x_2 \Rightarrow f(x_1) \neq f(x_2)$, f is said to be a *one-to-one* function. The *inverse* function exists only if $f^{-1} : A \rightarrow B$ is onto and one-to-one, so $f^{-1} : B \rightarrow A$ is the inverse function such that $f^{-1}(y) = x$ if and only if $y = f(x)$.

At this point, the most important set function that we can define is the *indicator* (or characteristic) function. Take a subset $A \subset X$, then $\chi_A : X \rightarrow \mathbb{R}$ is defined as

$$\chi_A(x) = \begin{cases} 1, & \text{if } x \in A \\ 0, & \text{if } x \notin A. \end{cases} \quad (\text{A.4})$$

The correspondence between subsets of X (not elements) and the indicator function is one-to-one.

Before going further into functions, let us give our abstract sets more structure.

Definition A.4. Take a non-empty set X with the function $\rho : X \times X \rightarrow \mathbb{R}$. X is said to be a **metric space** if it satisfies:

- (i) $\rho(x, y) = \rho(y, x) \geq 0, \quad \forall x, y \in X;$
- (ii) $\rho(x, y) = 0$, if and only if $x = y$;
- (iii) $\rho(x, y) \leq \rho(x, z) + \rho(z, y), \quad \forall x, y, z \in X.$

The function ρ agrees with our notion of distance in many spaces. On a metric space (X, ρ) , the open sphere of center x and radius $r > 0$ is a set given by $S(x, r) = \{y \mid \rho(x, y) < r\}$. We say that a set E on a metric space (X, ρ) is **open** if, for each $x \in E$, there is an $r > 0$ such that $S(x, r) \subset E$. From this definition, it follows that open spheres are open sets¹. With the definition of open sets, we can also define the closed sets. A set $E \subset X$ is said to be **closed** if $(X - E)$ is open. We can also define the closed sphere of center $x \in E \subset X$ and radius $r > 0$: $\bar{S}(x, r) = \{y \mid \rho(x, y) \leq r\}$, which is a closed set.

Definition A.5. On a metric space (X, ρ) , a sequence $\{x_n\}$ is said to be a **Cauchy sequence** if given $\varepsilon > 0$, there is an integer N such that

$$n, m \geq N \Rightarrow \rho(x_n, x_m) < \varepsilon \quad (\text{A.5})$$

¹ $y \in S(x, r)$, then $\rho(x, y) = r_1 < r$. So, $0 < r_2 \leq r - r_1$ such that $S(y, r_2) \subset S(x, r)$.

On a metric space (X, ρ) , any sequence $\{x_n\}$ that converges to $x \in X$ is a Cauchy sequence. A metric space is said to be **complete** if for each Cauchy sequence $\{x_n\}$ in X , there is a point $x \in X$ such that $x = \lim x_n$.

With the idea of open sets, we can construct the class of all open sets of X , denoted such a class as $\mathcal{G}$, then we have that

Theorem A.6. In a metric space X , the class $\mathcal{G}$ of open sets satisfies

- (i) $\emptyset, X \in \mathcal{G}$;
- (ii) $A_1, A_2, \dots, A_n \in \mathcal{G}$, then $\bigcap_{i=1}^n A_i \in \mathcal{G}$;
- (iii) $A_\alpha \in \mathcal{G}$ for $\alpha \in I$, then $\bigcup_{\alpha \in I} A_\alpha \in \mathcal{G}$.

Proof. For (i), we first notice that any statement about $\emptyset$ is true, then $\emptyset \in \mathcal{G}$. Note that $S(x, r) \subset X$ for any $x \in X$, so $X \in \mathcal{G}$.

(ii) Take $x \in \bigcap_{i=1}^n A_i$, so $x \in A_i$, $i = 1, 2, \dots, n$. By construction, each A_i is open, thus there exists $0 < r_i \in \mathbb{R}$ such that $S(x, r_i) \subset A_i$. Fix $r = \min_{1 \leq i \leq n} r_i$, then $S(x, r) \subset \bigcap_{i=1}^n A_i$.

(iii) Let $x \in \bigcup_{\alpha \in I} A_\alpha$, so, for some $\alpha \in I$, $x \in A_\alpha$. A_α is open, so there is $r_i > 0$ such that $S(x, r) \subset A_\alpha \subset \bigcup_{\alpha \in I} A_\alpha \subset \mathcal{G}$. ■

Worth noting that (ii) cannot be extended for infinite intersections². We could start from the class $\mathcal{G}$ and then define it as the open sets. The set X and the class $\mathcal{G}$ are said to form a **topological space**. The *topology* of a space can vary with the choices of the open sets that form $\mathcal{G}$.

Definition A.7. In a topological space $(X, \mathcal{G})$, any open set containing $x \in X$ is said to be a **neighbourhood** of x . If $E \subset X$, a point $x \in X$ is said to be a **limit point** or **point of accumulation** of E if every neighbourhood of x contains a point of E other than x .

The *closure* of a set $E \subset X$, denoted by $\bar{E}$, is the intersection of all closed sets that contain E . $\bar{E}$ is a closed set, and it contains all limit points of E .

Definition A.8. A set S in a metric space M is called **nowhere dense** if $\bar{S}$ has an empty interior³.

Theorem A.9. (Baire category theorem) A complete metric space is never the union of a countable of nowhere dense sets.

²Take $\mathbb{R}$ and the open intervals $(0, 1 + \frac{1}{n})$. $\bigcap_{n=1}^{\infty} (0, 1 + \frac{1}{n}) = (0, 1]$, which contains no open sphere with center at 1.

³ $\bar{S}$ contains no open set besides the empty set.

Proof. Take M a complete metric space such that $M = \bigcup_{n=1}^{\infty} A_n$, where each A_n is nowhere dense. So, there is some $x_1 \notin \overline{A_1}$. Construct the open sphere at centre at x_1 and radius less than the unity, r_1 , $S(x_1, r_1)$. By definition we have that $S(x_1, r_1) \cap A_1 = \emptyset$. A_2 is also nowhere dense, so there is $x_2 \notin \overline{A_2}$ and $x_2 \in B_1 \setminus \overline{A_2}$. Construct the open sphere $S(x_2, r_2)$, with $r_2 < 1/2$, so $\overline{S(x_2, r_2)} \subset S(x_1, r_1)$ and $S(x_2, r_2) \cap A_2 = \emptyset$. Proceeding n steps, we have $x_n \notin \overline{A_n}$, $x_n \in B_{n-1} \setminus \overline{A_n}$. Construct the open sphere $S(x_n, r_n)$, with $r_n < 2^{-n}$, so $\overline{S(x_n, r_n)} \subset S(x_{n-1}, r_{n-1})$ and $S(x_n, r_n) \cap A_n = \emptyset$.

The previous construction says that $\{x_n\}$ is a Cauchy sequence since for $m, n > N$ we have $x_n, x_m \in S(x_N, r_N)$, such that

$$\rho(x_n, x_m) \leq 2^{1-N} + 2^{1-N} = 2^{2-2N} \rightarrow 0, \quad \text{as } N \rightarrow \infty. \quad (\text{A.6})$$

Denote $x = \lim_{n \rightarrow \infty} x_n$, such that $x_n \in B_n$, $n \geq N$. So $x \in \overline{B_N} \subset B_{N-1}$. But $x \notin A_{N-1}$ for any N . This contradicts $M = \bigcup_{n=1}^{\infty} A_n$. So some A_n is not nowhere dense. ■

Back to functions, we can say that, for given two metric spaces (X, ρ_X) and (Y, ρ_Y) , a function $f : X \rightarrow Y$ is said to be *continuous* at $x = a$ if, given $\varepsilon > 0$, there is a $\delta > 0$ such that

$$\rho_X(x, a) < \delta \Rightarrow \rho_Y(f(x), f(a)) < \varepsilon. \quad (\text{A.7})$$

We say that f is continuous on $E \subset X$ if f is continuous on each point of E . Saying that $f : X \rightarrow Y$ is continuous means that f is continuous at each point of X .

Lemma A.10. If (X, ρ_X) and (Y, ρ_Y) are metric spaces, a function $f : X \rightarrow Y$ is continuous if and only if $f^{-1}(G)$ is an open set in X for each open set G in Y .

Proof. Suppose f is continuous and $G \in Y$ is open. If $f^{-1}(G) = \emptyset$, it is open. Now let $a \in f^{-1}(G)$, $f(a) \in G$, then, there is a $\varepsilon > 0$ for which the sphere $S(f(a), \varepsilon) \subset G$. Then we can find $\delta > 0$ such that

$$\rho_X(x, a) < \delta \Rightarrow f(x) \in S(f(a), \varepsilon) \subset G. \quad (\text{A.8})$$

So $S(a, \delta) \subset f^{-1}(G)$, that is, $f^{-1}(G)$ is open.

Now take f at the point $a \in X$. For each $\varepsilon > 0$, $S(f(a), \varepsilon) = H$ is an open set in Y . If $f^{-1}(H)$ is open, we can find $\delta > 0$ for which $S(a, \delta) \subset f^{-1}(H)$, then

$$\rho_X(x, a) < \delta \Rightarrow \rho_Y(f(x), f(a)) < \varepsilon, \quad (\text{A.9})$$

so f is continuous. ■

Definition A.11. A class $\mathcal{X}$ of subsets of a set X is said to be a **σ -algebra** (or **σ -field**) if it satisfies

- (i) $\emptyset, X$ belong to $\mathcal{X}$;
- (ii) If A belongs to $\mathcal{X}$, then the complement $X - A$ belongs to $\mathcal{X}$;
- (iii) If $\{A_n\}$ is a sequence of sets in $\mathcal{X}$, then the union $\bigcup_{n=1}^{\infty} A_n$ belongs to $\mathcal{X}$.

In a topological space X , the σ -algebra $\mathcal{B}^n$ generated by the open sets is called the class of *Borel sets*.

Lemma A.12. The class $\mathcal{P}^n$ of half-open intervals in $\mathbb{R}^n$ generates the σ -algebra $\mathcal{B}^n$ of Borel sets in $\mathbb{R}^n$.

Proof. Denote by $\mathcal{F}^n$ the σ -algebra generated by $\mathcal{P}^n$. Any set in $\mathcal{P}^n$ is given by

$$\mathcal{P}^n : \{(x_1, x_2, \dots, x_n) \mid a_i < x_i \leq b_i; i = 1, 2, \dots, n\}, \quad (\text{A.10})$$

such sets can be obtained by a countable intersection

$$\mathcal{P}^n : \bigcap_{k=1}^{\infty} \left\{ (x_1, x_2, \dots, x_n) \mid a_i < x_i < b_i + \frac{1}{k}; i = 1, 2, \dots, n \right\} = \bigcap_{k=1}^{\infty} R_k^n, \quad (\text{A.11})$$

but each R_k^n is an open rectangle, that is, $R_k^n \in \mathcal{B}^n$. So $\mathcal{P}^n \subset \mathcal{B}^n \Rightarrow \mathcal{F}^n \subset \mathcal{B}^n$.

Any open set $G \in \mathcal{B}^n$ is the union of rectangles of $\mathcal{P}^n$ with boundaries at a_i, b_i rational numbers, that is $a_i, b_i \in \mathbb{Q}$, but by lemma A.3, $\mathbb{Q} = \bigcup_{n=1}^{\infty} E_n$, where E_n is the set of real numbers of the form p/n , with $p \in \mathbb{Z}$. So E_n is countable, so $\mathbb{Q}$ is also countable. Then there are only a countable number of rectangles. Thus G is a countable union of sets in $\mathcal{P}^n$. It follows that $\mathcal{B}^n \subset \mathcal{P}^n \Rightarrow \mathcal{B}^n \subset \mathcal{F}^n$.

Thus $\mathcal{B}^n = \mathcal{F}^n$ ■

A set with the corresponding σ -algebra, $(X, \mathcal{X})$, is called a *measurable space*. So, the real line, $\mathbb{R}$, with the Borel sets, $(\mathbb{R}, \mathcal{B})$, is a measurable space.

With the previous basic concepts developed, we now can define what is measurability of a function.

Definition A.13. A function $f : X \rightarrow \mathbb{R}$ is said to be **$\mathcal{X}$ -measurable** (or **measurable**) if for every real number α , the set

$$\{x \in X \mid f(x) > \alpha\} \quad (\text{A.12})$$

belongs to $\mathcal{X}$.

Lemma A.14. Let f and g be measurable real-valued functions and let $c, a \in \mathbb{R}$. Then the functions

$$cf, f^2, f + g, fg, |f|, \quad (\text{A.13})$$

are also measurable.

Proof. If $c = 0$, $cf = 0$ then the statement follows trivially. Take $c > 0$, then

$$\{x \in X \mid cf(x) > \alpha\} = \{x \in X \mid f(x) > \alpha/c\}. \quad (\text{A.14})$$

If $c < 0$, it follows similarly.

If $\alpha > 0$, then $\{x \in X \mid (f(x))^2 > \alpha\} = X$; if $\alpha < 0$, then

$$\{x \in X \mid (f(x))^2 > \alpha\} = \{x \in X \mid f(x) > \sqrt{\alpha}\} \cup \{x \in X \mid f(x) < -\sqrt{\alpha}\} \quad (\text{A.15})$$

Take r a rational number and define $S_r = \{x \in X \mid f(x) > r\} \cup \{x \in X \mid g(x) > \alpha - r\} \in X$. So,

$$\{x \in X \mid (f + g)(x) > \alpha\} = \bigcup S_r \in X. \quad (\text{A.16})$$

Write $fg = \frac{1}{4} [(f + g)^2 - (f - g)^2]$, so fg is measurable.

If $\alpha < 0$, then $\{x \in X \mid |f(x)| > \alpha\} = X$. If $\alpha > 0$, then

$$\{x \in X \mid |f(x)| > \alpha\} = \{x \in X \mid f(x) > \alpha\} \cup \{x \in X \mid f(x) < -\alpha\}. \quad (\text{A.17})$$

■

For any function $f : X \rightarrow \mathbb{R}$, we can define

$$f^+(x) = \sup\{f(x), 0\}, \quad f^-(x) = \sup\{-f(x), 0\}. \quad (\text{A.18})$$

Where $f^+(x)$ is called *positive part* of f and $f^-(x)$ is the *negative part* of f . Of course we have that

$$\begin{aligned} f &= f^+ - f^-, & |f| &= f^+ + f^- \\ f^+ &= \frac{1}{2}(|f| + f), & f^- &= \frac{1}{2}(|f| - f). \end{aligned} \quad (\text{A.19})$$

From the last lemma, one concludes that f is measurable if and only if f^+ and f^- are measurable.

The previous discussion and results can be easily translated to complex-valued functions. If f is a complex values function we can write it as $f = f_1 + if_2$, so f is measurable if and only if its real and imaginary parts are measurable.

After such a lengthy discussion, we have some familiarity with the main structures that we need to push further our construction. Now we can sit tight and define what is a measure.

Definition A.15. A **measure** is an extended real-valued function⁴ μ defined on a σ -algebra $\mathcal{X}$ of subsets of X such that

- (i) $\mu(\emptyset) = 0$;
- (ii) $\mu(E) \geq 0$ for all $E \in \mathcal{X}$;
- (iii) μ is *countably additive*, that is, if $\{E_n\}$ is a disjoint sequence of sets in $\mathcal{X}$, then

$$\mu\left(\bigcup_{n=1}^{\infty} E_n\right) = \sum_{n=1}^{\infty} \mu(E_n). \quad (\text{A.20})$$

Note that μ may be $+\infty$, this means that for some set E_n on the Eq. (A.20) we have $\mu(E_n) = \infty$, or the series of positive numbers diverges. A set X , a σ -algebra $\mathcal{X}$, and a measure μ form a *measure space*, denoted by $(X, \mathcal{X}, \mu)$, or simply $\langle X, \mu \rangle$.

Theorem A.16. Suppose $\mu : \mathcal{X} \rightarrow \mathbb{R}^*$ is a measure defined on the σ -algebra $\mathcal{X}$ and $E, F \in \mathcal{X}$. Then

- (i) if $F \subset E$ and $\mu(F)$ is finite

$$\mu(E - F) = \mu(E) - \mu(F); \quad (\text{A.21})$$

- (ii) if $F \subset E$ and $\mu(F)$ is infinite

$$\mu(E) = \mu(F); \quad (\text{A.22})$$

Proof. (i) $\mathcal{X}$ is a σ -algebra, so $E - F \in \mathcal{X}$, using the countably additivity of μ and the fact that $F \cap (E - F) = \emptyset$ we have that

$$\mu(E) = \mu(E - F) + \mu(F), \quad (\text{A.23})$$

we can subtract the *finite* real number $\mu(F)$ from both sides to obtain $\mu(E - F) = \mu(E) - \mu(F)$.

(ii) if $\mu(F) = \infty$, the expression $\mu(E - F) = \mu(E) - \mu(F)$ has meaning only if $\mu(E - F) \neq -\infty$, so $\mu(E) = \infty$. ■

Like in the case of functions, we can define the continuity of measures.

⁴Extended real numbers are a compactification of real numbers adding the points $\{\pm\infty\}$, that is, $\mathbb{R}^* = \mathbb{R} \cup \{\pm\infty\}$. The operations of multiplication and sum with the symbols $\pm\infty$ follows the natural operations of reals. We adopt the convention that $0(\pm\infty) = 0$. Division by $\pm\infty$ is not allowed.

Definition A.17. Suppose $\mathcal{X}$ is a σ -algebra, and $\mu : \mathcal{X} \rightarrow \mathbb{R}^*$ is a measure. Then for all $E \in \mathcal{X}$ we say that

- (i) μ is **continuous from below** at E if

$$\lim_{n \rightarrow \infty} \mu(E_n) = \mu(E) \quad (\text{A.24})$$

for every monotone increasing sequence $\{E_n\}$ of sets in $\mathcal{X}$ which converges to E ;

- (ii) μ is **continuous from above** at E if $\lim_{n \rightarrow \infty} \mu(E_n) = \mu(E)$ is satisfied for any monotone decreasing sequence $\{E_n\}$ in $\mathcal{X}$ with limit E which is such that $\mu(E_n) < \infty$ for some n ;
- (iii) μ is **continuous** at E if it is continuous at E from below and from above (when $E = \emptyset$ the first requirement is trivially satisfied).

In the next theorem we show that our definition of measure (definition A.15) ensures the continuity of any measure.

Theorem A.18. Suppose $\mathcal{X}$ is a σ -algebra, and $\mu : \mathcal{X} \rightarrow \mathbb{R}^*$ is additive⁵ set function with $\mu(E) > -\infty$.

- (i) If μ is countably additive, then μ is continuous at E for all $E \in \mathcal{X}$;
- (ii) if μ is continuous from below at every set $E \in \mathcal{X}$, then μ is countably additive;
- (iii) if μ is finite and continuous from above at $\emptyset$, then μ is countably additive.

Proof. (i) Take $\mu(E_n) = \infty$ for some $n = N$, and assume that $\{E_n\}$ is monotone increasing. So, $\mu(E) = \infty$ and $\mu(E_n) = \infty$ for $n \geq N$. Then $\mu(E_n) \rightarrow \mu(E)$, as $n \rightarrow \infty$.

Now assume that $\mu(E_n) < \infty$ for all n and $\{E_n\}$ is monotone increasing to E . Then take the following disjoint decomposition of E

$$E = E_1 \bigcup_{n=1}^{\infty} (E_{n+1} \setminus E_n), \quad (\text{A.25})$$

⁵Additive means that, for $\{E_i\}$ a disjoint sequence, $\mu(\bigcup_{i=1}^n E_i) = \sum_{i=1}^n \mu(E_i)$, for n finite.

by hypothesis, μ is countably additive, so

$$\begin{aligned}\mu(E) &= \mu(E_1) + \sum_{n=1}^{\infty} \mu(E_{n+1} - E_n) \\ &= \mu(E_1) + \lim_{N \rightarrow \infty} \sum_{n=1}^N \mu(E_{n+1} - E_n) \\ &= \lim_{N \rightarrow \infty} \mu(E_N),\end{aligned}\tag{A.26}$$

so μ is continuous from below at E .

Now take $\{E_n\}$ as a monotone decreasing sequence that converges to E and assume that $\mu(E_N) < \infty$. Define $F_n = E_N - E_n$, such that $n \geq N$. By (ii) of theorem A.16, we have that $\mu(F_n) < \infty$ and the sequence $\{F_n\}$ is monotone increasing to $E_N - E$, so

$$\text{As } n \rightarrow \infty, \quad \mu(F_n) \rightarrow \mu(E_N - E) = \mu(E_N) - \mu(E).\tag{A.27}$$

On the other hand, $\mu(F_n) = \mu(E_N) - \mu(E_n)$, so $\mu(E_n) \rightarrow \mu(E)$ as $n \rightarrow \infty$, since $\mu(E_N)$ is finite. Then, μ is continuous from above at E . Thus, μ is continuous at E .

To prove (ii), we take $E \in \mathcal{X}$, and $E_i \in \mathcal{X}$, ($i = 1, 2, \dots$) such that $E = \bigcup_{i=1}^{\infty} E_i$ and E_i are disjoint. Define $F_n = \bigcup_{i=1}^n E_i$, so $\{F_n\}$ is an increasing sequence which converges to E .

By hypothesis, μ is additive and continuous from below at E , so

$$\begin{aligned}\sum_{i=1}^n \mu(E_i) &= \mu(F_n) \rightarrow \mu(E), \quad \text{as } n \rightarrow \infty \\ \Rightarrow \mu(E) &= \sum_{i=1}^{\infty} \mu(E_i),\end{aligned}\tag{A.28}$$

so μ is countably additive and, by (i), μ is continuous at E .

(iii) follows from denoting $G_n = E - F_n \in \mathcal{X}$, such that $F_n = \bigcup_{i=1}^n E_i$ and noticing that $\{G_n\}$ is a decreasing sequence converging to $\emptyset$. So, once again, by hypothesis μ is continuous from above at $\emptyset$, we have that

$$\begin{aligned}\mu(E) &= \sum_{i=1}^n \mu(E_i) + \mu(G_n) \\ \mu(G_n) &\rightarrow 0 \quad \text{as } n \rightarrow \infty \\ \Rightarrow \mu(E) &= \sum_{i=1}^{\infty} \mu(E_i),\end{aligned}\tag{A.29}$$

thus μ is countably additive and, therefore, μ is continuous. ■

So we have proved our claim that the definition A.15 ensures the continuity of measures. In light of the last theorem, we could define measures as the non-negative continuous additive maps $\mu : \mathcal{X} \rightarrow \mathbb{R}^*$, where $\mathcal{X}$ is a σ -algebra.

Before we start the construction that leads us to the integral, let us make one more definition and prove one more useful theorem.

Definition A.19. A measure $\mu : \mathcal{X} \rightarrow \mathbb{R}^*$ is said to be **σ -finite** if, for each $E \in \mathcal{X}$, there is a unique sequence of sets $C_i \in \mathcal{X}$, ($i = 1, 2, \dots$) such that $E \subset \bigcup_{i=1}^{\infty} C_i$ and $\mu(C_i)$ is finite for all i .

One should notice that a measure that is σ -finite may be infinite. But a finite measure is always σ -finite.

Theorem A.20. (Hahn-Jordan Decomposition) Given a countably additive set function $\mu : \mathcal{X} \rightarrow \mathbb{R}^*$, on a σ -algebra $\mathcal{X}$, there are measures μ_+ and μ_- on $\mathcal{X}$ and subsets P, N in $\mathcal{X}$ such that $P \cup N = X$, $P \cap N = \emptyset$, and for each $E \in \mathcal{X}$,

$$\begin{aligned} \mu_+(E) &= \mu(E \cap P) \geq 0, & \mu_-(E) &= -\mu(E \cap N) \geq 0, \\ \mu(E) &= \mu_+(E) - \mu_-(E), \end{aligned} \quad (\text{A.30})$$

so that μ is the difference of two measures μ_+ and μ_- on $\mathcal{X}$. At least one of μ_+ or μ_- is finite, and if μ is finite or σ -finite, so are both μ_+ and μ_- .

Proof. First, we observe that μ does not satisfy (ii) of definition A.15. Without loss of generality, we can assume that $-\infty < \mu(E) \leq +\infty$ for all $E \in \mathcal{X}$.

We begin by proving that if $E \in \mathcal{X}$ and $\lambda(E) = \inf_{B \subset E, B \in \mathcal{X}} \mu(B)$, then $\lambda(X) \neq -\infty$.

If our last statement is false, there exists a $B_1 \in \mathcal{X}$ such that $\mu(B_1) < -1$. Then, at least one of $\lambda(B_1)$ or $\lambda(X - B_1)$ must be $-\infty$; by our definitions, we have that $\lambda(A \cup B) \geq \lambda(A) + \lambda(B)$, for disjoint sets A, B in $\mathcal{X}$. Define

$$A_1 = \begin{cases} B_1, & \text{if } \lambda(B_1) = -\infty, \\ X - B_1, & \text{if } \lambda(X - B_1) = -\infty. \end{cases} \quad (\text{A.31})$$

By induction, for each integer n , take $B_{n+1} \subset A_n$ such that $\mu(B_{n+1}) < -(n+1)$ and

$$A_{n+1} = \begin{cases} B_{n+1}, & \text{if } \lambda(B_{n+1}) = -\infty, \\ A_n - B_{n+1}, & \text{if } \lambda(A_n - B_{n+1}) = -\infty, \end{cases} \quad (\text{A.32})$$

so, $\lambda(A_{n+1}) = -\infty$. We have two possibilities: (i) infinitely many integers n , such that $A_n = A_{n-1} - B_n$, (ii) for some $n \geq n_0$, $A_n = B_n$.

If (i) holds, there is a subsequence of disjoint sets $\{B_{n_i}\}$, and by the countable additivity of μ

$$\mu\left(\bigcup_{i=1}^{\infty} B_{n_i}\right) = \sum_{i=1}^{\infty} \mu(B_{n_i}) \leq \sum_{i=1}^{\infty} -(n_i + 1) = -\infty, \quad (\text{A.33})$$

so $\mu(E) = -\infty$ for $E = \bigcup_{i=1}^{\infty} B_{n_i} \in \mathcal{X}$, which contradicts the assumption that $-\infty < \mu(E) \leq +\infty$.

If (ii) is true, take $E = \bigcap_{n=n_0}^{\infty} B_n \in \mathcal{X}$, where $\{B_n\}$ is a decreasing sequence of sets. Then

$$\mu(E) = \lim_{n \rightarrow \infty} \mu(B_n) = -\infty, \quad (\text{A.34})$$

which also contradicts our assumption.

We conclude that $\lambda(X) \neq -\infty$.

We have that $\mu(\emptyset) = 0$, and $\lambda(X) \leq 0$, so $\lambda = \lambda(X)$ is finite. Take a sequence of sets $\{C_n\}$ in $\mathcal{X}$ such that $\mu(C_n) \leq \lambda + 2^{-n}$. We note that, using (vi) of proposition A.1, we can write

$$C_n \cup C_{n+1} = (C_n \setminus (C_n \cap C_{n+1})) \cup (C_{n+1} \setminus (C_n \cap C_{n+1})) \cup (C_n \cap C_{n+1}), \quad (\text{A.35})$$

and notice that the right-hand side is a disjoint decomposition of the left-hand side. By the countable additivity of μ , we have that

$$\begin{aligned} \mu(C_n \cap C_{n+1}) &= \mu(C_n) + \mu(C_{n+1}) - \mu(C_n \cup C_{n+1}) \\ &< \lambda + 2^{-n} + \lambda + 2^{-(n+1)} - \lambda = \lambda + 2^{-n} + 2^{-(n+1)}. \end{aligned} \quad (\text{A.36})$$

The same argument can be repeated for the intersection of $(C_n \cap C_{n+1})$ with C_{n+2} , proceeding by induction, one gets that

$$\mu\left(\bigcap_{r=n}^p C_r\right) < \lambda + \sum_{r=n}^p 2^{-r} < \lambda + 2^{1-n}. \quad (\text{A.37})$$

Now define $D_n = \bigcap_{r=n}^{\infty} C_r$, so $D_n \in \mathcal{X}$. By (i) of theorem A.18, our set function μ is continuous, so $\mu(D_n) \leq \lambda - 2^{1-n}$, which shows that $\{D_n\}$ is a monotone increasing sequence in $\mathcal{X}$. Take $N = \lim_{n \rightarrow \infty} D_n = \liminf_{n \rightarrow \infty} C_n \in \mathcal{X}$, so one gets that $\mu(N) = \lambda = \inf_{N \subset X, N \in \mathcal{X}} \mu(N)$.

Now take $P = X - N$. If $E \in \mathcal{X}$ and $E \subset P$, we must have that $\mu(E) \geq 0$, otherwise $\mu(E \cup N) = \mu(E) + \mu(N) < \lambda$. If $E \in \mathcal{X}$ and $E \subset N$, then $\mu(E) \leq 0$, otherwise $\mu(N - E) = \mu(N) - \mu(E) < \lambda$. Then, for any $E \subset X$ and $E \in \mathcal{X}$, define

$$\mu_+(E) = \mu(E \cap P), \quad \mu_-(E) = \mu(E \cap N), \quad (\text{A.38})$$

so the theorem is satisfied. ■

The decomposition $\mu = \mu_+ - \mu_-$ is called the *Jordan decomposition* and is unique. The decomposition of X into P and N is sometimes called the *Hahn decomposition*, and it is not unique. From our proof of the theorem, we can deduce that

$$\mu_-(E) = - \inf_{B \subset E, B \in \mathcal{X}} \mu(B), \quad \mu_+(E) = \sup_{B \subset E, B \in \mathcal{X}} \mu(B). \quad (\text{A.39})$$

Now we are able to continue along the path that culminates in the integral.

Definition A.21. A real-valued function is called **simple** if it has only a finite number of values. If $E_1, E_2, \dots, E_n$ are disjoint subsets of X , a simple function can be represented as

$$f(x) = \sum_{i=1}^n a_i \chi_{E_i}, \quad (\text{A.40})$$

where $a_i \in \mathbb{R}$ for $i = 1, 2, \dots, n$ and χ_{E_i} is the indicator function.

Just applying the previous representation shows that the sum and product of simple functions are simple functions. Now, using our definition of measurability, definition A.13, we can show that

Lemma A.22. Any simple function is measurable.

Proof. Using that $f = \sum_{i=1}^n a_i \chi_{E_i}$, we have that $E_c = \{x \mid f(x) > c\}$. Such a set E_c is the finite union of sets $E_i \in \mathcal{X}$, with $a_i > c$, so $E_c \in \mathcal{X}$. By our definition, f is measurable. ■

Theorem A.23. Any non-negative measurable function $f : X \rightarrow \mathbb{R}^+$ is the limit of a monotone increasing sequence of non-negative simple functions.

Proof. For each positive integer s , define

$$\begin{aligned} Q_{p,s} &= \left\{ x \mid \frac{p-1}{2^s} \leq f(x) < \frac{p}{2^s} \right\}, \quad (p = 1, 2, \dots, 2^{2s}) \\ Q_{0,s} &= X - \bigcup_{p=1}^{2^{2s}} Q_{p,s} = \{x \mid f(x) \geq 2^s\}, \end{aligned} \quad (\text{A.41})$$

f is measurable, $Q_{p,s} \in \mathcal{X}$, and $Q_{p,s}$ ($p = 0, 1, 2, \dots, 2^{2s}$) are disjoint. The function

$$f_s(x) = \begin{cases} \frac{p-1}{2^s}, & \text{if } x \in Q_{p,s} \ (p = 1, 2, \dots, 2^{2s}) \\ 2^s, & \text{if } x \in Q_{0,s} \end{cases} \quad (\text{A.42})$$

is a simple function. It follows directly that $0 \leq f_s < f$. If $x \in Q_{p,s}$, then either $x \in Q_{2p-1,s+1}$ or $x \in Q_{2p,s+1}$, so that, either $f_s(x) = f_{s+1}(x)$ or $f_s(x) + \frac{2}{2^{s+1}} = f_{s+1}(x)$.

If $x \in Q_{0,s}$, then $f_s(x) = 2^s \leq f(x)$, so that, in either case $x \in Q_{0,s+1}$ or $x \in Q_{p,s+1}$ for some $p \geq 2^{2s+1} + 1$. In either case, we have that for each integer s , $f_{s+1}(x) \geq f_s(x) \ \forall x \in X$. Thus, the sequence $\{f_s\}$ of simple functions is monotone increasing.

Take x such that $f(x)$ is finite and $2^s > f(x)$, then

$$0 \leq f(x) - f_s(x) < 2^{-s} \quad (\text{A.43})$$

$$\Rightarrow f_s(x) \rightarrow f(x), \quad \text{as } s \rightarrow \infty. \quad (\text{A.44})$$

If $f(x) = \infty$, then $f_s(x) = 2^s \Rightarrow f_s(x) \rightarrow f(x)$ as $s \rightarrow \infty$. ■

It is important to notice that the previous theorem does not establish the uniqueness of the monotone increasing sequence of simple functions that converges to the non-negative measurable function. There are many sequences of simple functions that may converge to f .

In a topological space, a function that is measurable with respect to the Borel sets is said to be *Borel measurable*.

Lemma A.24. Any continuous function $f : X \rightarrow \mathbb{R}$ on a topological space X is Borel measurable.

Proof. f is continuous, so the inverse image of an open set in $\mathbb{R}$ is an open set in X . So $\{x \mid f(x) < c\}$ is open for all $c \in \mathbb{R}$, and by the definition of Borel sets, it belongs to $\mathcal{B}$. ■

Before we define what an integral is, a final definition that will prove its importance later.

Definition A.25. We say that a function $f(x)$ has the property P **almost everywhere** with respect to μ , if there is a set $E \in \mathcal{X}$ with $\mu(E) = 0$ such that $f(x)$ has the property for all $x \in X - E$. We then write

$$f(x) \text{ has property } P \text{ a.e. } (\mu). \quad (\text{A.45})$$

If it raises no ambiguity, we may omit (μ) .

Now we have all the ingredients to define the integral in measure theory.

Definition A.26. If f is a non-negative simple function, we define the **integral** of f with respect to μ to be the extended real number

$$\int f d\mu = \sum_{i=1}^n a_i \mu(E_i), \quad (\text{A.46})$$

where the sequence $\{E_i\}$ is disjoint.

The expected linearity of the integral follows from the definition of simple functions, definition A.21, and from the definition of a measure, definition A.15.

Definition A.27. If f is a non-negative measurable function, we define the **integral** of f with respect to μ to be the extended real number

$$\int f d\mu = \sup \int f_s d\mu, \quad (\text{A.47})$$

where f_s is a simple function and the supremum is taken over all simple functions that satisfy $0 \leq f_s(x) \leq f(x)$ for all $x \in X$. If f is non-negative and measurable

and $E \in \mathcal{X}$, then $f\chi_E$ is non-negative and measurable, and we define the **integral** of f over E with respect to μ to be the extended real number

$$\int_E f d\mu = \int f\chi_E d\mu. \quad (\text{A.48})$$

Again, the linearity of the integral follows from the definitions. We observe that if we have f, g two non-negative measurable functions such that $f \geq g$, we may write $f = g + (f - g)$, such that $(f - g) \geq 0$, so

$$\int f d\mu = \int g d\mu + \int (f - g) d\mu \geq \int g d\mu. \quad (\text{A.49})$$

So the integral is a monotone operation.

We say that a function is *integrable* if its integral is finite. Note that a function can be measurable but not integrable.

Now we give some theorems about the continuity of the integral.

Theorem A.28. (Monotone convergence theorem) Suppose $\{f_n\}$ is a monotone increasing sequence of non-negative measurable functions: $X \rightarrow \mathbb{R}^+$ and $f_n \rightarrow f$ for all $x \in X$, then

$$\int f d\mu = \lim_{n \rightarrow \infty} \int f_n d\mu, \quad (\text{A.50})$$

in the sense that, if f is integrable, the integrals $\int f_n d\mu$ converge to $\int f d\mu$; while if f is not integrable, either f_n is integrable for all n and $\int f_n d\mu \rightarrow +\infty$ as $n \rightarrow +\infty$, or there is an integer N such that f_N is not integrable so that $\int f_n d\mu = \infty$ for $n \geq N$.

Proof. For each $n = 1, 2, \dots$ choose an increasing sequence $\{f_{n,k}\}$ ($k = 1, 2, \dots$) of non-negative simple functions converging to f_n . Set $g_k = \max_{n \leq k} f_{n,k}$, such that $\{g_k\}$ is a non-decreasing sequence of non-negative simple functions, so $g = \lim_{k \rightarrow \infty} g_k$, and g is non-negative and measurable. But $f_{n,k} \leq g_k \leq f_k \leq f$, $n \leq k$, so $f_n \leq g \leq f$, as $k \rightarrow \infty \Rightarrow f = g$ as $n \rightarrow \infty$. Using the fact that the integral is monotone, Eq. (A.49), we may write that

$$\begin{aligned} \int f_{n,k} d\mu &\leq \int g_k d\mu \leq \int f_k d\mu, \quad n \leq k, \\ \int f_n d\mu &\leq \int g d\mu \leq \lim_{k \rightarrow \infty} \int f_k d\mu, \quad \text{as } k \rightarrow \infty, \text{ and } n \text{ fixed,} \\ \lim_{n \rightarrow \infty} \int f_n d\mu &\leq \int g d\mu \leq \lim_{k \rightarrow \infty} \int f_k d\mu, \quad \text{as } n \rightarrow \infty, \\ \lim_{n \rightarrow \infty} \int f_n d\mu &= \int g d\mu = \int f d\mu. \end{aligned} \quad (\text{A.51})$$

■

Corollary A.29. (Absolute continuity) If f is integrable over X , then, for $A \in \mathcal{X}$,

$$\int_A f d\mu \rightarrow 0 \quad \text{as } \mu(A) \rightarrow 0 \quad (\text{A.52})$$

Proof. Take

$$f_n(x) = \begin{cases} f, & \text{if } |f| \leq n, \\ n, & \text{if } |f| \geq n. \end{cases} \quad (\text{A.53})$$

so $|f_n|$ is monotonic increasing to $|f|$ as $n \rightarrow \infty$. By Eqs. (A.19), it follows that $|f|$ is integrable and

$$\left| \int f d\mu \right| = \left| \int f_+ d\mu - \int f_- d\mu \right| \leq \int f_+ d\mu + \int f_- d\mu = \int |f| d\mu. \quad (\text{A.54})$$

Once $|f|$ is integrable, we have that $\int |f_n| d\mu \rightarrow \int |f| d\mu$ as $n \rightarrow \infty$.

Given $\varepsilon > 0$, take N such that

$$\int f d\mu < \int |f_n| d\mu + \frac{\varepsilon}{2}, \quad \text{as } n \geq N, \quad (\text{A.55})$$

if $A \in \mathcal{X}$ is such that $\mu(A) < \varepsilon/2$, then

$$\left| \int_A f d\mu \right| \leq \int_A |f| d\mu = \int_A |f_N| d\mu + \int_A (|f| - |f_N|) d\mu < \frac{\varepsilon}{2} + \int_X (|f| - |f_N|) d\mu < \varepsilon. \quad (\text{A.56})$$

■

Theorem A.30. (Fatou's lemma) If $\{f_n\}$ is a sequence of measurable functions which is bounded below by an integrable function, then

$$\int \liminf_{n \rightarrow \infty} f_n d\mu \leq \liminf_{n \rightarrow \infty} \int f_n d\mu. \quad (\text{A.57})$$

Proof. First, we notice that $\liminf$ picks out the smallest value of a sequence. So the theorem says that if we pick the smallest values and integrate, it is smaller or equal to the integral of the smallest values.

Set g as the integrable function that bounds from below the sequence $\{f_n\}$. Without loss of generality, we can assume that $f_n \geq 0$ for all n . So define $h_n = f_n - g \geq 0$ a.e.

$$\begin{aligned} \int h_n d\mu &= \int f_n d\mu - \int g d\mu \\ \liminf h_n &= \liminf f_n - g \text{ a.e.,} \end{aligned} \quad (\text{A.58})$$

Define $g_n = \liminf_{k \geq n} f_k$, so g_k is an increasing sequence of measurable functions and $\lim_{n \rightarrow \infty} g_n = \liminf_{n \rightarrow \infty} f_n$. But $f_n \geq g_n$ for all n , so, using the monotone convergence theorem (Theorem A.28), we get

$$\liminf_{n \rightarrow \infty} \int f_n d\mu \geq \lim_{n \rightarrow \infty} \int g_n d\mu = \int \lim_{n \rightarrow \infty} g_n d\mu = \int \liminf_{n \rightarrow \infty} f_n d\mu. \quad (\text{A.59})$$

■

Repeating the last proof but setting $g_n = -f_n$ ($n = 1, 2, \dots$), we can prove that

Corollary A.31. If $\{f_n\}$ is a sequence of measurable functions which is bounded above by an integrable function, then

$$\int \limsup_{n \rightarrow \infty} f_n d\mu \geq \limsup_{n \rightarrow \infty} \int f_n d\mu. \quad (\text{A.60})$$

Theorem A.32. (Lebesgue dominated convergence theorem)

- (i) If $g : X \rightarrow \mathbb{R}^+$ is integrable, $\{f_n\}$ is a sequence of measurable functions $X \rightarrow \mathbb{R}^*$, such that $|f_n| \leq g$ ($n = 1, 2, \dots$) and $f_n \rightarrow f$ as $n \rightarrow \infty$, then f is integrable and

$$\int f_n d\mu \rightarrow \int f d\mu, \quad \text{as } n \rightarrow \infty; \quad (\text{A.61})$$

- (ii) Suppose $g : X \rightarrow \mathbb{R}^+$ is integrable, $-\infty \leq a < b \leq +\infty$, and for each $t \in (a, b)$, f_t is a measurable function X to $\mathbb{R}^*$. Then if $|f_t| \leq g$ for all $t \in (a, b)$ and $f_t \rightarrow f$ as $t \rightarrow a^+$ or $t \rightarrow b^-$, then f is integrable and

$$\int f_t d\mu \rightarrow \int f d\mu. \quad (\text{A.62})$$

Proof. For (i), first consider the case where $f_n \geq 0$ and $f_n \rightarrow 0$ as $n \rightarrow \infty$. Using Fatou's Lemma and its corollary (theorems A.30 and A.31), we obtain that

$$\begin{aligned} \limsup \int f_n d\mu &\leq \int \limsup f_n d\mu = \int 0 d\mu = 0 \\ \int \liminf f_n d\mu &= 0 \leq \liminf \int f_n d\mu \leq \limsup \int f_n d\mu \\ &\Rightarrow \lim \int f_n d\mu = 0. \end{aligned} \quad (\text{A.63})$$

In the general case, take $h_n = |f_n - f|$, such that $0 \leq h_n \leq 2g$, where g is integrable. Thus, h_n is integrable and $h_n \rightarrow 0$ as $n \rightarrow \infty$, and

$$\left| \int f_n d\mu - \int f d\mu \right| \leq \int |f_n - f| d\mu \rightarrow 0 \quad \text{as } n \rightarrow \infty, \quad (\text{A.64})$$

hence $\int f_n d\mu \rightarrow \int f d\mu$ as $n \rightarrow \infty$, and f is measurable.

For (ii), suppose that $f_t \rightarrow f$ as $t \rightarrow a^+$. Then take $f_n = f_{t_n}$, where $\{t_n\}$ is any sequence in (a, b) converging to a . Thus, $f = \lim f_n$, and by (i) we obtain that

$$\int f_n d\mu \rightarrow \int f d\mu, \quad \text{as } n \rightarrow \infty, \text{ for any } \{t_n\}. \quad (\text{A.65})$$

Therefore, $\int f_t d\mu$ approaches $\int f d\mu$ as $t \rightarrow a$ through values in (a, b) . $\blacksquare$

We end this section with a short discussion about Lebesgue measure, culminating in the Riemann-Stieltjes integral. We also present one final theorem (in this section) and analyze its consequences. We note that we have not developed enough concepts to give a proper construction of such objects, so some of our conclusions can be proved using a more detailed construction.

First, we observe that we can define over the real line, $\mathbb{R}$, the class $\mathcal{F}$ of all finite unions of sets of the forms $(a, b]$, $(-\infty, b]$, $(a, +\infty)$, and $(-\infty, +\infty)$, and we can define the measure l as the length of the interval. Similarly to the proof of proposition A.12, we can show that $\mathcal{F}$ generates the σ -algebra $\mathcal{F}^*$. Sets that are measurable in the $\mathcal{F}^*$ are said to be **Lebesgue measurable**. We can restrict the measure l to the Borel sets $\mathcal{B}$, which are all $\mathcal{F}^*$ -measurable. When such a restriction is adopted, l is called **Borel** or **Lebesgue measure**. An analogous argument can be used to construct the Lebesgue measure in $\mathbb{R}^k$.

Instead of using the notation dl for integration with the Lebesgue measure, we use dx , and in the case of an integral over a single interval $E = (a, b]$, we use the endpoints of the interval in the integral. That is,

$$\begin{aligned} \text{we use } \int f(x)dx & \text{ instead of } \int f dl \\ \text{we use } \int_a^b f(x)dx & \text{ instead of } \int_E f dl \end{aligned}$$

The Lebesgue measure is not the unique measure possible in $\mathbb{R}^k$. Suppose $F : \mathbb{R} \rightarrow \mathbb{R}$ is a monotone increasing function which is everywhere continuous on the right. Such a function can be used to define a measure of an interval by setting

$$\mu_F(a, b] = F(b) - F(a) \quad (\text{A.66})$$

for each $(a, b] \in \mathcal{P}$. Such a measure is called **Stieltjes measure**. This measure can be used to define the **Riemann-Stieltjes integral**, which is denoted by

$$\int f(x) \mu_F = \int f(x) dF(x). \quad (\text{A.67})$$

It can also be directly generalized if F is a multivariable function, that is, if $F : \mathbb{R}^k \rightarrow \mathbb{R}$. In addition, if we have that $\int dF = 1$, $F(x)$ is said a **probability measure** and the space $(X, \mathcal{X}, F)$ is called a **probability space**.

All the previous theorems have been proved for *any* measure, so all of them hold in the case of either Lebesgue or Stieltjes measures.

Definition A.33. Take $\mathcal{X}$ as a σ -algebra of subsets of X and μ as a measure on $\mathcal{X}$. The set function $\nu : \mathcal{X} \rightarrow \mathbb{R}^*$ is said to be **absolutely continuous** with respect to μ if $\nu(E) = 0$ for every $E \in \mathcal{X}$ with $\mu(E) = 0$. In this case, we write $\nu \ll \mu$. Furthermore, we say that ν is **singular** with respect to μ if there exists a set $E_0 \in \mathcal{X}$ such that $\mu(E_0) = 0$ and $\nu(E) = \nu(E \cap E_0)$ for all $E \in \mathcal{X}$.

Clearly, any function which is μ -integrable is also ν -integrable if $\nu \ll \mu$.

Lemma A.34. If $(X, \mathcal{X}, \mu)$ is a measure space and $\nu : \mathcal{X} \rightarrow \mathbb{R}$ is finite-valued, countably additive, and $\nu \ll \mu$, then for any $\varepsilon > 0$, there exists a $\delta > 0$ such that for all $E \in \mathcal{X}$,

$$\mu(E) < \delta \Rightarrow |\nu(E)| < \varepsilon. \quad (\text{A.68})$$

Proof. From the Hahn-Jordan decomposition (theorem A.20), any such ν is the difference of two finite measures. Thus, it is enough to consider ν as a measure. Suppose that Eq. (A.68) is false, so there exists an $\varepsilon > 0$ and a sequence $\{E_n\}$ of sets in $\mathcal{X}$ such that $\nu(E_n) > \varepsilon$ and $\mu(E_n) < 2^{-n}$. Take $E = \limsup E_n$. Then,

$$\mu(E) \leq \mu\left(\bigcup_{r=n+1}^{\infty} E_r\right) \leq \sum_{r=n+1}^{\infty} \mu(E_r) < 2^{-n}, \quad (\text{A.69})$$

so that $\mu(E) = 0$, while

$$\nu(E) = \lim \nu\left(\bigcup_{r=n+1}^{\infty} E_r\right) \geq \limsup \nu(E_r), \quad (\text{A.70})$$

which leads to $\nu(E) \geq \varepsilon$, contradicting $\nu \ll \mu$. Thus, Eq. (A.68) holds. $\blacksquare$

Theorem A.35. (Radon-Nikodým theorem) Given a σ -finite measure space $(X, \mathcal{X}, \mu)$ and a countably additive, σ -finite set function ν , there exists a unique decomposition

$$\nu = \nu_1 + \nu_2, \quad (\text{A.71})$$

into countably additive set functions ν_i which are σ -finite and such that ν_1 is singular with respect to μ and $\nu_2 \ll \mu$. Furthermore, there exists a finite-valued measurable function $f : X \rightarrow \mathbb{R}$ such that

$$\nu_2(E) = \int_E f d\mu, \quad \text{for all } E \in \mathcal{X}. \quad (\text{A.72})$$

The function f is unique in the sense that if we also have

$$\nu_2(E) = \int_E g d\mu, \quad (\text{A.73})$$

for all $E \in \mathcal{X}$, then $f(x) = g(x)$ except in a set of zero measure.

Proof. We can express X as a union of a countable set of disjoint sets on which both μ and ν are finite, so we can consider them both finite on X . This applies to both the existence and uniqueness proofs. We start by proving that the decomposition is unique.

Let

$$\nu = \nu_1 + \nu_2 = \nu_3 + \nu_4, \quad (\text{A.74})$$

where ν_1 and ν_3 are singular and ν_2 and ν_4 are absolutely continuous. Then $\nu_1 - \nu_3 = \nu_4 - \nu_2$. The union of the support sets of ν_1 and ν_3 gives a set E_0 such that

$$(\nu_1 - \nu_3)(E) = (\nu_1 - \nu_3)(E \cap E_0), \quad \mu(E_0) = 0. \quad (\text{A.75})$$

But $(\nu_4 - \nu_2)$ is absolutely continuous and therefore zero on any null set, so

$$(\nu_1 - \nu_3)(E) = (\nu_4 - \nu_2)(E) = (\nu_1 - \nu_3)(E \cap E_0) = (\nu_4 - \nu_2)(E \cap E_0) = 0. \quad (\text{A.76})$$

Thus, $\nu_1 = \nu_3$ and $\nu_4 = \nu_2$. The uniqueness of the integral representation of ν_2 follows trivially from Eq. (A.49). Now, we must find the decomposition and the integral representation.

From Theorem A.20, we can decompose ν into the difference of two measures, so it is enough to prove the theorem assuming ν is a measure. Let $\mathcal{M}$ be the class of non-negative measurable functions $f : X \rightarrow \mathbb{R}$ such that

$$\nu(E) \geq \int_E f d\mu, \quad \forall E \in \mathcal{X}. \quad (\text{A.77})$$

and define

$$\alpha = \sup \left\{ \int f d\mu \mid f \in \mathcal{M} \right\}. \quad (\text{A.78})$$

Consider a sequence $\{f_n\}$ of functions in $\mathcal{M}$ such that

$$\int f_n d\mu > \alpha - \frac{1}{n}. \quad (\text{A.79})$$

Define $g_n = \max\{f_1(x), f_2(x), \dots, f_n(x)\}$. Then, for any $E \in \mathcal{X}$ and fixed n , we can decompose E into a disjoint union of sets $E = E_1 \cup E_2 \cup \dots \cup E_n \in \mathcal{X}$ such that $g_n = f_i$ on E_i . Hence,

$$\int_E g_n d\mu = \sum_{i=1}^n \int_{E_i} g_n d\mu = \sum_{i=1}^n \int_{E_i} f_i d\mu \leq \sum_{j=1}^n \nu(E_j) = \nu(E), \quad (\text{A.80})$$

so that $g_n \in \mathcal{M}$ for all n . Since g_n is monotone increasing, by the Monotone Convergence Theorem (Theorem A.28), $f_0(x) = \lim_{n \rightarrow \infty} g_n(x) \in \mathcal{M}$. Since $f_0(x) \geq f_n(x)$ for all n , we must have

$$\alpha = \int f_0(x) d\mu. \quad (\text{A.81})$$

For each $E \in \mathcal{X}$, define

$$v_2(E) = \int_E f_0 d\mu, \quad v_1(E) = v(E) - v_2(E). \quad (\text{A.82})$$

Then $v_2 \leq \mu$, and it remains to show that v_1 is singular.

Take the countably additive set function $\lambda_n = v_1 - \frac{1}{n}\mu$ and use Theorem A.20 to decompose X into positive and negative sets N_n, P_n such that $P_n \cup N_n = X$, $P_n \cap N_n = \emptyset$, $E \subset P_n \Rightarrow \lambda_n(E) \geq 0$, and $E \subset N_n \Rightarrow \lambda_n(E) \leq 0$. Take $E \subset P_n$:

$$v(E) = v_1(E) + v_2(E) \geq v_2(E) + \frac{1}{n}\mu(E) = \int_E \left(f_0 + \frac{1}{n}\right) d\mu. \quad (\text{A.83})$$

Thus, $f = f_0$ on N_n and $f = (f_0 + \frac{1}{n})$ on P_n , which belongs to $\mathcal{M}$. This gives an integral less than α , by the definition of α , unless $\mu(P_n) = 0$. If $P = \bigcup_{n=1}^{\infty} P_n$, then $\mu(P) = 0$. Further, $X - P \subset N_n$ for all n , so that $v(X - P) = 0$ and

$$v_1(E) = v_1(E \cap P), \quad \forall E \in \mathcal{X}. \quad (\text{A.84})$$

That is, v_1 is singular. ■

If $(X, \mathcal{X}, \mu)$ is a σ -finite measure space and

$$v(E) = \int_E f d\mu \quad \text{for } E \in \mathcal{X}, \quad (\text{A.85})$$

then we write $f = \frac{dv}{d\mu}$ and call f the *Radon-Nikodým derivative* of v with respect to μ .

A.2 Different Kinds of Spaces

In this section, we intend to present some spaces and their principal properties that will be useful in later constructions. At present, we focus on normed linear and inner-product spaces and their key properties for the further development of physical concepts. More detailed references on such subjects can be easily found; for example, see Refs. [16, 17, 303].

A.2.1 Banach Spaces

Definition A.36. A **normed linear space** is a vector space V , over $\mathbb{R}$ (or $\mathbb{C}$), and a function $\|\cdot\|$ from V to $\mathbb{R}$ which satisfies

- (i) $\|v\| \geq 0$ for all $v \in V$;
- (ii) $\|v\| = 0$ if and only if $v = 0$;
- (iii) $\|\alpha v\| = |\alpha|\|v\|$, for all $v \in V$ and for all $\alpha \in \mathbb{R}$ (or $\mathbb{C}$);
- (iv) $\|v + w\| \leq \|v\| + \|w\|$, for all $v, w \in V$.

If we drop condition (ii), the function $\|\cdot\|$ is said to be a **semi-norm** or **pseudo-norm** for V .

It is direct to see that if we define our metric, from definition A.4, as $\rho(v, w) = \|v - w\|$, then the normed linear space $(V, \|\cdot\|)$ is a metric space. If the metric space induced by $(V, \|\cdot\|)$, denoted by X , is incomplete in the Cauchy sense (definition A.5), we can add the missing Cauchy sequences, denoted by $C_a = \{x = \lim x_n \mid x \notin X, x_n \in X\}$, and define the completion of the space as $\tilde{X} = X \cup C_a$. Since by construction, every Cauchy sequence of X converges to some element of $\tilde{X}$, we say that X is **dense** in $\tilde{X}$. Using the metric now defined over $\tilde{X}$, we can make it into a normed linear space, say $(\tilde{V}, \|\cdot\|)$. We say that $\tilde{V}$ is the *completion* of V .

We say that a normed linear space $(V, \|\cdot\|)$ is complete if its metric-induced space is complete.

Definition A.37. A **bounded linear transformation** (or **bounded operator**) from a normed linear space $(V_1, \|\cdot\|_1)$ to a normed linear space $(V_2, \|\cdot\|_2)$ is a map, $T : V_1 \rightarrow V_2$, which satisfies

- (i) $T(\alpha v + \beta w) = \alpha T(v) + \beta T(w)$ for all $v, w \in V$ and for all $\alpha, \beta \in \mathbb{R}$ (or $\mathbb{C}$);
- (ii) For some $C \geq 0$, $\|Tv\|_2 \leq C\|v\|_1$.

We say that the smallest C is the **norm of T** , so

$$\|T\| = \inf_{\|v\|_1=1} \|Tv\|_2. \quad (\text{A.86})$$

With these definitions, we now present an important theorem of functional analysis.

Theorem A.38. (Bounded Linear Transformation Theorem, or B.L.T. Theorem) Suppose T is a bounded linear transformation from a normed linear space $(V_1, \|\cdot\|_1)$ to a complete normed linear space $(V_2, \|\cdot\|_2)$. Then T can be uniquely extended to a bounded linear transformation (with the same bound), $\tilde{T}$, from the completion of V_1 to $(V_2, \|\cdot\|_2)$.

Proof. Denote by $\tilde{V}_1$ the completion of V_1 . For each $x \in \tilde{V}_1$, there is a Cauchy sequence $\{x_n\} \in V_1$ such that $x_n \rightarrow x$ as $n \rightarrow \infty$. That is, for some N , there exist $n, m < N$ and a $\epsilon = \epsilon/\|T\| > 0$ such that

$$\|x_n - x_m\|_1 \leq \frac{\epsilon}{\|T\|}. \quad (\text{A.87})$$

By the linearity and boundedness of the transformation T , we can write that

$$\|Tx_n - Tx_m\|_2 = \|T(x_n - x_m)\|_2 \leq \|T\|\|x_n - x_m\|_1 < \epsilon, \quad (\text{A.88})$$

so it is a Cauchy sequence in V_2 . Since V_2 is complete, we have $Tx_n \rightarrow y \in V_2$.

Define $\tilde{T}x = y$. Take two sequences that converge to the same element: $\{x_n\} \rightarrow x$, $\{x'_n\} \rightarrow x$. Then, the sequence $\{x_n, x'_n\}$ also converges to x . By the boundedness of T , we have that $\{Tx_n, Tx'_n\} \rightarrow y'$ and $\lim_{n \rightarrow \infty} Tx_n = \lim_{n \rightarrow \infty} Tx'_n = y'$. So, our definition does not depend on the sequence.

Observing that $\|\tilde{T}x\|_2 = \lim_{n \rightarrow \infty} \|Tx_n\|_2 \leq \limsup_{n \rightarrow \infty} C\|x_n\|_1 = C\|x\|_1$, we conclude that $\tilde{T}$ is bounded and has the same bound as T .

Linearity of $\tilde{T}$ follows directly, noting that $\tilde{T}(\alpha x + \beta x') = \lim_{n \rightarrow \infty} (\alpha Tx_n + \beta Tx'_n)$.

To prove uniqueness, take $\tilde{T}'x = y'$, such that $Tx_n \rightarrow y'$ as $\{x_n\} \rightarrow x$. But $\lim_{n \rightarrow \infty} Tx_n = y' = T \lim_{n \rightarrow \infty} x_n = Tx = y$, so $y = y' \Rightarrow \tilde{T}' = \tilde{T}$. ■

Since, from now on, we are interested in integrable functions, it is convenient to use set notation for functions that are Borel integrable. For that, we define

$$L^1(\mathbb{R}) = \left\{ f(x) \mid \int f(x) dx < \infty, x \in \mathbb{R} \right\} \quad (\text{A.89})$$

as the set of real-valued integrable functions. Now assume that we fix the norm on L^1 as

$$\|f\|_1 = \int |f(x)| dx. \quad (\text{A.90})$$

From the linearity and monotonicity of the integral, it follows directly that $L^1(\mathbb{R})$ is a linear normed space. We must check if such a space is complete. For that, take the following sequence $g_n(x) = \min[n, -\ln(x)]$. If $m > n$, it follows that

$$\|g_n - g_m\| = \int |g_n(x) - g_m(x)| dx \leq \int |g_n(x)| dx - 1, \quad (\text{A.91})$$

$g_n \rightarrow -\ln(x)$ ⁶, as $n \rightarrow \infty$ and $-\ln(x) \notin L^1$, so $L^1(\mathbb{R})$ is not a complete space.

⁶See definition A.25.

In order to obtain a complete space preserving integrability, we must consider the space of equivalence classes⁷. We say that two functions $f, g \in L^1(\mathbb{R})$ are equivalent if $f = g$ a.e., equivalently, if $\int |f - g| dx = 0$. Since there are many functions that can be taken and are equal almost everywhere, we must choose a representative. Since we will only work with the set of equivalence classes, we will not distinguish the representative of a function from the function itself. However, we define the set of equivalence classes of integrable functions as $\mathcal{L}^1(\mathbb{R})$. With the norm defined in Eq. (A.90), it is direct to prove that the space $(\mathcal{L}^1(\mathbb{R}), \|\cdot\|_1)$ is a linear normed space, usually denoted only by $\mathcal{L}^1$. Soon we will also prove that $\mathcal{L}^1$ is complete. Before that, let us introduce a more general notion.

Definition A.39. If $1 \leq p < \infty$, the space $\mathcal{L}^p = (\mathcal{L}^p(\mathbb{R}), \|\cdot\|_p)$ of all equivalent Borel measurable real-valued functions f for which $|f|^p$ has a finite integral. We set

$$\|f\|_p = \left[\int |f|^p dx \right]^{\frac{1}{p}}. \quad (\text{A.92})$$

Before analyzing the completeness of this space, let us prove a set of important inequalities.

Theorem A.40. (i) (Hölder's inequality) Let $f \in \mathcal{L}^p$ and $g \in \mathcal{L}^q$, where $p > 1$ and $1/p + 1/q = 1$. Then $fg \in \mathcal{L}^1$ and $\|fg\|_1 \leq \|f\|_p \|g\|_q$.

(ii) (Schwarz's inequality) If f and g belong to $\mathcal{L}^2$, then fg is integrable and

$$\left| \int fg dx \right| \leq \int |fg| dx \leq \|f\|_2 \|g\|_2. \quad (\text{A.93})$$

(iii) (Minkowski's inequality) If f and h belong to $\mathcal{L}^p$, $p \geq 1$, then $f+h$ belongs to $\mathcal{L}^p$ and $\|f+h\|_p \leq \|f\|_p + \|h\|_p$.

Proof. (i): Take $\alpha \in (0, 1)$ and define the function $\phi(t) = \alpha t - t^\alpha$. It is immediate that $\phi'(t) < 0$, if $0 < t < 1$ and $\phi'(t) > 0$, if $t > 1$. From the mean value theorem of calculus, one takes that $\phi(t) \geq \phi(1)$, from that follows, for $t \geq 0$,

$$t^\alpha \leq \alpha t + (1 - \alpha). \quad (\text{A.94})$$

For any a, b non-negative numbers, take $t = a/b$ and multiply the last expression by b to get

$$a^\alpha b^{1-\alpha} \leq \alpha a + (1 - \alpha)b. \quad (\text{A.95})$$

⁷An equivalence relation must be reflexive, symmetric, and transitive.

Choose p, q satisfying $1/p + 1/q = 1$, $1 < p < \infty$. Take $y = x^{p-1}$ and compute the area of this function between $(0, A)$,

$$A_1 = \int_0^A x^{p-1} dx = \frac{A^p}{p}. \quad (\text{A.96})$$

Similarly, we can take the area of $x = y^{1/(p-1)} = y^{q-1}$ between $(0, B)$:

$$A_2 = \int_0^B x^{p-1} dx = \frac{B^p}{p}. \quad (\text{A.97})$$

Clearly, the area of the rectangle AB is greater than or equal to $A_1 + A_2$, so for any two nonnegative real numbers, we obtain:

$$AB \leq \frac{A^p}{p} + \frac{B^p}{p}. \quad (\text{A.98})$$

Using this previous result and fixing $\alpha = 1/p$, we can take $f \in \mathcal{L}^p$ and $g \in \mathcal{L}^q$, and set $A = \frac{|f(x)|}{\|f\|_p}$, $B = \frac{|g(x)|}{\|g\|_q}$ to write:

$$\frac{|f(x)g(x)|}{\|f\|_p \|g\|_q} \leq \frac{|f(x)|^p}{p \|f\|_p^p} + \frac{|g(x)|^q}{q \|g\|_q^q}. \quad (\text{A.99})$$

Both sides are integrable, so $fg \in \mathcal{L}^1$. Integrating both sides:

$$\begin{aligned} \frac{\|f(x)g(x)\|_1}{\|f\|_p \|g\|_q} &\leq \frac{1}{p} + \frac{1}{q} = 1 \\ \Rightarrow \|f(x)g(x)\|_1 &\leq \|f\|_p \|g\|_q. \end{aligned} \quad (\text{A.100})$$

(ii) follows by taking $p = q = 2$ in Hölder's inequality.

In (iii), the case for $p = 1$ follows directly from $|f + h| \leq |f| + |h|$. Assume $p > 1$, since

$$|f + h|^p \leq [2 \sup\{|f|, |h|\}]^p \leq 2^p[|f|^p + |h|^p]. \quad (\text{A.101})$$

$f + h$ is measurable by lemma A.14. Moreover, we notice that

$$|f + h|^p = |f + h||f + h|^{p-1} \leq |f||f + h|^{p-1} + |h||f + h|^{p-1}, \quad (\text{A.102})$$

so $f + h \in \mathcal{L}^p$ and $|f + h|^p \in \mathcal{L}^1$. Taking $1/p + 1/q = 1 \Rightarrow p = (p-1)q$, we

have that $|f + h|^{p-1} \in \mathcal{L}^q$, so by (i), we get:

$$\begin{aligned} \int |f| |f + h|^{p-1} dx &\leq \|f\|_p \left[\int |f + h|^{(p-1)q} dx \right]^{\frac{1}{q}} = \|f\|_p \|f + h\|_p^{\frac{1}{q}} \\ \int |h| |f + h|^{p-1} dx &\leq \|h\|_p \left[\int |f + h|^{(p-1)q} dx \right]^{\frac{1}{q}} = \|h\|_p \|f + h\|_p^{\frac{1}{q}} \\ \|f + h\|_p^p &\leq \|f\|_p \|f + h\|_p^{\frac{1}{q}} + \|h\|_p \|f + h\|_p^{\frac{1}{q}} = [\|f\|_p + \|h\|_p] \|f + h\|_p^{\frac{p}{q}}. \end{aligned} \quad (\text{A.103})$$

If $\|f + h\|_p = 0$, the relation is trivially satisfied. If $\|f + h\|_p \neq 0$, we can divide the last relation by $\|f + h\|_p^{\frac{p}{q}}$ to obtain:

$$\|f + h\|_p \leq \|f\|_p + \|h\|_p. \quad (\text{A.104})$$

■

With this last set of results, in particular with Minkowski's inequality, it is trivial to show that $\mathcal{L}^p$ with the norm from Eq. (A.92) is complete. The following theorem proves its completeness.

Theorem A.41. (Riesz-Fischer Theorem or Completeness Theorem) If $1 \leq p < \infty$, then the space $\mathcal{L}^p$ is a complete normed linear space under the norm given by Eq. (A.92).

Proof. $\mathcal{L}^p$ with the norm from Eq. (A.92) is a linear normed space. To prove completeness, we need to show that for a sequence $\{f_n\}$, there exists an $\varepsilon > 0$ and a N such that for $m, n \geq N$, we have

$$\int |f_m - f_n|^p dx = \|f_m - f_n\|_p^p < \varepsilon^p. \quad (\text{A.105})$$

Take a subsequence $\{g_k\}$ of $\{f_n\}$ such that $\|g_{k+1} - g_k\|_p < 2^{-k}$, $k \in \mathbb{N}$, and define the Borel measurable function $g(x)$ as

$$g(x) = |g_1(x)| + \sum_{k=1}^{\infty} |g_{k+1}(x) - g_k(x)|. \quad (\text{A.106})$$

Using Fatou's lemma (Theorem A.30), we have that

$$\int |g|^p dx \leq \liminf_{n \rightarrow \infty} \int \left[|g_1| + \sum_{k=1}^{\infty} |g_{k+1} - g_k| \right]^p dx, \quad (\text{A.107})$$

taking the p th root and using Minkowski's inequality ((iii) of Theorem A.40) we have that

$$\begin{aligned} \left[\int |g|^p dx \right]^{\frac{1}{p}} &\leq \liminf_{n \rightarrow \infty} \left[\|g_1\|_p + \sum_{k=1}^{\infty} \|g_{k+1} - g_k\|_p \right] \\ &\leq \|g_1\|_p + 1, \end{aligned} \quad (\text{A.108})$$

where we have used the fact that $\sum_{k=2}^{\infty} \|g_{k+1} - g_k\|_p < \sum_{k=1}^{\infty} 2^{-k} = 1$. Take the set E as the set where g is Borel measurable and $g\chi_E \in \mathcal{L}^p$. So the Lebesgue measure of $\mathbb{R} - E$ is zero.

Now define f on $\mathbb{R}$ as

$$f(x) = \begin{cases} g_1 + \sum_{k=1}^{\infty} [g_{k+1} - g_k], & \text{if } x \in E \\ 0, & \text{if } x \notin E, \end{cases} \quad (\text{A.109})$$

but we know that $|g_k| \leq |g_1| + \sum_{j=1}^{k-1} |g_{j+1} - g_j|$ and $\{g_k\}$ converges to f a.e., so, by the Lebesgue dominated convergence theorem (Theorem A.32) we have that $f \in \mathcal{L}^p$. Since $|f - g_k| \leq 2^p g^p$ by the Lebesgue dominated theorem, we get $\lim_{k \rightarrow \infty} \|f - g_k\|_p = 0$. So $\{g_k\}$ converges to f in $\mathcal{L}^p$.

Take $m, k \geq M$, so $\int |f_m - g_k|^p dx < \varepsilon^p$. Using Fatou's lemma

$$\int |f_m - f|^p dx \leq \liminf_{k \rightarrow \infty} \int |f_m - g_k|^p dx \leq \varepsilon^p, \quad (\text{A.110})$$

for any $m \geq M$. So f_n converges to f in the $\mathcal{L}^p$ norm. Therefore, $\mathcal{L}^p$ is complete. $\blacksquare$

All the previous discussion of $\mathcal{L}^p$ spaces has been focused on the functions defined over $\mathbb{R}$ with the usual Lebesgue measure. We choose such an approach because such functions are going to appear in the main applications. However, all the previous discussion can be directly generalized to any space $\mathcal{L}^p = \mathcal{L}^p(X, \mathcal{X}, \mu)$, that is, the space of functions defined over a measure space $(X, \mathcal{X}, \mu)$.

Definition A.42. A complete linear normed space is called a **Banach space**.

Denote the set of all bounded linear functionals from X to Y by $\mathcal{L}(X, Y)$ and assume that for any $A \in \mathcal{L}(X, Y)$, the operator norm is given by

$$\|A\| = \sup_{x \in X, x \neq 0} \frac{\|Ax\|_Y}{\|x\|_X}, \quad (\text{A.111})$$

where $\|\cdot\|_{X,Y}$ denotes the norm in X and Y . We then have the following theorem.

Theorem A.43. If Y is complete, then $\mathcal{L}(X, Y)$ is a Banach space.

Proof. Linear combinations of bounded operators are bounded operators, so $\mathcal{L}(X, Y)$ is a vector space. Our definition of $\|\cdot\|$ in Eq. (A.111) trivially satisfies (i), (ii), and (iii) of definition A.36. To verify (iv) of definition A.36, we write

$$\begin{aligned} \|A + B\| &= \sup_{x \in X, x \neq 0} \frac{\|(A + B)x\|_Y}{\|x\|_X} \leq \sup_{x \in X, x \neq 0} \frac{\|Ax\|_Y + \|Bx\|_Y}{\|x\|_X} \\ &\leq \sup_{x \in X, x \neq 0} \left(\frac{\|Ax\|_Y}{\|x\|_X} + \frac{\|Bx\|_Y}{\|x\|_X} \right) = \|A\| + \|B\|, \end{aligned} \quad (\text{A.112})$$

so $\mathcal{L}(X, Y)$ is a normed linear space under the norm $\|\cdot\|$.

Take $\{A_n\}$ as a Cauchy sequence in the operator norm. For each $x \in X$, $\{A_n x\}$ is a Cauchy sequence in Y . By hypothesis, Y is complete, so $A_n x \rightarrow y \in Y$. Define $Ax = y$, where A is a linear operator. By the triangle inequality, we have that $|\|A_n\| - \|A_m\|| \leq \|A_n - A_m\|$. Therefore, $\{\|A_n\|\}$ is a Cauchy sequence of real numbers that converge to some real number C . Thus,

$$\|Ax\|_Y = \lim_{n \rightarrow \infty} \|A_n x\|_Y \leq \lim_{n \rightarrow \infty} \|A_n\| \|x\|_X = C \|x\|_X, \quad (\text{A.113})$$

which shows that A is a bounded operator.

We have that $\|(A - A_n)x\|_Y = \lim_{m \rightarrow \infty} \|(A_m - A_n)x\|_Y$, which implies that

$$\begin{aligned} \frac{\|(A - A_n)x\|_Y}{\|x\|_X} &\leq \lim_{m \rightarrow \infty} \|A_m - A_n\| \\ \|A - A_n\| &= \sup_{x \neq 0} \frac{\|(A - A_n)x\|_Y}{\|x\|_X} \leq \lim_{m \rightarrow \infty} \|A_m - A_n\| \\ &\leq \lim_{m, n \rightarrow \infty} \|A_m\| - \|A_n\| = \lim_{m \rightarrow \infty} \|A_m\| - C < \varepsilon \quad \text{arbitrary.} \end{aligned} \quad (\text{A.114})$$

So, $\|A\| = C$. ■

If $Y = \mathbb{C}$, the space $\mathcal{L}(X, \mathbb{C})$ is denoted by X^* and is called the **Dual Space of X** . Since the complex numbers, $\mathbb{C}$, are complete⁸, the last theorem shows that X^* is complete, and therefore we can define its dual, denoted by X^{**} , which is called the **double dual**.

Lemma A.44. Let X and Y be linear normed spaces. Then a linear map $T : X \rightarrow Y$ is bounded if and only if $T^{-1}[\{y \mid \|y\|_Y \leq 1\}]$ has nonempty interior.

⁸Take $z_n = x_n + iy_n$, an $\varepsilon > 0$, and $m, n > N$, so $|z_n - z_m| < \varepsilon$ is a Cauchy sequence. But $|z_m - z_n| \geq |x_m - x_n|$ and $|z_m - z_n| \geq |y_m - y_n|$, so $\{x_n\}, \{y_n\} \in \mathbb{R}$ and are Cauchy sequences. Reals are complete, so $x_n \rightarrow x$ and $y_n \rightarrow y$, therefore $z_n \rightarrow x + iy = z \in \mathbb{C}$.

Proof. Suppose that T is given and that the set contains the open sphere $\{x \mid \|x - x_0\|_X < \varepsilon\}$. If $\|x\| < \varepsilon$, we have that $\|Tx\| \leq \|T(x + x_0)\| + \|T(x_0)\| \leq 1 + \|Tx_0\|$. So, for all $x \in X$,

$$\|Tx\| \leq \varepsilon^{-1} (\|Tx_0\| + 1) \|x\|, \quad (\text{A.115})$$

thus, T is bounded.

Now assume that T is bounded. By definition A.37, $\|Tx\| \leq C\|x\|$. Take $x \in \{x \mid \|x - x_0\|_X < \varepsilon\} \subset X$, then $\|Tx\| = \|T(x + x_0)\| \leq C\|x\|$. Denote $Tx = y$ and $T(x + x_0) = y_0$, by our last relation,

$$\begin{aligned} \|y\| &= \|y_0\| \leq C\|x\| \\ \Rightarrow \|y - y_0\| &\leq C\|x\|, \end{aligned} \quad (\text{A.116})$$

which is a (closed) sphere of center y_0 and radius $C\|x\|$. So, $T^{-1}[\{y \mid \|y - y_0\|_Y \leq 1\}]$ has nonempty interior. ■

Theorem A.45. (Open mapping theorem) Let $T : X \rightarrow Y$ be a bounded linear transformation from one Banach space to another Banach space Y . Then, if M is an open set in X , $T[M]$ is open in Y .

Proof. We need to show that for any neighbourhood N of x , $T[N]$ is a neighbourhood of $T(x)$. T is linear, so $T[x + N] = T[x] + T[N]$, then we need only prove for a neighbourhood of $x = 0$. Since the neighbourhoods contain open spheres, it is enough to prove that $S(y, r') \subset T[S(x, r)]$ for some r' . But $T[S(x, r)] = rT[S(x, 1)]$, so we must prove that $T[S(x, r)]$ is a neighbourhood of zero for some r . Using the result of lemma A.44, we must show that $T[S(x, r)]$ has nonempty interior for some r .

T is onto, so $Y = \bigcup_{n=1}^{\infty} T[S(0, r_n)]$. By the Baire category theorem (theorem A.9), some $\overline{T[S(0, r_n)]}$ has nonempty interior. Suppose that $S(0, \varepsilon) \subset \overline{T[S(0, r_1)]}$. Take $y \in \overline{T[S(0, r_1)]}$. If $x_1 \in S(0, r_1)$, then $y - Tx_1 \in S(0, \varepsilon/2) \subset \overline{T[S(0, r_1/2)]}$. If $x_1 \in S(0, r_1/2)$, then $y - Tx_1 - Tx_2 \in S(0, \varepsilon/4) \subset \overline{T[S(0, r_1/4)]}$. If $x_n \in S(0, r_n)$, then $y - \sum_{j=1}^n Tx_j \in S(0, 2^{1-n}\varepsilon)$.

Set $x = \sum_{j=1}^{\infty} x_j \in S(0, r_1/2)$, thus $y = \sum_{j=1}^{\infty} Tx_j = Tx$, so $y \in T[S(0, r_1/2)]$, so some $T[S(x, r)]$ has nonempty interior and the theorem follows. ■

Corollary A.46. (Inverse mapping theorem) A continuous bijection from one Banach space to another has a continuous inverse.

Proof. By the last theorem, if T is open, T^{-1} is continuous. ■

Banach spaces are useful to construct functionals with some desired properties. In order to understand why it is useful to define functionals on Banach spaces, the next important theorem is necessary.

Theorem A.47. (Hahn-Banach theorem) Let X be a real vector space, p a real valued function defined on X satisfying $p(\alpha x + (1 - \alpha)y) \leq \alpha p(x) + (1 - \alpha)p(y)$ for all $x, y \in X$ and all $\alpha \in [0, 1]$. Suppose that λ is a linear functional defined on a subspace Y of X which satisfies $\lambda(x) \leq p(x)$ for all $x \in Y$. Then, there is a linear functional Λ , defined on X , satisfying $\Lambda(x) \leq p(x)$ for all $x \in X$, such that $\Lambda(x) = \lambda(x)$ for all $x \in Y$.

Proof. Denote the space spanned by z and Y by $\tilde{Y}$. The extension of λ , defined on Y satisfying $\lambda(y) \leq p(y)$ for all $y \in Y$, to $\tilde{Y}$ is denoted by $\tilde{\lambda}$. Define $\tilde{\lambda}(z)$ using $\tilde{\lambda}(az + y) = a\tilde{\lambda}(z) + \lambda(y)$.

Take $y_1, y_2 \in Y$ and $\alpha, \beta > 0$, so

$$\begin{aligned} \beta\lambda(y_1) + \alpha\lambda(y_2) &= \lambda(\beta y_1 + \alpha y_2) = (\alpha + \beta)\lambda\left(\frac{\beta}{\alpha + \beta}y_1 + \frac{\alpha}{\alpha + \beta}y_2\right) \\ &\leq (\alpha + \beta)p\left(\frac{\beta}{\alpha + \beta}y_1 + \frac{\alpha}{\alpha + \beta}y_2\right) \\ &\leq (\alpha + \beta)p\left(\frac{\beta}{\alpha + \beta}y_1 + \frac{\alpha}{\alpha + \beta}y_2 + \frac{\alpha\beta}{\alpha + \beta}z - \frac{\alpha\beta}{\alpha + \beta}z\right) \\ &\leq (\alpha + \beta)p\left(\frac{\beta}{\alpha + \beta}(y_1 - \alpha z) + \frac{\alpha}{\alpha + \beta}(y_2 + \beta z)\right) \\ &\leq \beta p(y_1 - \alpha z) + \alpha p(y_2 + \beta z), \end{aligned} \quad (\text{A.117})$$

therefore, for all $\alpha, \beta > 0$ and $y_1, y_2 \in Y$

$$\frac{1}{\alpha}[-p(y_1 - \alpha z) + \lambda(y_1)] \leq \frac{1}{\beta}[-p(y_2 + \beta z) + \lambda(y_2)]. \quad (\text{A.118})$$

We can always find a real number a such that

$$\sup_{y \in Y, \alpha > 0} \frac{1}{\alpha}[-p(y_1 - \alpha z) + \lambda(y_1)] \leq a \leq \inf_{y \in Y, \alpha > 0} \frac{1}{\beta}[-p(y_2 + \beta z) + \lambda(y_2)], \quad (\text{A.119})$$

which means that we can thus define $\tilde{\lambda}(z) = a$. Thus, λ can be extended “one direction at a time”.

It remains to show that λ can be extended to the whole space X . Take $\mathcal{E}$ as the collection of extensions e of λ , which satisfies $e(x) \leq p(x)$ on each subspace. Define a partial order in $\mathcal{E}$ by setting that $e_1(x) \leq e_2(x)$ if $e_2(x)$ is defined on a larger set than $e_1(x)$, and $e_1(x) = e_2(x)$ where they are both defined.

Take $\{e_\alpha\}_{\alpha \in A}$ as a partially ordered subset of $\mathcal{E}$. Define e on $\bigcup_{\alpha \in A} X_\alpha$ by $e(x) = e_\alpha(x)$ if $x \in X_\alpha$. So $e_\alpha \leq e$ for any $e_\alpha \in \mathcal{E}$, therefore, each partially ordered subset of $\mathcal{E}$ has an upper bound in $\mathcal{E}$. By Zorn’s lemma, $\mathcal{E}$ has a maximal element, Λ , defined in some subset X' and satisfying $\Lambda(x) \leq p(x)$ for $x \in X'$.

But, if X' is not the whole X , we can extend it to $\tilde{\Lambda}$ by the previous procedure. This contradicts the maximality of Λ ; therefore $X' = X$, and the extension Λ is defined everywhere in X . ■

The extension of the Hahn-Banach theorem to a complex vector space X is straightforward.

Now we can see why Banach spaces are useful. If we need a functional with some properties, we need only to define it on a subspace of the Banach space, then we use the Hahn-Banach theorem to extend it to the whole space.

Corollary A.48. Let X be a normed linear space, Y a subset of X , and λ an element of Y^* . Then there exists a $\Lambda \in X^*$ extending λ and satisfying $\|\Lambda\|_{X^*} = \|\lambda\|_{Y^*}$.

Proof. Take $p(x) = \|\lambda\|_{Y^*}\|x\|$ in the Hahn-Banach theorem. ■

Corollary A.49. Let y be an element of a normed linear space X . Then there is a nonzero $\Lambda \in X^*$ such that $\Lambda(y) = \|X\|_{X^*}\|y\|$

Proof. Take Y as the subspace of all scalar multiples of y and define $\lambda(ay) = a\|y\|$. By the last corollary, we can construct Λ , such that $\|\Lambda\| = \|\lambda\|$, which extends λ for the whole X . But $\Lambda(y) = \|y\|$, once that $\|\Lambda\| = 1$, thus, $\Lambda(y) = \|\Lambda\|_{X^*}\|y\|$. ■

We finish our brief discussion about Banach spaces with the definition of a graph and a theorem which has future use.

Definition A.50. Let T be a mapping of a normed linear space X into another linear normed space Y . The **graph** of T , denoted by $\Gamma(T)$, is defined by

$$\Gamma(T) = \{\langle x, y \rangle \mid \langle x, y \rangle \in X \times Y, y = Tx\}. \quad (\text{A.120})$$

Theorem A.51. (Closed graph theorem) Let X and Y be Banach spaces and T a linear map of X into Y . Then T is bounded if and only if the graph of T is closed.

Proof. Suppose that $\Gamma(T)$ is closed. T is linear, therefore, $\Gamma(T)$ is a subspace of the Banach space $X \times Y$. Since $\Gamma(T)$ is closed⁹, it is a Banach space in the norm

$$\|\langle x, Tx \rangle\| = \|x\| + \|Tx\|. \quad (\text{A.121})$$

Now consider the maps $\Pi_1 : \langle x, Tx \rangle \rightarrow x$ and $\Pi_2 : \langle x, Tx \rangle \rightarrow Tx$. Π_1 is a bijection, so by the inverse map theorem (corollary A.46), Π_1^{-1} is continuous. Since $T = \Pi_2 \circ \Pi_1^{-1}$, T is continuous and bounded.

⁹Remember that a closed set contains all its limit points.

Conversely, assume that T is bounded. Then, $\|Tx\| \leq C\|x\|$, so

$$\begin{aligned}\|\Gamma(T)\| &= \|\langle x, Tx \rangle\| = \|x\| + \|Tx\| \leq \|x\|(1 + C) \\ \Rightarrow \frac{\|\Gamma(T)\|}{\|x\|} &\leq 1 + C,\end{aligned}\tag{A.122}$$

thus $\Gamma(T)$ is closed. ■

Of course, there are many results that could be obtained in the context of Banach spaces. However, we believe that the set of results that we have chosen to present has a low level of difficulty and is useful in physics, especially those involving integrable functions.

A.2.2 Hilbert spaces

Vector and metric spaces have a plethora of physics literature due to their applicability in the physical world. However, the inner-product space, which is used as the basis of quantum mechanics and some classical physics as well, does not receive that much attention. Many quantum mechanics books do not even give a proper definition of what a Hilbert space is. To avoid repeating the same oversight, let us analyze with care the main properties and results of inner product spaces.

Definition A.52. A complex vector space V is called an **inner product space** if there is a complex-valued function $(\bullet, \bullet)$, called the **inner product**, on $V \times V$ that satisfies the following conditions for any $x, y, z \in V$ and $\alpha \in \mathbb{C}$

- (i) $(x, x) \geq 0$ and $(x, x) = 0$ if and only if $x = 0$;
- (ii) $(x, y + z) = (x, y) + (x, z)$;
- (iii) $(\alpha x, y) = \alpha(x, y)$;
- (iv) $(x, y) = \overline{(y, x)}$.

We can use the same geometrical nomenclature of vectors in the inner product space. That is, if $(x, y) = 0$ they are said to be *orthogonal*, and if we have a collection of vectors $\{x_i\}_{i \in A}$, such that $(x_i, x_i) = 1$ for all $i \in A$ and $(x_i, x_j) = 0$ for all $i, j \in A$, we say that we have an *orthonormal set*. We directly see that if we fix $\|x\| = \sqrt{(x, x)}$, then (i), (ii), and (iii) of definition A.36 are directly satisfied. To prove that $\|\bullet\| = \sqrt{(\bullet, \bullet)}$ is a norm, we need only check (iv) of definition A.36.

Theorem A.53. (Pythagorean theorem) Let $\{x_n\}$, $n = 1, 2, \dots, N$ be an orthonormal set in an inner product space V . Then for all $x \in V$

$$\|x\|^2 = \sum_{n=1}^N |(x, x_n)|^2 + \left\| x - \sum_{n=1}^N (x_n, x)x_n \right\|^2. \quad (\text{A.123})$$

Proof. First we note that

$$\begin{aligned} \left(\sum_{n=1}^N (x_n, x)x_n, x - \sum_{n=1}^N (x_n, x)x_n \right) &= \left(\sum_{n=1}^N (x_n, x)x_n, x \right) - \left(\sum_{n=1}^N (x_n, x)x_n, \sum_{n=1}^N (x_n, x)x_n \right) \\ &= \sum_{n=1}^N (x_n, x) \overline{(x_n, x)} - \sum_{n=1}^N (x_n, x) \overline{(x_n, x)} \\ &= 0, \end{aligned} \quad (\text{A.124})$$

so, $x = \sum_{n=1}^N (x_n, x)x_n + \left(x - \sum_{n=1}^N (x_n, x)x_n \right)$ is a decomposition of any $x \in V$ into two orthogonal components. Now we use this decomposition to directly compute

$$\begin{aligned} (x, x) &= \left\| \sum_{n=1}^N (x_n, x)x_n \right\|^2 + \left\| x - \sum_{n=1}^N (x_n, x)x_n \right\|^2 \\ &= \sum_{n=1}^N |(x, x_n)|^2 + \left\| x - \sum_{n=1}^N (x_n, x)x_n \right\|^2 \end{aligned} \quad (\text{A.125})$$

■

Corollary A.54. (Bessel's inequality) Let $\{x_n\}$, $n = 1, 2, \dots, N$ be an orthonormal set in an inner product space V . Then for all $x \in V$

$$\|x\|^2 \geq \sum_{n=1}^N |(x, x_n)|^2. \quad (\text{A.126})$$

Proof. Follows directly from the Pythagorean theorem. ■

Corollary A.55. (Cauchy-Schwarz's inequality) Let x and y be any elements of an inner product space V , then $|(x, y)| \leq \|x\|\|y\|$.

Proof. If $y = 0$ it is trivial. Suppose $y \neq 0$, then $y/\|y\|$ is an orthonormal set. Take $x \in V$ and apply Bessel's inequality to obtain

$$\begin{aligned}\|x\|^2 &\geq \left| \left(x, \frac{y}{\|y\|} \right) \right|^2 = \frac{|(x, y)|^2}{\|y\|^2} \\ &\Rightarrow |(x, y)| \leq \|x\| \|y\|.\end{aligned}\tag{A.127}$$

■

Now we can directly calculate

$$\begin{aligned}\|x + y\|^2 &= (x, x) + (x, y) + (y, x) + (y, y) \\ &= (x, x) + 2\Re(x, y) + (y, y),\end{aligned}\tag{A.128}$$

but, $\Re(x, y) \leq |(x, y)|$ and by Schwarz's inequality $|(x, y)| \leq (x, x)^{\frac{1}{2}}(y, y)^{\frac{1}{2}}$, therefore

$$\begin{aligned}\|x + y\|^2 &\leq (x, x) + 2(x, x)^{\frac{1}{2}}(y, y)^{\frac{1}{2}} + (y, y), \\ &\Rightarrow \|x + y\| \leq \|x\| + \|y\|,\end{aligned}\tag{A.129}$$

which is item (iv) of definition A.36. That is, we have proved the following theorem.

Theorem A.56. Every inner product space is a linear normed space with the norm $\|\cdot\| = \sqrt{(\cdot, \cdot)}$.

By the last theorem, it is direct to see that we have a natural definition of a metric on the inner product space

$$\rho(x, y) = \sqrt{(x - y, x - y)}.\tag{A.130}$$

That is, all the construction of Section A.1 can be applied.

Definition A.57. A complete inner product space is called **Hilbert space**.

It is worth noting that, if we sum up the following expression

$$\|x - y\|^2 = (x, x) - (x, y) - (y, x) + (y, y),\tag{A.131}$$

with Eq. (A.128) we obtain that for any x, y in a Hilbert space we have

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2,\tag{A.132}$$

which is the *Parallelogram law*. This law is satisfied whenever the norm is obtained by an inner product. The emergence of such a law is a consequence of

the fact that in Hilbert spaces, we have a geometric notion, making it easier to handle than Banach spaces.

Assume that we have $f = \chi_{[0,1]}(x)$ and $g = \chi_{[1,2]}(x)$, where χ_E is the indicator function. It is direct to check that $f, g \in \mathcal{L}^p$, and it follows that $\|f\|_p = \|g\|_p = 1$, and $\|f + g\|_p = \|f - g\|_p = 2^{\frac{1}{p}}$. So, applying the parallelogram law, we have that $4 = 2(2)^{\frac{2}{p}}$. This relation is satisfied only if $p = 2$. This quick analysis shows us that $\mathcal{L}^p$ is a Hilbert space *only* if $p = 2$. That is, $\mathcal{L}^2$ is the only one of the $\mathcal{L}^p$ spaces whose norm is obtained by an inner product.

As we have explained, the geometric properties of Hilbert spaces are useful. In particular, if we have a Hilbert space $\mathcal{H}$, we can construct a closed subspace $\mathcal{M}$ with the same inner product. Now denote by $\mathcal{M}^\perp$ the set of all elements that are orthogonal to $\mathcal{M}$. Now take the subspace $\mathcal{M}$ as the following set $\mathcal{M} = \{\phi\} \subset \mathcal{H}$, then, for any $\psi \in \mathcal{M}^\perp$, we have that $(\phi, \psi)_{\mathcal{H}} = 0$. Let $\psi = \psi_1 + \psi_2$, with $\psi_1, \psi_2 \in \mathcal{M}^\perp$, then $(\phi, \psi) = 0 = (\phi, \psi_1) + (\phi, \psi_2)$, so $(\phi, \psi_1) = (\phi, \psi_2) = 0$ and $(\psi_1, \psi_2)_{\mathcal{M}^\perp} = (\psi_1, \psi_2)_{\mathcal{H}}$, and all the linearity properties follow. So, $\mathcal{M}^\perp$ is a linear subspace of $\mathcal{H}$.

Further, take the open sphere $S(\psi_2, r) = \{\psi_1 \mid \psi_1 \in \mathcal{H}, \rho(\psi_1, \psi_2) < r\}$, with $\rho(\psi_1, \psi_2) = \sqrt{(\psi_1 - \psi_2, \psi_1 - \psi_2)}$. Assume that $\psi_1, \psi_2 \in \mathcal{M}^\perp$ and write $\psi_1 = \psi + \psi'$, then

$$\begin{aligned} \rho(\psi_1, \psi_2) &= \sqrt{(\psi + \psi' - \psi_2, \psi + \psi' - \psi_2)} < r \\ &= \sqrt{(\psi - \psi_2 + \psi', \psi - \psi_2) + (\psi - \psi_2 + \psi', \psi')} < r \\ &= \sqrt{(\psi_3 + \psi', \psi) + (\psi_3 + \psi', \psi')} < r \\ &= \sqrt{(\psi_3 + \psi', \psi + \psi')} < r, \end{aligned} \tag{A.133}$$

where we have defined $\psi_3 = \psi - \psi_2$. By the last equation, we have that $\psi_3 \in S(\psi_2, r)$, and by the linearity of $\mathcal{M}^\perp$, $\psi_3 \in \mathcal{M}^\perp$. Therefore, $S(\psi_2, r) \cap \mathcal{M}^\perp \neq \emptyset$, so ψ_3 is a limit point of $\mathcal{M}^\perp$, once the decomposition $\psi_1 = \psi + \psi'$ is arbitrary, also it is ψ_3 , so $\mathcal{M}^\perp$ is closed. We conclude that $\mathcal{M}^\perp$ is a closed linear subspace of $\mathcal{H}$.

Lemma A.58. Let $\mathcal{H}$ be a Hilbert space, $\mathcal{M}$ a closed linear subspace of $\mathcal{H}$, and suppose that $\phi \in \mathcal{H}$. Then, there is a unique $\psi \in \mathcal{M}$ closest to ϕ .

Proof. Let $d = \inf_{\psi \in \mathcal{M}} \|\phi - \psi\|$ and take a sequence $\{\psi_n\} \in \mathcal{M}$ such that $\|\phi - \psi_n\| \rightarrow d$, then, using the parallelogram law (Eq. (A.132)), we get that

$$\begin{aligned} \|\psi_n - \psi_m\|^2 &= \|(\psi_n - \phi) - (\psi_m - \phi)\|^2 = 2\|\psi_n - \phi\|^2 + 2\|\psi_m - \phi\|^2 - \|2\phi + \psi_n + \psi_m\|^2 \\ &= 2\|\psi_n - \phi\|^2 + 2\|\psi_m - \phi\|^2 - 4\left\|\phi + \frac{1}{2}(\psi_n + \psi_m)\right\|^2 \\ &\leq 2\|\psi_n - \phi\|^2 + 2\|\psi_m - \phi\|^2 - 4d^2 \\ &\rightarrow 2d^2 + 2d^2 - 4d^2 = 0, \quad \text{as } n \rightarrow \infty \text{ and } m \rightarrow \infty, \end{aligned} \tag{A.134}$$

once that $\mathcal{M}$ is closed, $\{\psi_n\}$ is Cauchy. Take $\{\psi_n\} \rightarrow \psi$, then $\|x - z\| = d$.

Now take a different sequence $\{\psi'_n\}$, all the calculations follow as the same. We conclude that $\{\psi'_n\}$ is Cauchy and $\{\psi'_n\} \rightarrow \psi' \in \mathcal{M}$ and $\|\phi - \psi'\| = d$. But $\|\phi - \psi'\| - \|\phi - \psi\| = 0$, then $\psi = \psi'$. ■

Theorem A.59. (Projection theorem) Let $\mathcal{H}$ be a Hilbert space, and $\mathcal{M} \subset \mathcal{H}$ a closed subspace. Then, every $\phi \in \mathcal{H}$ can be uniquely written as $\phi = \psi + \xi$, where $\psi \in \mathcal{M}$ and $\xi \in \mathcal{M}^\perp$.

Proof. Take $\phi \in \mathcal{H}$. By the last lemma, there is a unique $\psi \in \mathcal{M}$ closest to ϕ . Define $\xi = \phi - \psi$. Take any $\psi' \in \mathcal{M}$ and $t \in \mathbb{R}$, if $d = \|\phi - \psi\| = \|\omega\|$, then

$$\begin{aligned} d^2 &\leq \|\phi - (\psi + t\psi')\|^2 = \|\xi - t\psi'\|^2 \\ &\leq \|\xi\|^2 - 2t\Re(\xi, \psi') + t^2\|\psi'\|^2 = d^2 - 2t\Re(\xi, \psi') + t^2\|\psi'\|^2, \end{aligned} \quad (\text{A.135})$$

therefore it follows that $-2\Re(\xi, \psi') + t\|\psi'\|^2 \geq 0$, this can only be satisfied if $\Re(\xi, \psi') = 0$. Repeating the same thing but with it , we get $\Im(\xi, \psi')$. So we conclude that $(\xi, \psi') = 0$, so $\xi \in \mathcal{M}^\perp$.

Repeating the same procedure but with $\xi' = \phi - \psi$, we get $(\xi, \psi') = 0$, so $\xi' \in \mathcal{M}^\perp$. But $d^2 = \|\xi\|^2 = \|\xi'\|^2$, on the other hand $d^2 = \|\phi - \psi\|^2$, so $\xi = \xi'$. ■

This last theorem indicates that we can write any Hilbert space as $\mathcal{H} = \mathcal{M} \oplus \mathcal{M}^\perp$.

Just like in the case of Banach spaces (see the discussion of Eq. (A.111)), we can define the set of bounded linear transformations from $\mathcal{H}$ to $\mathcal{H}'$ by $\mathcal{L}(\mathcal{H}, \mathcal{H}')$, and the theorem A.43 ensures that this space is complete. Again, if $\mathcal{H}' = \mathbb{C}$, the space $\mathcal{L}(\mathcal{H}, \mathbb{C})$ is denoted by $\mathcal{H}^*$ and called the **dual space** of $\mathcal{H}$. The elements of $\mathcal{H}^*$ are called **continuous linear functionals**.

Theorem A.60. (Riesz's Representation theorem in Hilbert spaces) Any linear functional $\Phi(\psi)$ in the Hilbert space $\mathcal{H}$ can be represented *uniquely* in the form

$$\Phi(\psi) = (\phi, \psi), \quad (\text{A.136})$$

where $(\cdot, \cdot)$ denotes the inner-product in $\mathcal{H}$, and ϕ is defined *uniquely* by the functional Φ . Moreover,

$$\|\Phi\| = \|\phi\|. \quad (\text{A.137})$$

Proof. Let $\Phi(\psi)$ be a continuous linear functional acting over the complex Hilbert space $\mathcal{H}$. Denote by L the set of zeros of this functional, that is,

$$L = \{\psi \in \mathcal{H} \mid \Phi(\psi) = 0\}. \quad (\text{A.138})$$

L is a subspace of $\mathcal{H}$. Linearity and continuity of $\Phi(\psi)$ implies that L is a linear and closed manifold.

For any $\psi \in \mathcal{H}$, let ψ_0 be the projection of ψ into the subspace $\mathcal{H} \setminus L$. Then, $\Phi(\psi_0) = C$, and $C \neq 0$. Set $\psi_1 = \psi_0/C$, by the linearity of the functional we have that $\Phi(\psi_1) = 1$. For any $\psi \in \mathcal{H}$ we have $\Phi(\psi) = C'$, again using the linearity of the functional, we can write that

$$\Phi(\psi) - C'\Phi(\psi_1) = \Phi(\psi - C'\psi_1) = 0, \quad (\text{A.139})$$

from which one can conclude that $\psi - C'\psi_1 = \xi$, $\xi \in L$, equivalently $\psi = C'\psi_1 + \xi$. So we get that $\mathcal{H}$ is the sum of two orthogonal spaces, one of them is L and the other is the space spanned by ψ_1 .

Once $\psi_1 \perp \xi$, follows that $(\psi_1, \psi) = C'\|\psi_1\|$, since $C' = \Phi(\psi)$ we can write

$$\Phi(\psi) = \left(\frac{\psi_1}{\|\psi_1\|}, \psi \right). \quad (\text{A.140})$$

Set $\phi = \psi_1/\|\psi_1\|$, then

$$\Phi(\psi) = (\phi, \psi). \quad (\text{A.141})$$

Suppose that $\Phi(\psi) = (\omega, \psi)$, then $0 = (\phi - \omega, \psi)$, $\forall \psi \in \mathcal{H}$, which implies that $\phi = \omega$. Taking the absolute value of the previous equation, one gets that

$$|\Phi(\psi)| = |(\phi, \psi)| \leq \|\phi\| \|\psi\| \Rightarrow \|\Phi\| \leq \|\phi\|. \quad (\text{A.142})$$

However, $\Phi(\phi) = (\phi, \phi) = \|\phi\|^2$, then $\|\Phi\| \geq \|\phi\|$, hence $\|\Phi\| = \|\phi\|$. ■

Theorem A.61. Let $\mathcal{H}$ be a Hilbert space, and let $A \in \mathcal{L}(\mathcal{H})$. If

$$f\langle\phi, \psi\rangle = (A\phi, \psi), \quad (\text{A.143})$$

then f is a bounded sesquilinear¹⁰ functional and $\|f\| = \|A\|$. Conversely, if f is a bounded sesquilinear functional, there exists a unique $A \in \mathcal{L}(\mathcal{H})$ such that $f\langle\phi, \psi\rangle = (A\phi, \psi)$.

Proof. Two linear transformations A_1 and A_2 , each mapping $\mathcal{H}$ into itself, satisfy $(A_1\phi, \psi) = (A_2\phi, \psi)$ for all $\phi, \psi \in \mathcal{H}$, then $A_1 = A_2$. If A_1 and A_2 satisfy the weaker condition $(A_1\phi, \phi) = (A_2\phi, \phi)$, this also implies that $A_1 = A_2$. Let us consider two sesquilinear functionals $f\langle\phi, \psi\rangle = (A_1\phi, \psi)$ and $g\langle\phi, \psi\rangle = (A_2\phi, \psi)$. Therefore, $f = g$, and then $A_1 = A_2$ for all $\phi, \psi \in \mathcal{H}$.

Now let $A \in \mathcal{L}(\mathcal{H})$ and consider $f\langle\phi, \psi\rangle = (A\phi, \psi)$. Using the Cauchy-Schwarz inequality (corollary A.55), we have

$$|f\langle\phi, \psi\rangle| = |(A\phi, \psi)| \leq \|A\| \|\phi\| \|\psi\|, \quad (\text{A.144})$$

¹⁰See footnote 4 on page 16.

so f is a bounded sesquilinear functional and $\|f\| \leq \|A\|$. For any $\phi \in \mathcal{H}$, we have

$$\|A\phi\|^2 = (A\phi, A\phi) = f(\phi, A\phi) = |f(\phi, A\phi)| \leq \|f\| \|\phi\| \|A\phi\|, \quad (\text{A.145})$$

so it follows that $\|A\phi\| \leq \|f\| \|\phi\| \Rightarrow \|A\| \leq \|f\|$. Therefore, $\|A\| = \|f\|$.

Conversely, suppose that f is a bounded sesquilinear functional and consider the functional $g_\phi(y) = \overline{f(\phi, y)}$. It directly follows that g_ϕ is a linear functional. The fact that g_ϕ is bounded follows directly from the definition and the Cauchy-Schwarz inequality. By Riesz's Representation theorem, there exists a unique $\xi \in \mathcal{H}$ such that

$$g_\phi(\psi) = \overline{f(\phi, \psi)} = (\psi, \xi), \quad (\text{A.146})$$

and $\|g_\phi\| = \|\xi\|$. If we denote $\xi = A\phi$, we have that $f(\phi, \psi) = (A\phi, \psi)$. It remains to show that A is a bounded linear transformation. From linearity, we have that $g_{\phi_1 + \phi_2}(\psi) = (\psi, A(\phi_1 + \phi_2))$, and from the definition of g_ϕ , it follows immediately that $A(\phi_1 + \phi_2) = A\phi_1 + A\phi_2$. The multiplication by scalar follows similarly. Then A is linear. Its boundedness follows from

$$\|g_\phi\| = \|\xi\| = \|A\phi\| \leq \|f\| \|\phi\|. \quad (\text{A.147})$$

■

To push further the ideas of finite-dimensional spaces into an infinite-dimensional space like Hilbert spaces, we must ask ourselves if it is possible to define a set of orthonormal basis.

We say that if S is an orthonormal subset of a Hilbert space and there is no other orthogonal set which contains S as a proper subset, then we say that S is an **orthonormal basis** for $\mathcal{H}$.

Theorem A.62. Every Hilbert space has an orthonormal basis.

Proof. Take $\mathcal{C}$ as the collection of orthonormal sets of $\mathcal{H}$. Partially order $\mathcal{C}$ by inclusion, that is $S_1 < S_2$ if $S_1 \subset S_2$. Since for any $\psi \in \mathcal{H}$, we have that $\psi/\|\psi\|$ is an orthonormal set, $\mathcal{C}$ is a nonempty collection.

Take $\{S_\alpha\}_{\alpha \in A}$ as any partially ordered subset of $\mathcal{C}$, so $\bigcup_{\alpha \in A} S_\alpha$ is an orthonormal set which contains each S_α , also, it is an upper bound for $\{S_\alpha\}_{\alpha \in A}$. Each partially ordered subset of $\mathcal{C}$ has an upper bound, so we can apply Zorn's Lemma, therefore $\mathcal{C}$ has a maximal element. That is, $\mathcal{C}$ contains an orthonormal system which is not contained by any other orthonormal system. ■

Theorem A.63. Let $\mathcal{H}$ be a Hilbert space and $s = \{\phi_\alpha\}_{\alpha \in A}$ an orthonormal basis. Then, for each $\psi \in \mathcal{H}$

$$\psi = \sum_{\alpha \in A} (\phi_\alpha, \psi) \phi_\alpha, \quad (\text{A.148})$$

where the equality means that the sum (independent of the order) converges to $\psi \in \mathcal{H}$, and

$$\|\psi\|^2 = \sum_{\alpha \in A} |(\phi_\alpha, \psi)|^2. \quad (\text{A.149})$$

Conversely, if $\sum_{\alpha \in A} |c_\alpha|^2 < \infty$, with $c_\alpha \in \mathbb{C}$, then $\sum_{\alpha \in A} c_\alpha \phi_\alpha$ converges to an element of $\mathcal{H}$.

Proof. Using Bessel's inequality (corollary A.54), we have that for any finite subset $A' \subset A$, $\sum_{\alpha \in A'} |(\phi_\alpha, \psi)|^2 \leq \|\psi\|^2$. If $(\phi_\alpha, \psi) \neq 0$, there is at most a countable number of α 's in A for which we can establish an order in some way: $\alpha_1, \alpha_2, \dots$. Since $\sum_{j=1}^N |(\phi_{\alpha_j}, \psi)|^2$ is monotone increasing and bounded, it converges to a finite quantity as $N \rightarrow \infty$. Assume that $\psi_n = \sum_{j=1}^n (\phi_{\alpha_j}, \psi) \phi_{\alpha_j}$, then, for any $n > m$

$$\|\psi_n - \psi_m\|^2 = \left\| \sum_{j=m+1}^n (\phi_{\alpha_j}, \psi) \phi_{\alpha_j} \right\|^2 = \sum_{j=m+1}^n |(\phi_{\alpha_j}, \psi)|^2, \quad (\text{A.150})$$

thus, $\{\psi_n\}$ is a Cauchy sequence that converges to some $\psi' \in \mathcal{H}$. Therefore, we have that

$$\begin{aligned} (\psi - \psi', \phi_{\alpha_l}) &= \lim_{n \rightarrow \infty} \left(\psi - \sum_{j=1}^n (\phi_{\alpha_j}, \psi) \phi_{\alpha_j}, \phi_{\alpha_l} \right) \\ &= (\psi, \phi_{\alpha_l}) - (\psi, \phi_{\alpha_l}) = 0, \end{aligned} \quad (\text{A.151})$$

the previous holds for any $\alpha \neq \alpha_l$, which means that we have $(\psi - \psi', \phi_\alpha) = 0$, so $\psi - \psi'$ is orthogonal to all $\phi_\alpha \in S$. But S is a complete orthonormal set, then $\psi - \psi' = 0$ and it follows that

$$\psi = \sum_{\alpha \in A} (\phi_\alpha, \psi) \phi_\alpha. \quad (\text{A.152})$$

Furthermore, we have that

$$\begin{aligned} 0 &= \left\| \psi - \sum_{\alpha \in A} (\phi_\alpha, \psi) \phi_\alpha \right\|^2 = \lim \left(\|\psi\|^2 - \sum_{j=1}^n |(\phi_{\alpha_j}, \psi)|^2 \right) \\ &= \|\psi\|^2 - \sum_{\alpha \in A} |(\phi_\alpha, \psi)|^2, \end{aligned} \quad (\text{A.153})$$

and Eq. (A.149) follows. ■

The Eq. (A.149) is sometimes called *Parseval's relation*.

Definition A.64. A metric space which has a countable dense subset is said to be topologically **separable**.

Theorem A.65. A Hilbert space $\mathcal{H}$ is separable if and only if it has a countable orthonormal basis S . If there are $N < \infty$ elements in S , then $\mathcal{H}$ is isomorphic to $\mathbb{C}^N$. If there are countably many elements in S , then $\mathcal{H}$ is isomorphic to l_2 ¹¹.

Proof. Suppose $\mathcal{H}$ is separable and take $\{\phi_n\}$ as a countable dense set. Take out of the sequence some of the ϕ_n to get a subcollection of independent vectors. Such a subcollection spans the same dense space as $\{\phi_n\}$. Apply the Gram-Schmidt procedure to obtain a countable orthonormal system.

Now take $\{\psi_n\}$ as a complete orthonormal system of $\mathcal{H}$. By the theorem A.63, the set of finite linear combinations of ψ_n is dense in $\mathcal{H}$, such a set is countable, therefore $\mathcal{H}$ is separable.

Take $\mathcal{H}$ separable and $\{\psi_n\}$, $n = 1, 2, \dots$, a complete orthonormal system. Define $\mathcal{U} : \mathcal{H} \rightarrow l_2$ by $\mathcal{U} : \phi \rightarrow \{(\psi_n, \phi)\}$, $n = 1, 2, \dots$. By the theorem A.63 it is well defined and onto, by Parseval's relation, it is unitary.

In the case $N < \infty$, an analogous map can be defined. ■

Using the fact that $\mathcal{L}^2$ is a Hilbert space and the last theorem, we have that $\mathcal{L}^2$ is isomorphic to l_2 .

We end the discussion about Hilbert spaces with an important theorem in mathematical physics. First, we say that an operator $A : X \rightarrow Y$ is *everywhere defined* if $D(A) = X$.

Theorem A.66. (Hellinger-Toeplitz theorem) Let A be an everywhere defined linear operator on a Hilbert space $\mathcal{H}$ with $(A\phi, \psi) = (\phi, A\psi)$, for all $\phi, \psi \in \mathcal{H}$. Then A is bounded.

Proof. Suppose that $\langle \phi_n, A\phi_n \rangle \rightarrow \langle \phi, \psi \rangle$. Then, for any $\xi \in \mathcal{H}$ we have that

$$\begin{aligned} (\xi, \psi) &= \lim_{n \rightarrow \infty} (\xi, A\phi_n) = \lim_{n \rightarrow \infty} (A\xi, \phi_n) \\ &= (A\xi, \phi) = (\xi, A\phi), \end{aligned} \tag{A.154}$$

thus $A\phi = \psi$, which means that $\Gamma(A)$ is a closed graph. By the closed graph theorem (theorem A.51), A is bounded. ■

¹¹ l_2 is the set of sequences $\{x_n\}$, $n = 1, 2, \dots$, of complex numbers which satisfy $\sum_{n=1}^{\infty} |x_n|^2 < \infty$.

A.3 Spectral Theorem

We dedicate this section to explore constructions about bounded operators that allow us to culminate into the spectral theorem. For such a section do not extend too much, we focus only on the minimum concepts needed to prove the spectral theorem for bounded operators.

Definition A.67. Let X and Y be Banach spaces, $T : X \rightarrow Y$ a bounded linear operator. The Banach space **adjoint** of T , denoted by T' , is the bounded linear operator from Y^* to X^* defined by

$$(T'l)(x) = l(Tx) \quad (\text{A.155})$$

for all $l \in Y^*$, $x \in X$.

Theorem A.68. Let X and Y be Banach spaces. The map $T \rightarrow T'$ is an isomorphism of $\mathcal{L}(X, Y)$ into $\mathcal{L}(X^*, Y^*)$.

Proof. The linearity of $T \rightarrow T'$ follows from the definition of T' . To prove the isometry¹² we use the operator norm, Eq. (A.111) and the corollary A.48 to get

$$\begin{aligned} \|T\|_{\mathcal{L}(X,Y)} &= \sup_{\|x\| \leq 1} \|Tx\|_Y = \sup_{\|x\| \leq 1} \|l(Tx)\|_{Y^*} = \sup_{\|x\| \leq 1} \left(\sup_{\|l\| \leq 1} |l(Tx)| \right) \\ &= \sup_{\|l\| \leq 1} \left(\sup_{\|x\| \leq 1} |(T'l)(x)| \right) = \sup_{\|l\| \leq 1} \|T'l\| \\ &\Rightarrow \|T\|_{\mathcal{L}(X,Y)} = \|T'\|_{\mathcal{L}(X^*,Y^*)}. \end{aligned} \quad (\text{A.156})$$

■

Most of the time we are concerned about operators which map a Hilbert space $\mathcal{H}$ into itself, that is $T : \mathcal{H} \rightarrow \mathcal{H}$. The Banach space adjoint does the map $T' : \mathcal{H}^* \rightarrow \mathcal{H}^*$. Let us consider $C : \mathcal{H} \rightarrow \mathcal{H}^*$, by the Riesz representation theorem (theorem A.60), C is the functional $(\psi, \cdot)$ acting on $\mathcal{H}$.

Define $T^* : \mathcal{H} \rightarrow \mathcal{H}$ as $T^* = C^{-1}T'C$, so we have that

$$(T\phi, \psi) = (C\psi)(T\phi) = (T'C\psi)(\phi) = (\phi, C^{-1}T'C\psi) = (\phi, T^*\psi), \quad (\text{A.157})$$

T^* is called the **Hilbert space adjoint** of T . Since we are mostly interested in the Hilbert space case, we will call it only the adjoint and let $'$ and $*$ differentiate the cases.

¹² T is said to be an isometry if $\|Tx\| = \|x\|$.

Proposition A.69. Any adjoint operators $A, B \in \mathcal{L}(X)$, satisfies the following properties

- (i) $\|A' A\| = \|A\|^2$;
- (ii) $(AB)' = B' A'$;
- (iii) $(A + B)' = A' + B'$.

Proof. To prove (i) we note that $\|A' A\| \leq \|A'\| \|A\| = \|A\| \|A\| = \|A\|^2$. On the other hand we have

$$\begin{aligned} \|A\|^2 &= \left(\sup_{\|\phi\|=1} \|A\phi\| \right)^2 = \sup_{\|\phi\|=1} \|A\phi\|^2 = \sup_{\|\phi\|=1} (A\phi, A\phi) \\ &= \sup_{\|\phi\|=1} (A' A\phi, \phi) \leq \sup_{\|\phi\|=1} \|A' A\phi\| \|\phi\| = \|A' A\|, \end{aligned} \quad (\text{A.158})$$

therefore, $\|A' A\| = \|A\|^2$.

In order to show (ii), assume A, B adjoint and define $\xi = B\phi$, then it follows

$$(A\xi, \psi) = (\xi, A'\psi) = (B\phi, A'\psi) = (\phi, B' A'\psi), \quad (\text{A.159})$$

but $((AB)\phi, \psi) = (\phi, (AB)'\psi)$. Thus, $(AB)' = B' A'$.

(iii) follows similarly to (ii). ■

Definition A.70. A bounded operator A on a Hilbert space is called **self-adjoint** if $A = A^*$.

Another important kind of operators are the projections.

Definition A.71. If $P \in \mathcal{L}(\mathcal{H})$ and $P^2 = P$, then P is called a **projection**. If in addition $P = P^*$, then P is called an **orthogonal projection**.

Definition A.72. If the range of $\lambda I - A$, $\text{Ran}(\lambda I - A)$, is dense in $\mathcal{H}$ and if $\lambda I - A$ has a bounded inverse on $\text{Ran}(\lambda I - A)$, then λ is said to belong to the **resolvent set** of A , $\rho(A)$.

Theorem A.73. Let X be a Banach space and suppose that $A \in \mathcal{X}$. Then $\rho(A)$ is an open subset of $\mathbb{C}$ and $(\lambda I - A)^{-1}$ is an analytic $\mathcal{L}(X)$ -valued function on each component (maximal connected subset) of D . For any two points $\lambda, \mu \in \rho(A)$, $(\lambda I - A)^{-1}$ and $(\mu I - A)^{-1}$ commute and

$$(\lambda I - A)^{-1} - (\mu I - A)^{-1} = (\mu - \lambda)(\mu I - A)^{-1}(\lambda I - A)^{-1} \quad (\text{A.160})$$

Proof. Let us take $\lambda_0 \in \rho(A)$ and, momentarily, ignore questions about convergence, then we can write

$$\begin{aligned} \frac{1}{\lambda I - A} &= \frac{1}{\lambda - \lambda_0 I + (\lambda_0 I - A)} = \frac{1}{\lambda_0 I - A} \left(\frac{1}{1 - \frac{\lambda_0 - \lambda}{\lambda_0 I - A}} \right) \\ &= \frac{1}{\lambda_0 I - A} \left[1 + \sum_{n=1}^{\infty} \left(\frac{\lambda_0 - \lambda}{\lambda_0 I - A} \right)^n \right], \end{aligned} \quad (\text{A.161})$$

this last equation suggests us to define

$$(\lambda I - A)^{-1} = (\lambda_0 I - A)^{-1} \left\{ I + \sum_{n=1}^{\infty} (\lambda_0 - \lambda)^n [(\lambda_0 I - A)^{-1}]^n \right\}. \quad (\text{A.162})$$

The previous series converges if $|\lambda - \lambda_0| < \|(\lambda_0 I - A)^{-1}\|^{-1}$, in such a scenario, $(\lambda I - A)^{-1}$ is well defined. Therefore, $\lambda \in \rho(A)$ if $|\lambda - \lambda_0| < \|(\lambda_0 I - A)^{-1}\|^{-1}$ and $\rho(A)$ is open. Once that $(\lambda I - A)^{-1}$ has a convergent power series expansion, $(\lambda I - A)^{-1}$ is analytic.

By direct computation of the following expression

$$(\lambda I - A)^{-1} - (\mu I - A)^{-1} = (\lambda I - A)^{-1}(\mu I - A)(\mu I - A)^{-1} - (\lambda I - A)^{-1}(\lambda I - A)(\mu I - A)^{-1}, \quad (\text{A.163})$$

we conclude that $(\lambda I - A)^{-1}$ and $(\mu I - A)^{-1}$ commute and the Eq. (A.160) follows. ■

Sometimes the quantity $(\lambda I - A)^{-1}$ is called the **resolvent** of A , denoted $R_\lambda(A) = (\lambda I - A)^{-1}$, and the Eq. (A.160) is called the **first resolvent formula**. Note that, if we take formally

$$\frac{1}{\lambda I - A} = \left(\frac{1}{\lambda} \right) \frac{1}{I - \frac{A}{\lambda}} = \frac{1}{\lambda} \left[1 + \sum_{n=1}^{\infty} \left(\frac{A}{\lambda} \right)^n \right] \quad (\text{A.164})$$

it suggests that we have

$$R_\lambda(A) = \frac{1}{\lambda} \left[I + \sum_{n=1}^{\infty} \left(\frac{A}{\lambda} \right)^n \right], \quad (\text{A.165})$$

such a series is called the **Neumann series** for $(\lambda I - A)^{-1}$.

Theorem A.74. The resolvent of A , $R_\lambda(A)$, is analytic in the set of regular points¹³.

¹³Set of numbers $x \in \mathbb{C}$ for which an operator has a bounded inverse.

Proof. Take λ and λ_0 to be regular points. By the first resolvent formula, Eq. (A.160), we have that

$$\lim_{\lambda \rightarrow \lambda_0} \frac{R_\lambda(A) - R_{\lambda_0}(A)}{\lambda - \lambda_0} = \lim_{\lambda \rightarrow \lambda_0} R_{\lambda_0}(A)R_\lambda(A) = R_{\lambda_0}(A) \lim_{\lambda \rightarrow \lambda_0} R_\lambda(A). \quad (\text{A.166})$$

Let $\{R_{\lambda,n}(A)\}$ be a sequence which converges to $R_\lambda(A)$. Then $R_\lambda(A)^{-1}R_{\lambda,n}(A) \rightarrow I$, and for any $\varepsilon > 0$, there must exist an $n > N$ such that

$$\|R_\lambda(A)^{-1}R_{\lambda,n}(A) - I\| < \varepsilon. \quad (\text{A.167})$$

Now take N_1 such that for $n > N_1$ we have $\|R_\lambda(A)^{-1}R_{\lambda,n}(A) - I\| < 1$, and consider the series

$$I + \sum_{k=1}^{\infty} [I - R_\lambda(A)^{-1}R_{\lambda,n}(A)]^k. \quad (\text{A.168})$$

By the same argument used in the proof of theorem A.73, and since $\|R_\lambda(A)^{-1}R_{\lambda,n}(A) - I\| < 1$, the series must converge to $(R_\lambda(A)^{-1}R_{\lambda,n}(A))^{-1} = R_{\lambda,n}(A)^{-1}R_\lambda(A)$. Therefore, we have

$$\begin{aligned} \|R_\lambda(A)^{-1}R_{\lambda,n}(A) - I\| &\leq \sum_{k=1}^{\infty} \|[I - R_\lambda(A)^{-1}R_{\lambda,n}(A)]^k\| \\ &= \sum_{k=1}^{\infty} \|R_\lambda(A)^{-k} [R_\lambda(A) - R_{\lambda,n}(A)]^k\| \\ &\leq \sum_{k=1}^{\infty} \|R_\lambda(A)^{-1}\|^k \|[R_\lambda(A) - R_{\lambda,n}(A)]^k\| = \delta, \end{aligned} \quad (\text{A.169})$$

Once that $R_\lambda(A) \rightarrow R_{\lambda,n}(A)$, we can take N_2 such that $n > N_2$ will make δ as small as desired; hence

$$\begin{aligned} \|I - R_{\lambda,n}(A)^{-1}R_\lambda(A)\| &\rightarrow 0 \\ R_{\lambda,n}(A)^{-1}R_\lambda(A) &\rightarrow I \\ R_{\lambda,n}(A)^{-1} &\rightarrow R_\lambda(A)^{-1}, \end{aligned} \quad (\text{A.170})$$

therefore, taking the inverse is continuous.

Using the continuity of taking the inverse, we can write

$$\lim_{\lambda \rightarrow \lambda_0} R_\lambda(A) = \lim_{\lambda \rightarrow \lambda_0} (\lambda I - A)^{-1} = (\lambda_0 I - A)^{-1} = R_{\lambda_0}(A), \quad (\text{A.171})$$

thus, the limit of Eq. (A.166) exists, and symbolically we have that $R'_\lambda(A)|_{\lambda=\lambda_0} = R_{\lambda_0}^2(A)$. ■

Remembering that every Hilbert space is a Banach space, we can define some important quantities.

Definition A.75. If the range of $\lambda I - A$, $\text{Ran}(\lambda - A)$, is dense in $\mathcal{H}$ and if $\lambda I - A$ has an unbounded inverse, then λ is said to belong to the **continuous spectrum** of A , $\sigma_c(A)$.

Definition A.76. If the range of $\lambda I - A$, $\text{Ran}(\lambda - A)$, is not dense in $\mathcal{H}$ but $\lambda I - A$ has an inverse, bounded or unbounded, then λ is said to belong to the **residual spectrum** of A , $\sigma_r(A)$.

Definition A.77. If $(\lambda I - A)^{-1}$ does not exist, then λ is said to belong to the **point spectrum** (or **discrete spectrum**) of A , σ_p .

Note that the set σ_p is just the eigenvalues of A .

Definition A.78. The set $\sigma(A) = \sigma_c(A) \cup \sigma_r(A) \cup \sigma_p(A)$ is called the **spectrum** of A .

Definition A.79. Let

$$r(T) = \sup_{\lambda \in \sigma(T)} |\lambda| \quad (\text{A.172})$$

$r(T)$ is called the **spectral radius** of T .

Theorem A.80. Let X be a Banach space, $T \in \mathcal{L}(X)$. Then $\lim_{n \rightarrow \infty} \|T^n\|^{\frac{1}{n}}$ exists and is equal to $r(T)$.

Proof. Take $a_n = \ln \|T^n\|$, then we have

$$\begin{aligned} a_{m+n} &= \ln \|T^{m+n}\| \leq \ln (\|T^m\| \|T^n\|) = \ln \|T^m\| + \ln \|T^n\|, \\ &\Rightarrow a_{m+n} \leq a_m + a_n. \end{aligned} \quad (\text{A.173})$$

Setting $n = mq + r$ where m, q and r are positive integers such that $0 \leq r \leq m - 1$, we obtain the following

$$a_n \leq a_{mq} + a_r, \quad (\text{A.174})$$

$$a_{mq+r} \leq a_{mq} + a_r, \quad (\text{A.175})$$

$$a_r \leq a_m + a_{-1} \leq a_m, \quad (\text{A.176})$$

therefore, for any $n \in [m, 2m - 1]$, we have that

$$\limsup \frac{a_n}{n} \leq \frac{a_m}{m}. \quad (\text{A.177})$$

Once that $a_n \geq \frac{1}{n}$, we have

$$\lim_{n \rightarrow \infty} \frac{a_n}{n} = \inf \frac{a_n}{n}. \quad (\text{A.178})$$

Then $\lim_{n \rightarrow \infty} \ln \|T^n\|$ exists, and $\lim_{n \rightarrow \infty} \|T^n\|^{\frac{1}{n}}$ exists.

Once that $R_\lambda(T)$ is analytic in $\rho(T)$, and $\{\lambda \mid |\lambda| > r(T)\} \subset \rho(T)$, the convergence of the Neumann series (Eq. A.165) cannot be smaller than $r^{-1}(T)$. Using the Cauchy-Hadamard theorem, we have that the radius of convergence of the Neumann series is the inverse of $\limsup_n \|T\|^{1/n} = \lim_{n \rightarrow \infty} \|T\|^{1/n}$, therefore

$$r(T) = \lim_{n \rightarrow \infty} \|T\|^{\frac{1}{n}}. \quad (\text{A.179})$$

■

If $X = \mathcal{H}$ and $T = A$ is a self-adjoint operator, we can use the property (i) of proposition A.69 to see that

$$\begin{aligned} r(A) &= \lim_{k \rightarrow \infty} \|A^k\|^{\frac{1}{k}} = \lim_{n \rightarrow \infty} \|A^{2^n}\|^{2^{-n}} = \|A\| \\ &\Rightarrow r(A) = \|A\|. \end{aligned} \quad (\text{A.180})$$

Theorem A.81. (Phillips' Theorem) Let X be a Banach space, $T \in \mathcal{L}(X)$. Then $\sigma(T) = \sigma(T')$ and $R_\lambda(T) = R_\lambda(T')$. If $X = \mathcal{H}$ is a Hilbert space, then $\sigma(T^*) = \{\lambda \mid \bar{\lambda} \in \sigma(T)\}$ and $R_{\bar{\lambda}}(T^*) = R_\lambda(T)^*$.

Proof. First, we use property (ii) of proposition A.69 and notice that

$$I_X = I_{X'} = (T^{-1}T)' = T' (T^{-1})^{-1} = (TT^{-1})' = (T^{-1})^{-1} T'. \quad (\text{A.181})$$

Then, T being an isomorphism implies that T' is an isomorphism, and $\rho(T) \subset \rho(T')$. Repeating the same reasoning, we get that $\rho(T') = \rho(T)$. Therefore, $\sigma(T) = \sigma(T')$.

Now we notice that

$$I_{X'} = [R_\lambda(T)(T - \lambda I_X)]' = (T - \lambda I_X)' R_\lambda(T)' = (T' - \lambda I_{X'}) R_\lambda(T'). \quad (\text{A.182})$$

Thus, $R_\lambda(T) = R_\lambda(T')$.

The case for Hilbert spaces follows similarly using that $I = I^*$. ■

Assume that A is a self-adjoint operator acting over a Hilbert space. By the last theorem, we have that $\sigma(A^*) = \{\lambda \mid \bar{\lambda} \in \sigma(A)\}$, but $\sigma(A^*) = \sigma(A)$, therefore $\{\lambda \mid \bar{\lambda} \in \sigma(A)\} = \{\lambda \mid \lambda \in \sigma(A)\}$. Then, $\Im \lambda = \Im \bar{\lambda}$, which implies that $\lambda \in \mathbb{R}$ and $\sigma(A) \subset \mathbb{R}$. Actually, we can restrict the spectrum of a bounded self-adjoint operator to an interval of $\mathbb{R}$.

Theorem A.82. Let A be a bounded self-adjoint operator $A \in \mathcal{L}(\mathcal{H})$. Then, there exist m and M real numbers such that $\sigma(A) \subset [m, M]$. Furthermore, m and M belong to $\sigma(A)$.

Proof. We have that $\|A\| = \sup_{\|\phi\|=1} |(A\phi, \phi)|$, so we define

$$m = \inf_{\|\phi\|=1} (A\phi, \phi), \quad M = \sup_{\|\phi\|=1} (A\phi, \phi), \quad (\text{A.183})$$

then $\|A\| = \max(|m|, |M|)$. Now assume that $\phi \neq 0$, then $(A\phi/\|\phi\|, \phi/\|\phi\|) < M$. Then, for every ϕ we have $(A\phi, \phi) \leq M(\phi, \phi)$.

Suppose that $\lambda \notin [m, M]$, so $\lambda < m$ or $\lambda > M$. Take $\lambda > M$, so there is $\varepsilon > 0$ such that $\lambda = M + \varepsilon$. Thus

$$((A - \lambda)\phi, \phi) \leq M(\phi, \phi) - \lambda(\phi, \phi) \leq -\varepsilon(\phi, \phi) < 0 \quad (\text{A.184})$$

or, in terms of absolute values

$$|((A - \lambda)\phi, \phi)| \geq \varepsilon\|\phi\|^2. \quad (\text{A.185})$$

By the Cauchy-Schwarz inequality (Corollary A.55), we have $|((A - \lambda)\phi, \phi)| \leq \|(A - \lambda)\phi\|\|\phi\|$, which implies $\|(A - \lambda)\phi\| \geq \varepsilon\|\phi\|$. It is worth noting that the values μ which satisfy $\|(A - \mu)\phi\| > \varepsilon\|\phi\|$ are sometimes called *approximate eigenvalues* of A . Now take the set of all approximated eigenvalues of A and denote it by $\pi(A)$, called the *approximate spectrum* of A . Then, it follows directly that $\lambda \notin \pi(A)$.

Now take any complex number μ and any $\phi \neq 0$, then

$$\begin{aligned} 0 < |\mu - \bar{\mu}|\|\phi\|^2 &= ((A - \mu)\phi, \phi) - ((A - \bar{\mu})\phi, \phi) = ((A - \mu)\phi, \phi) - (\phi, (A^* - \mu)\phi) \\ &= ((A - \mu)\phi, \phi) - (\phi, (A - \mu)\phi) \leq 2\|(A - \mu)\phi\|\|\phi\|. \end{aligned} \quad (\text{A.186})$$

If $\Im\mu = 0$ and $\mu \in \sigma(A)$, there is some ϕ_n such that $\|(A - \mu)\phi_n\| \rightarrow 0$, therefore $\pi(A) = \sigma(A)$.

So, by the last result, $\lambda \notin \sigma(A)$. This is a contradiction, so $\lambda < M$. It follows similarly that $\lambda > m$, therefore $\lambda \in [m, M]$.

There is some real number ν such that $M - \nu \geq m - \nu \geq 0$. So we have that

$$\sup_{\|\phi\|=1} ((A - \nu)\phi, \phi) = M - \nu = \|A - \nu\|. \quad (\text{A.187})$$

We need to show that $M \in \sigma(A)$. There must exist a sequence of ϕ_n , $\|\phi_n\| = 1$ for every n such that $(A\phi_n, \phi_n) \rightarrow M$. By the definition of M , the sequence $\{(A\phi_n, \phi_n)\}$ must approach from below

$$(A\phi_n, \phi_n) = M - \varepsilon_n, \quad \text{where } \varepsilon_n \rightarrow 0 \text{ and } \varepsilon_n > 0, \forall n. \quad (\text{A.188})$$

Consider

$$\begin{aligned}\|A\phi_n - M\phi_n\| &= \|A\phi_n\|^2 - 2M(A\phi_n, \phi_n) + M^2\|\phi_n\|^2 \\ &\leq \|A\|2M(A\phi_n, \phi_n) + M^2 = 2M\varepsilon_n \rightarrow 0.\end{aligned}\quad (\text{A.189})$$

Which implies that $M \in \pi(A) = \sigma(A)$. Analogously, one shows that $m \in \sigma(A)$. ■

Theorem A.83. (Spectral Decomposition Theorem) To every bounded self-adjoint transformation A in a Hilbert space, such that $\|A\| = \max(|m|, |M|)$, we can assign a **spectral family** on the interval $[m, M]$. That is, a family of projections $\{E_\lambda\}$ depending on the real parameter λ such that

- (i) $E_\lambda \leq E_\mu$, or equivalently $E_\lambda E_\mu = E_\lambda$ for $\lambda \leq \mu$;
- (ii) $E_{\lambda+0} = E_\lambda$;
- (iii) $E_\lambda = 0$ for $\lambda < m$ and $E_\lambda = I$ for $\lambda > M$.

In such a way that we have

$$A = \int_m^M \lambda dE_\lambda. \quad (\text{A.190})$$

Moreover, these properties uniquely determine the family $\{E_\lambda\}$. For every fixed value of the parameter, E_λ is the limit of a sequence of polynomials in A .

Proof. Take the function $e_\mu(\lambda)$ depending on the real parameter μ , which is 1 if $\lambda \leq \mu$ and 0 for $\lambda > \mu$. This function is a projection and is a continuous function. Denote then the analogous projection $e_\mu(A)$ by E_μ . It is clear that $e_\mu(\lambda)e_\nu(\lambda) = e_\mu(\lambda)$ for $\mu < \nu$, therefore $E_\mu E_\nu = E_\mu$. Once that we have $m \leq \lambda \leq M$, we have $E_\mu = 0$ if $\mu < m$ and E_μ for $\mu \geq M$.

To prove that our map E_μ is meaningful, it needs to be continuous from the right. For that, let's pick a sequence of polynomials $p_n(\lambda)$ which decrease in $[m, M]$ to e_μ , and in addition satisfy

$$p_n(\lambda) \geq \mu_{\mu+\frac{1}{n}}(\lambda). \quad (\text{A.191})$$

Then we have

$$p_n(A) \geq E_{\mu+\frac{1}{n}} \geq E_\mu. \quad (\text{A.192})$$

Since $p_n(A) \rightarrow \mu$, we have that $E_{\mu+\frac{1}{n}} \rightarrow E_\mu$ as $n \rightarrow \infty$, E_μ is a monotone function of μ , so $E_{\mu+\varepsilon} \rightarrow E_\mu$ as $\varepsilon \rightarrow 0$. If $\mu < \nu$ we have

$$\mu[e_\nu(\lambda) - e_\mu(\lambda)] \leq \lambda[e_\nu(\lambda) - e_\mu(\lambda)] \leq \nu[e_\nu(\lambda) - e_\mu(\lambda)], \quad (\text{A.193})$$

then

$$\mu[E_\nu - E_\mu] \leq A[E_\nu - E_\mu] \leq \nu[E_\nu - E_\mu]. \quad (\text{A.194})$$

Take a sequence $\mu_0 < m < \mu_1 < \dots < \mu_{n-1} < M \leq \mu_n$. Take $\mu = \mu_{k-1}$ and $\nu = \mu_k$ ($k = 1, 2, \dots, n$) in the previous equation, taking its sum

$$\sum_{k=1}^n \mu_{k-1}(E_{\mu_k} - E_{\mu_{k-1}}) \leq A \sum_{k=1}^n (E_{\mu_k} - E_{\mu_{k-1}}) \leq \sum_{k=1}^n \mu_k(E_{\mu_k} - E_{\mu_{k-1}}), \quad (\text{A.195})$$

in the middle we have $A(E_{\mu_n} - E_{\mu_0}) = A(I - 0) = A$. If $\max(\mu_k - \mu_{k-1}) \leq \varepsilon$, the difference of the first and third members is less than εI . Take λ_k as any point between μ_{k-1} and μ_k , so

$$\left\| A - \sum_{k=1}^n (E_{\mu_k} - E_{\mu_{k-1}}) \right\| \leq \varepsilon. \quad (\text{A.196})$$

Now, increasing the number n of the decomposition of the intervals (μ_{k-1}, μ_k) , in such a way that the maximum length tends to zero, the sums $\sum_{k=1}^n \lambda_k(E_{\mu_k} - E_{\mu_{k-1}})$ tend to A in norm. Since E_λ is constant for $\lambda \geq M$ and for $\lambda < m$, we can use the Riemann-Stieltjes integral (see Eq (A.67)) to write

$$A = \int_{-\infty}^{\infty} \lambda dE_\lambda = \int_m^M \lambda dE_\lambda. \quad (\text{A.197})$$

Remains to prove the uniqueness. For that, let us explore the last representation of A further. Since $\left[\sum_{k=1}^n \lambda_k(E_{\mu_k} - E_{\mu_{k-1}}) \right]^r = \sum_{k=1}^n \lambda_k^r(E_{\mu_k} - E_{\mu_{k-1}})$, we have that

$$A^r = \int_m^M \lambda^r dE_\lambda. \quad (\text{A.198})$$

That ensures that for any polynomial $p(\lambda)$ we can write

$$p(A) = \int_m^M p(\lambda) dE_\lambda. \quad (\text{A.199})$$

Using the fact that polynomials are dense in the set of continuous functions $u(\lambda)$ in the interval $[m, M]$, we can extend this result to any $u(\lambda)$. Given any ε , we can find a polynomial $p(\lambda)$ such that $-\varepsilon/3 \leq u(\lambda) - p(\lambda) \leq \varepsilon/3$ in $[m, M]$; therefore

$$\frac{\varepsilon}{3} I \leq u(A) - p(A) \leq \frac{\varepsilon}{3} I, \quad (\text{A.200})$$

hence $\|u(A) - p(A)\| \leq \varepsilon/3$.

For every decomposition on the λ -axis we must have

$$S_u = \sum_{k=1}^n u(\lambda_k)(E_{\mu_k} - E_{\mu_{k-1}}), \quad (\text{A.201})$$

and analogous S_p for $p(\lambda)$. Hence, by the same argument, we have

$$\|S_u - S_p\| \leq \frac{\varepsilon}{3}. \quad (\text{A.202})$$

If the decomposition has enough parts, we shall have $\|p(A) - S_p\| \leq \varepsilon/3$. Thus

$$\|u(A) - S_u\| \leq \|u(A) - p(A)\| + \|p(A) - S_p\| + \|S_p - S_u\| \leq \varepsilon. \quad (\text{A.203})$$

Then, for every continuous function $u(\lambda)$, we have

$$u(A) = \int_m^M u(\lambda) dE_\lambda. \quad (\text{A.204})$$

So, for any $\phi, \psi \in \mathcal{H}$, we have that

$$(u(A)\phi, \psi) = \int_m^M u(\lambda) d(E_\lambda \phi, \psi). \quad (\text{A.205})$$

It is clear that the right-hand side of the last equation does not depend on the choice of $\{E_\lambda\}$. Therefore $(E_\lambda \phi, \psi)$ is determined. Such a function is continuous from the right and has the value (f, g) at M , then it is uniquely determined everywhere. ■

Just in the study of bounded self-adjoint operators, we could spend a lot of time and pages. However, to keep it as brief as possible, we wrap up this section with a final case of the spectral theorem.

Theorem A.84. Every unitary¹⁴ transformation U has a spectral decomposition

$$U = \int_0^{2\pi} e^{i\theta} dE_\theta \quad (\text{A.206})$$

where $\{E_\theta\}$ is a spectral family over the segment $0 \leq \theta \leq 2\pi$. We can require that E_θ be continuous at the point $\theta = 0$, that is, $E_0 = 0$; $\{E_\theta\}$ will then be determined uniquely by U . Moreover, E_θ is the limit of a sequence of polynomials in U and U^{-1} .

¹⁴We call a unitary transformation one such that its inverse coincides with its adjoint, that is, $U^*U = I$.

Proof. First, we take the trigonometric polynomial

$$p(e^{i\mu}) = \sum_{k=-n}^n c_k e^{ik\mu}, \quad (\text{A.207})$$

and assign it to

$$p(U) = \sum_{k=-n}^n c_k U^k. \quad (\text{A.208})$$

We admit c_k to be complex. Such a correspondence is obviously linear. The conjugate polynomial, $\overline{p(e^{i\mu})} = \sum_{k=-n}^n \bar{c}_k e^{-ik\mu}$, is the adjoint of $p(e^{i\mu})$. If $p(e^{i\mu})$ is real, then $p(U)$ is self-adjoint. And if we have $p(e^{i\mu}) \geq 0$, then $p(U) \geq 0$.

Now take the function $e_\theta(\mu)$, which depends on the parameter $0 \leq \theta \leq 2\pi$, and is defined as

$$e_\theta(\mu) = \begin{cases} 1, & \text{if } 2k\pi < \mu \leq 2k\pi + \theta, \\ 0, & \text{if } 2k\pi + \theta < \mu \leq 2(k+1)\pi, \end{cases} \quad (\text{A.209})$$

where $k = 0, \pm 1, \pm 2, \dots$. These functions are equal to their squares, so the corresponding transformation E_μ is a projection. In particular, $E_0 = 0$ and $E_{2\pi} = I$, and if $\mu \leq \nu$, then $E_\mu E_\nu = E_\mu$.

The function E_μ is continuous on the right. Consider $0 \leq \theta < 2\pi$, the functions $e'_\mu(\theta) = e_\mu(\theta) + e'_0(\theta)$, where $e'_0(\theta)$ is equal to 1 at $\theta = 2k\pi$ and zero elsewhere. Then, for each fixed θ , we can construct trigonometric polynomials $p_n(e^{i\mu})$ which decrease to $e'_\theta(\mu)$, and for n large enough, $p_n(e^{i\mu}) \geq e'_{\theta+\frac{1}{n}}(\mu)$. So, the corresponding transformations $E'_{\mu+\frac{1}{n}} \rightarrow E'_\mu$, more generally, we have $\lim_{\xi \rightarrow \mu^+} E_\xi = E_\mu$.

Thus, the transformation E_μ forms a spectral family over $[0, 2\pi]$, and $E_0 = 0$. By the construction, E_μ is the limit of polynomials in U and $U^* = U^{-1}$.

Now consider a decomposition of the interval $[0, 2\pi]$ using the points $0 = \theta_0 < \theta_1 < \dots < \theta_n = 2\pi$, such that $\max(\theta_k - \theta_{k-1}) \leq \varepsilon$. Take any θ such that $\theta_{k-1} < \theta \leq \theta_k$, so we have

$$\left| e^{i\theta} - \sum_{k=1}^n e^{i\theta_k} [e_{\theta_k}(\theta)a - e_{\theta_{k-1}}(\theta)] \right| = |e^{i\theta} - e^{i\theta_k}| \leq |\theta - \theta_k| \leq \varepsilon. \quad (\text{A.210})$$

The analogous follows for $\theta = 0$. Then, for any value of θ , we have

$$0 \leq \overline{\left[e^{i\theta} - \sum_{k=1}^n e^{i\theta_k} [e_{\theta_k}(\theta)a - e_{\theta_{k-1}}(\theta)] \right]} \left[e^{i\theta} - \sum_{k=1}^n e^{i\theta_k} [e_{\theta_k}(\theta)a - e_{\theta_{k-1}}(\theta)] \right] \leq \varepsilon^2. \quad (\text{A.211})$$

Using the corresponding transformations, we get

$$\left\| U - \sum_{k=1}^n e^{i\theta_k} (E_{\mu_k} - E_{\mu_{k-1}}) \right\| \leq \varepsilon. \quad (\text{A.212})$$

Which, in the limit, is the desired representation. By the same way that in the previous theorem, it follows that

$$U^n = \int_0^{2\pi} e^{in\theta} dE_\theta. \quad (\text{A.213})$$

Also, using the same construction, we have for any continuous function u

$$u(U) = \int_0^{2\pi} u(e^{i\theta}) dE_\mu, \quad (\text{A.214})$$

from which it follows for any $\phi, \psi \in \mathcal{H}$, that

$$(u(U)\phi, \psi) = \int_0^{2\pi} u(e^{i\theta}) d(E_\theta\phi, \psi). \quad (\text{A.215})$$

And the uniqueness follows from the same reasoning. ■

A.4 Generalized Functions

Roughly speaking, the theory of generalized functions is the theory of how to work with “functions” that diverge at some point. Here we base our discussion on Ref. [34] to provide just an introductory and intuitive notion about such objects. For this reason, we relax the mathematical rigor of this section. However, we must bear in mind that all the results presented here have rigorous theorems that ensure their validity. We choose not to develop these here because their side constructions would greatly enlarge the previous sections. These theorems and the main ingredients needed for a proper construction of the generalized functions can be found in Ref. [304].

The simplest case of a singular function is given by a function that is zero everywhere except at the point, say x_0 , where it diverges. If we have in mind that the following equation is meaningless, we can represent such a singular function by

$$\delta(x - x_0) = \begin{cases} 0, & \text{if } x \neq x_0 \\ \infty, & \text{if } x = x_0. \end{cases} \quad (\text{A.216})$$

To give a proper meaning to the last equation, we must integrate it with a “sufficiently good” function.

By a sufficiently good function, we must require that the function has a bounded support¹⁵ and with derivatives of all orders. We call these functions test functions and represent their space by K . It is direct to see that the space K is a linear space.

We can define linear functionals over the space K by using an inner product. So, f is a linear functional on K if for all $\phi(x) \in K$, the real number (f, ϕ) exists, satisfying the linearity and continuity conditions. If f is absolutely integrable in every bounded region of $\mathbb{R}^n$, we can represent our inner product by

$$(f, \phi) = \int_{\mathbb{R}^n} f(x)\phi(x). \quad (\text{A.217})$$

We remark that this is a special kind of continuous linear functional; there are others. We have two kinds of continuous linear functionals. In order to be clear, let us search for a locally summable¹⁶ function that evaluates $\phi(x) \in K$ at $x = 0$, that is, let us find an f , such that

$$\int_{\mathbb{R}^n} f(x)\phi(x) = \phi(0). \quad (\text{A.218})$$

If such a function does exist, it should act in the same way for all functions $\phi \in K$. Denote $x^2 = x_1^2 + \dots + x_n^2$ and take

$$\phi(x, a) = \begin{cases} e^{-\frac{a^2}{a^2-x^2}}, & \text{if } x < a \\ 0, & \text{if } x \geq a, \end{cases} \quad (\text{A.219})$$

then we have that $\phi(0, a) = e^{-1}$; however,

$$\lim_{a \rightarrow 0} \int_{\mathbb{R}^n} f(x)\phi(x, a) = \int_{\mathbb{R}^n} f(x) \lim_{a \rightarrow 0} \phi(x, a) = 0 \neq e^{-1}. \quad (\text{A.220})$$

Therefore, such a summable function does not exist. The function that acts as we desire is called the δ -function (remember that it is not a function) and is defined by its action on $\phi \in K$

$$(\delta(x), \phi(x)) = \phi(0), \quad (\text{A.221})$$

or its translated version $(\delta(x - x_0), \phi(x)) = \phi(x_0)$.

¹⁵The support of the function f is the region where $f(x) \neq 0$. Therefore, a bounded support means that the function is nonzero in a finite region.

¹⁶Can also be referred to as locally integrable. A function is locally summable if it is integrable in each compact subset.

So, with the previous discussion, we fix some nomenclature. We call a **generalized function** any functional defined on K . Functionals associated with locally summable functions are called **regular generalized functions**. Functionals which are defined by their action, similar to the δ -function, are called **irregular generalized functions**.

Clearly, for an irregular generalized function, say $\delta(x)$, the representation

$$(\delta(x), \phi(x)) = \int_{\mathbb{R}^n} \delta(x) \phi(x) dx, \quad (\text{A.222})$$

is meaningless and must be taken just as symbolic manipulation.

As we can see, it is meaningless to talk about the values of a generalized function at a given point. They need always to be “smeared out” by the test functions. The value of generalized functions in a neighborhood N of a point can be taken. If a generalized function vanishes in the neighborhood of every point, it vanishes, $(f, \phi) = 0$. If two generalized functions coincide on the open set G , $f - g$ vanishes in G . That is, any generalized function is uniquely determined by its local properties. The linear properties of generalized functions are defined straightforwardly using the integral representation.

We can also define the derivative and the integral of generalized functions. Worth noting is that not all ordinary functions have derivatives, but *all generalized functions have derivatives of all orders*, which are also generalized functions. To see that, let us first consider a regular generalized function defined by some continuous function $f(x)$ with a continuous first derivative and $\phi \in K$. Then, integrating by parts, we have

$$(f', \phi) = f(x)\phi(x) \Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} f(x)\phi'(x) dx = (f, -\phi'(x)), \quad (\text{A.223})$$

where the first contribution vanishes because ϕ has compact support. We can use the previous relation to define the derivative of generalized functions. Consider any generalized function (regular or irregular) f in K . Define the functional g by

$$(g, \phi) = (f, -\phi'). \quad (\text{A.224})$$

Then g is the derivative of f . The continuity and linearity of g follows trivially, so g is a generalized function. Usually, it is denoted by f' or $\frac{df}{dx}$. The rules of differentiation are preserved.

In particular, let us compute the derivative of the step function defined by

$$\theta(x) = \begin{cases} 0, & \text{if } x < 0 \\ 1, & \text{if } x > 0. \end{cases} \quad (\text{A.225})$$

using our previous definition, for any $\phi \in K$, we get

$$\begin{aligned} (\theta'(x), \phi(x)) &= (\theta(x), -\phi'(x)) = - \int_{-\infty}^{\infty} \theta(x) \phi'(x) dx = - \int_0^{\infty} \phi(x) dx = \phi(0) \\ \Rightarrow (\theta'(x), \phi(x)) &= (\delta(x), \phi(x)). \end{aligned} \quad (\text{A.226})$$

Thus, $\theta'(x) = \delta(x)$. By the same manipulations, one recovers that $\theta'(x+h) = \delta(x+h)$.

Using the same construction that we used for the first derivative, we can define the k -th derivative of a generalized function by

$$(f^{(k)}, \phi) = (f, (-1)^k \phi^{(k)}). \quad (\text{A.227})$$

Using this definition, it is straightforward to compute the k -th derivative of the δ -function

$$(\delta^{(k)}(x-h), \phi(x)) = (\delta(x-h), (-1)^k \phi^{(k)}(x)) = (-1)^k \phi^{(k)}(h) \quad (\text{A.228})$$

Once we have the possibility of functionals defined by non-locally summable functions f , the integral representation may diverge. Let's say that the function f is not locally summable at x_0 , then if we take $\phi \in K$ such that it vanishes in the neighborhood of x_0 , we can make the integral representation finite. The procedure of making the integrals finite is called **regularization**.

We shall introduce the regularization procedure using an example. Consider the function $f(x) = 1/x$, so

$$(f, \phi) = \int_{-\infty}^{\infty} \frac{\phi(x)}{x} dx \quad (\text{A.229})$$

diverges at $x = 0$. So, the procedure that we described in the last paragraph can be implemented if we ensure that our test function is zero in the neighborhood of $x = 0$. If in the interval $[-a, b]$ we subtract $\phi(0)$, we ensure that $\phi(x) - \phi(0)$ vanishes in a neighborhood of zero. Therefore, the last divergent integral can be represented by

$$(f, \phi) = \int_{-\infty}^{-a} \frac{\phi(x)}{x} dx + \int_{-a}^b \frac{\phi(x) - \phi(0)}{x} dx + \int_b^{\infty} \frac{\phi(x)}{x} dx, \quad (\text{A.230})$$

which is convergent and agrees with the previous expression everywhere except in the neighborhood of zero.

It is just a matter of repeating the same reasoning to conclude that any algebraic singularity can be regularized by an analogous procedure. That is, if $f(x)x^m$

$(x = \sqrt{\sum_i x_i^2})$ is locally summable for some $m > 0$, we can regularize (f, ϕ) by

$$(f, \phi) = \int_{\mathbb{R}^n} f(x) \left\{ \phi(x) - \left[\phi(0) + \frac{\partial \phi(x)}{\partial x_1} \Big|_{x=0} x_1 + \dots + \frac{\partial^m \phi(x)}{\partial x_n^m} \Big|_{x=0} \frac{x_n^m}{m!} \right] \theta(1-x) \right\}. \quad (\text{A.231})$$

Therefore, the last expression is the meaningful version of any irregular generalized function with algebraic singularities.

Now let us consider the following regular functional: define the generalized function x_+^λ by

$$x_+^\lambda = \begin{cases} 0, & \text{if } x \leq 0 \\ x^\lambda, & \text{if } x > 0, \end{cases} \quad (\text{A.232})$$

For $\Re \lambda > -1$. So the functional given by (x_+^λ, ϕ) is regular for $\Re \lambda > -1$. However, we notice that

$$\begin{aligned} (x_+^\lambda, \phi) &= \int_0^\infty x^\lambda \phi(x) dx = \int_0^1 x^\lambda \phi(x) dx + \int_1^\infty x^\lambda \phi(x) dx \\ &= \int_0^1 x^\lambda [\phi(x) - \phi(0)] dx + \int_0^1 x^\lambda \phi(0) dx + \int_1^\infty x^\lambda \phi(x) dx \\ &= \int_0^1 x^\lambda [\phi(x) - \phi(0)] dx + \int_1^\infty x^\lambda \phi(x) dx + \frac{\phi(0)}{\lambda + 1}, \end{aligned} \quad (\text{A.233})$$

this last expression is regular for $\Re \lambda > -2$ and $\lambda \neq -1$. Therefore, we have an **analytic extension** of the functional x_+^λ . By successive applications of the previous reasoning, we can obtain the following expression

$$\begin{aligned} (x_+^\lambda, \phi) &= \int_0^1 x^\lambda \left[\phi(x) - \sum_{k=1}^{m-1} \frac{x^{k-1}}{(k-1)!} \phi^{(k-1)}(0) \right] + \int_1^\infty x^\lambda \phi(x) dx \\ &\quad + \sum_{k=1}^m \frac{\phi^{(k-1)}(0)}{(k-1)!(\lambda + k)}, \end{aligned} \quad (\text{A.234})$$

which is regular for $\Re \lambda > -m-1$ and $\lambda \neq -1, -2, \dots, -m$. The previous expression is the regularization of the generalized function as a function of λ , and it follows directly that for any $\lambda = -k$, it has a pole with residue

$$\frac{\phi^{(k-1)}(0)}{(k-1)!} = \frac{(-1)^{k-1}}{(k-1)!} (\delta^{(k-1)}(x), \phi(x)), \quad (\text{A.235})$$

which means that the functional has a pole at $\lambda = -k$ with residue $\frac{(-1)^{k-1}}{(k-1)!} \delta^{(k-1)}(x)$.

With that, we finish the discussion about generalized functions. One must bear in mind that we only discussed simple examples and properties to avoid extending ourselves. As we can notice, some of the concepts that are key ideas of quantum field theory have already appeared in the generalized functions. Besides this direct connection, the theory of generalized functions is also useful to obtain practical results; for example, the Cauchy problem can be solved using such objects.

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