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Lucas de Souza Menicucci

Entanglement entropy of free scalar fields, a numerical study

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Prof. Nelson de Oliveira Yokomizo
Orientador do estudante
Departamento de Física/UFMG

Prof. Gláuber Carvalho Dorsch
Departamento de Física/UFMG

Prof. Pablo Lima Saldanha
Departamento de Física/UFMG

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Resumo

Investigações sobre a origem microscópica da entropia de buracos negros revelaram uma propriedade interessante sobre a quantidade de emaranhamento entre duas regiões espaciais complementares para o estado de vácuo de um campo escalar real livre [17], sua proporcionalidade à área da superfície que separa as duas regiões. Desde então, a entropia de emaranhamento se tornou uma ferramenta importante para explorar a estrutura interna de campos quânticos. Apesar da lei de área se provar um caso específico, novos estudos revelaram a dependência dessa quantidade a propriedades geométricas do espaço-tempo, pela presença de coeficientes universais [39]. Nesta dissertação, um estudo numérico da entropia de emaranhamento de um campo escalar real livre com uma curvatura de fundo é apresentado. Dois coeficientes universais são estimados. Os valores obtidos concordam bem com os previstos analiticamente. Uma descrição das técnicas usadas assim como uma breve revisão das teorias necessárias são também inclusas.

Palavras-chave: Entropia de emaranhamento, Teoria quântica de campos, Teoria de campos na rede, Computação Numérica

Abstract

Investigations towards the microscopic origin of the entropy of black holes revealed an interesting property of the amount of entanglement between two complementary spatial regions for the vacuum state of a real free scalar field [17], its proportionality with the area separating the regions. From that point, a measure of entanglement on pure states, called entanglement entropy, became an important tool for exploring the internal structure of quantum field theories. Although the area law proved to be a specific case, new studies have unveiled the dependency of this quantity on geometric features of spacetime by the presence of universal coefficients. In this dissertation, a numerical study of the entanglement entropy of a real scalar field on a curved background is presented. Two universal coefficients are estimated with good agreement with its predicted values. A description of the used techniques as well as a brief revision of the necessary theories are also included.

Keywords: Entanglement entropy, Quantum Field Theory, Lattice field theory, Numerical Computation.

Contents

1 Introduction

In this chapter, we present a short historical motivation for the study of the entanglement entropy of quantum fields by describing the development of the area law for the entropy of black holes. The presentation is followed by a non-extensive review of the numerical and analytical methods which revealed the geometric dependency of the entanglement entropy on quantum fields and, in particular, the proportionality of such quantity to the area of the entangling surface. Finally, we cite further references which point out the impact of such quantity in other areas.

1.1 Entropy of black holes

Under certain circumstances, the Einstein equations, provided by the theory of general relativity, allows for the gravitational collapse of matter and the subsequent formation of a black hole [18, 33, 59]. As suggested by its name, a black hole defines a region in spacetime where no light ray nor observer can escape. As a consequence, an object captured by the black hole can have no causal relation with the future of the outside region. The boundary of the black hole is then called an event horizon.

The event horizon of a spherically symmetric, static and non-charged black hole with mass m is a two-dimensional spherical surface in a spacetime described by the Schwarzschild metric [18, 33, 59]. The area of such horizon is given by:

$$A = 16\pi G^2 m^2. \tag{1.1}$$

A capture of a body by a black hole results in an increase of its mass and, as a consequence of eq. (1.1), an increase in A.

Since there is no way for a particle to escape from the region defined by the event horizon, it is reasonable to ask whether any energy can be extracted from a black hole. In the case of a rotating black hole with angular momentum L and mass m, Penrose suggested that energy can be extracted by means of what became known as the **Penrose process** [47]. Such process consists in sending a particle with four-momentum p_1 which decays into a pair of particles with four-momenta p_2 and p_3, where the latter has negative energy $p_3^0 < 0$ when measured at the infinity. Conservation of four-momentum requires that:

$$p_1 = p_2 + p_3. \tag{1.2}$$

Penrose showed that a possible process where the first particle (with four momentum p_2) is swallowed and the second is ejected away, results in $p_3^0 > p_1^0$ at the cost of decreasing the black hole's rotational energy.

The efficiency of the Penrose process described above was later studied by Christodoulou who showed [23] that the total mass energy m of a Black hole can be written in the form

$$m^2 = m_{ir}^2 + \frac{L^2}{4m_{ir}^2}, \tag{1.3}$$

where m_{ir} is the irreducible mass, which cannot be decreased by any process. It was also shown that an irreversible process is associated with an increase in m_{ir}. In the case of a charged black hole, the rest mass is given by [24]

$$m^2 = \left(m_{ir} + \frac{e^2}{4m_{ir}}\right)^2 + \frac{L^2}{4m_{ir}^2}. \tag{1.4}$$

Regarding the capture of a particle, it was pointed out by Penrose that the horizon area of a black hole is increased even if its mass decreases. Such property was explored by Hawking [30] in a general setting to derive the famous **area theorem**, which states that the area A of a black hole never decreases with time:

$$dA \geq 0. \tag{1.5}$$

Hawking also showed that, in the specific case of two black holes merging, the area of the final black hole is strictly greater than the sum of the initial ones. The result puts the quantity A in close analogy with the thermodynamic entropy S which, by the second law of thermodynamics, is also non-decreasing:

$$dS \geq 0. \tag{1.6}$$

The analogy between black hole physics and thermodynamics was developed further by Bardeen, Carter and Hawking [5], who obtained an expression that relates the parameters of two neighboring stationary solutions of the black hole. By comparison with the first law of thermodynamics, one notes that the quantity

$$T_{bh} = \frac{\kappa}{2\pi}, \tag{1.7}$$

where κ measures the magnitude of the acceleration of a test particle near the horizon, plays the same role as the temperature in the suggested analogy.

The authors of [5] pointed out, however, that the thermodynamic temperature of the black hole is absolute zero. Since it is unable to emit radiation, it could not be in equilibrium with black body radiation at a non-zero temperature and thus, the thermodynamic temperature and the analog given by $\kappa/2\pi$ quantify distinct physical parameters.

A stationary black hole in four dimensions is characterized by three quantities only: mass, angular momentum and charge. Such result is known as the *no hair theorem* [19, 20, 31, 36]. This property seems to violate the second law of thermodynamics, since a system with arbitrary entropy falling into the black hole ends up in a state which has none. A similar case, considered by Bekenstein [7, 8], indicated a violation of the law of Baryon-Number conservation.

These results indicated that, in order to fix the second law of thermodynamics, one would need to account for the entropy of a black hole. A candidate which was strongly suggested by Bekenstein is the rationalized area of the horizon

$$S_{bh} = \frac{A}{4\pi}. \tag{1.8}$$

In addition to that, only the sum of this entropy (1.8) and the common entropy S_c is never decreasing [10]:

$$d(S_{bh} + S_c) \geq 0. \tag{1.9}$$

This proposition puts S_{bh} and S_c on equal footing since one may balance the other in order to fulfill eq. (1.9). An interesting point arises regarding the microscopic source of S_{bh}. Because a system constituted of Ω microstates at thermal equilibrium has a thermodynamic entropy proportional to $\ln \Omega$ [54], one might ask what degrees of freedom are associated to the apparent $e^{S_{bh}}$ states indicated by S_{bh}. Investigations on the microscopic source of such entropy will be revised in the next section.

As pointed out earlier, the entropy S_{bh} is associated with a non-zero parameter T_{bh}. In order to interpret T_{bh} as a temperature, one needs to consider outgoing black body radiation from the black hole. This process is, however, prohibited by classical means since the horizon, from its definition, is a region which no particle can escape. Such tension was suspended by Hawking, who showed that a distant observer would indeed observe a thermal radiation with temperature T_{bh} coming from an isolated Schwarzschild black hole if a scalar quantum field is considered using a semiclassical treatment [32]. The particle creation process originates from the curvature induced by the presence of the black hole. A loss of energy by such creation process would then cause a slow decrease of the area of the horizon over time and the evaporation of the black hole over a long period.

The calculation by Hawking was later generalized for the case of an incident number of particles [12] thus supporting the radiative aspect of the phenomena.

1.2 Emergence of an area law

Interesting observations can be made from the establishment of S_{bh} as a correction to the second law. From the microscopic derivation of thermodynamics, one defines

the entropy as $S_{bol} = k_p \ln \Omega(p_{mac})$, where $\Omega(p_{mac})$ measures the volume of states with macroscopic parameters p_{mac} [54]. Note that:

- The Boltzmann entropy S_{bol} is then an extensive quantity $S_{bol} \propto V$ whereas $S_{bh} \propto A$.
- S_{bol} is related to a set of degrees of freedom, which parametrizes the state space where the surface with volume Ω lies. Assuming the same relation for S_{bh}, one might induce that a set of e^{S_{bh}/k_b} states is related to the presence of such quantity.
- On an informational theoretic perspective [55], S_{bol} measures the ignorance on the microstate of a physical system. This is in close analogy to the proposal that the entropy of the black hole is originated from an inability to determine its interior state from the exterior [9].

A model called "**Brick wall**" was proposed by 't Hooft [11] as an attempt to provide the degrees of freedom necessary to the emergency of an entropy S_{bh}. The model considered a scalar field on the outside vicinity of the horizon under a series of assumptions about the quantum treatment of the black hole. Added to the assumptions, the model suffered a drawback on the addition of a parameter to guarantee the agreement with previous results.

An alternative approach was given by Bombelli [17] in the following year. In an enlightening work, Bombelli considered a free scalar field ϕ on the ground state given by $\rho = |0\rangle\langle 0|$, situated on a flat spacetime. The black hole is modeled as a spatial region of which one can have no knowledge about the associated degrees of freedom. Because the states inside and outside might be correlated through entanglement, one should expect that an ignorance of the inside state corresponds to an ignorance of the outside state. Such "*ignorance*" can be viewed as one of the possible sources of entropy and can be quantified by computing the von Neumann entropy of the reduced density matrix associated to the outside region.

A reduced density matrix ρ_{red} is given by tracing the degrees of freedom ψ_{in} which are inaccessible to an outside observer:

$$\rho_{red} = \sum_{\psi_{in}} \langle \psi_{in} | \rho | \psi_{in} \rangle \,. \tag{1.10}$$

Because ρ is a pure state, the von Neumann entropy of ρ_{red},

$$S_{ent} = \mathrm{Tr}(\rho_{red} \ln \rho_{red}), \tag{1.11}$$

is known to measure the degree of entanglement between the two spatial regions [45]. The relation between the amount of entanglement of a pure state and the von Neumann entropy will be treated in detail in chapter 2. To compute ρ_{red} and evaluate the trace in

eq. (1.11), Bombelli considered a short distance cutoff ϵ which maps the field ϕ into a lattice of coupled harmonic oscillators separated by a distance of ϵ.

As a result, it is found that $S_{ent} \propto A$, where A is the area of the surface separating the two regions. The proportionality constant depends on ϵ and is divergent in the continuum limit $\epsilon \to 0$. Despite the divergence, it was a surprising discovery that such formula holds on a flat background geometry.

The same method was revisited by Srednicki [57], who evaluated S_{ent} numerically for a scalar field on flat spacetime and explicitly demonstrated the dependence of such quantity on the area of the sphere separating two spatial regions. The expressions which permitted this computation of S_{ent} will be derived in detail in section 5.1.

A drawback of these methods is that the calculation of S_{ent} depends on the explicit computation of ρ_{red} by tracing the degrees of freedom of the complement system. An optimization aiming at such problem was later introduced to obtain S_{ent} only in terms of the field correlations inside the region of ρ_{red} [21, 49]. The updated method is known as "real time approach" and is the basis for the calculation of S_{ent} developed further in this work (published in [56]). Details of the formalism can be found in section 5.3.

This approach has been applied to several cases [21, 22, 35, 41, 42, 52, 56, 57] and has revealed itself to be a robust tool for computing S_{ent} numerically.

1.3 Deviations from the area law

An important analytical tool for the calculation of S_{ent} in QFT follows from the path integral description of quantum mechanics. By writing the ground state of the field as a functional integral, one can relate the functions

$$S_\alpha[\rho_{red}] = \frac{1}{1-\alpha} \ln \mathrm{Tr}\, \rho_{red}^\alpha \tag{1.12}$$

to the partition functions Z_α. Such functions are known as **Renyi entropies** and the entanglement entropy can be obtained when $\alpha \to 1$. This method is referred to as the "**Euclidean formalism**".

It follows from a generic analysis of a QFT in d dimensions, using the Euclidean formalism, that the entropy S_{ent} in the limit $\epsilon \to 0$ should take the form of [39, 46]

$$S_{ent} = \frac{c_2}{\epsilon^{d-2}} + \frac{c_4}{\epsilon^{d-4}} + \frac{c_6}{\epsilon^{d-6}} + \ldots, \tag{1.13}$$

where the coefficients c_{2k} involve an integration over the entangling surface Σ and depend on the parameter ϵ. The area law is recovered if $c_2 \propto A(\Sigma)$, where $A(\Sigma)$ is the area of the entangling surface.

Smaller contributions to S_{ent} on eq. (1.13) may appear, such as a logarithmic divergence, $\ln \epsilon$. An interesting feature of these contributions is that they can be accompanied

by a multiplicative factor which is independent of ϵ. This factor is called a universal coefficient and can reveal fundamental aspects of the underlying QFT. In chapter 6 we use the real time approach to compute S_{ent} and estimate two of these universal coefficients.

1.4 Further developments and connections

As we saw earlier, the area law proved to be a feature of a quantum field even in the absence of a curved background. Further investigations led to the suggestion that the fundamental degrees of freedom of a field are in fact embedded on a hypersurface of lower dimension [34, 58]. Such proposal is known as the **holographic principle**.

The entanglement entropy has also a wide range of applications outside the scope of fundamental physics. It plays an important role in some condensed matter systems [38], for example, where entanglement serves as a mechanism for collective phenomena.

We will not list here the many areas in which the study of this quantity has a great impact. The reader interested in such broad view might refer to the introduction of [46].

2 Quantum Mechanics

Quantum mechanics is a theory which revolutionized the description of microscopic physics in the 20th century. Despite the initial criticism related to its radical premises, the theory has proved to be a robust set of rules from which a wide range of predictions can be made. Such coverage includes accurate descriptions of chemical reactions, material properties and atomic processes which no other contemporary theory is capable of achieving.

In this chapter, a short description of quantum mechanics is given from a fundamental perspective [45, 48, 53]. The mathematical framework is directly connected to the postulates of the theory. Furthermore, the concepts of entanglement and (quantum) entropy are developed, as they serve of basis for the content developed in the following chapters.

2.1 Hilbert spaces and state vectors

Quantum mechanics prescribes the description of the physical state of a system by an element of a Hilbert space. Before giving a refined statement of that postulate, let us define the properties of a Hilbert space:

Definition 2.1: Hilbert Space

A complex vector space V is called an **inner space** if there is a complex-valued operation of two vectors $|a\rangle, |b\rangle \in V$, denoted as $\langle a|b\rangle \in \mathbb{C}$, which satisfies the following properties [50]:

1. **Linearity**: $\langle a| (\alpha |b\rangle + \beta |c\rangle) = \alpha \langle a|b\rangle + \beta \langle a|c\rangle$.
2. **Conjugacy**: $\overline{\langle a|b\rangle} = \langle b|a\rangle$.
3. **Positive definiteness**: $\langle a|a\rangle \geq 0$, and $\langle a|a\rangle = 0$ if and only if $a = 0$.

An operation satisfying the above requirements is called a **inner product** in V. The presence of a inner product induces a metric

$$||a|| = \sqrt{\langle a|a\rangle}. \tag{2.1}$$

We also reefer to $||a||$ as the norm of the vector $|a\rangle$. It follows from the above properties that $||a||$ is always non-negative.
A **Hilbert space** is an inner space which is also complete (we refer the reader to [50] for a definition of completeness in terms of Cauchy sequences).

Now we might postulate that, if an experiment involving a physical system is carried with the same preparation and produces the same statistical distribution of results, the physical entity is said to be in a particular state $|\psi\rangle$ [48], which is an element of a Hilbert space $\mathcal{H}$.

Postulate 2.1: State vectors

The state of a particular entity is given in terms of a complex vector $|\psi\rangle$ (also called "*ket*") which is an element of a Hilbert space $\mathcal{H}$. This space $\mathcal{H}$ contains all the possible state vectors $|\psi\rangle$ which the physical entity can be found. Physical states $|\psi\rangle$, in particular, have to be normalized:

$$\langle\psi|\psi\rangle = 1. \tag{2.2}$$

Every ket $|\psi\rangle$ has a unique correspondent $\langle\psi|$, which is called "*bra*" and describes the same physical state.

The normalization condition stated in eq. (2.2) is necessary for connecting inner products with probability theory, as will be shown latter. The fact that the state of a physical entity is described by an element of a Hilbert space enables us to *compare* two arbitrary states by using the inner product defined in definition 2.1. Since physical states are normalized vectors, the inner product resembles the traditional notion of angle between vectors of finite vector spaces. More precisely, the inner product measures the projection of a vector on another vector. Whenever the length of that component is zero, the two vectors are said to be orthogonal:

Definition 2.2: Orthogonality between states

Two arbitrary vectors $|a\rangle$, $|b\rangle$ are orthogonal whenever

$$\langle a|b\rangle = 0. \tag{2.3}$$

For every Hilbert space there exists a set of vectors which can be used to represent any other vector as a linear combination. If we further impose that every element of that special set is normalized just as in eq. (2.2), and any pair of such vectors is orthogonal in the sense of eq. (2.3), then this set is called an orthonormal basis for that Hilbert space:

Definition 2.3: Orthonormal Basis

A set of vectors $B \in \mathcal{H}$ such that its elements $|k\rangle, |j\rangle$ satisfy the orthonormality condition

$$\langle k|j\rangle = \delta_{k,j} = \begin{cases} 1 & \text{if } k = j \\ 0 & \text{if } k \neq j \end{cases} \tag{2.4}$$

and can be used in conjunction to a set of complex coefficients α_k to express any vector $|\psi\rangle \in \mathcal{H}$ as

$$|\psi\rangle = \sum_{k \in B} \alpha_k |k\rangle , \tag{2.5}$$

is called an orthonormal basis for $\mathcal{H}$. Also, an arbitrary element $|i\rangle$ from the basis is linearly independent of all others. This is, if $|\psi\rangle = |i\rangle$ in eq. (2.5), we must have $\alpha_k = \delta_{ik}$.

The number of coefficients necessary to represent an arbitrary state as a linear combination of the elements of an orthonormal basis is called the dimension of that space. For a generic Hilbert space, one might need an infinite number of coefficients, which turns the expression (2.5) an infinite sum. In this case, questions about convergence, which will not be treaded here, have to be addressed.

If the orthonormality condition of definition 2.3 is weakened into a linear independence requirement, the resulting set which spans $\mathcal{H}$ is simply called a **basis** (or a **Hamel basis**) [37]. It is possible to show that every space $\mathcal{H}$ admits a basis and, contrary to the orthonormal case, every element of $\mathcal{H}$ can be represented as a finite sum of basis elements, even on the infinite dimensional case.

2.1.1 Example: qubit

Consider a generalization of the *quantum coin* introduced together with the concept of superposition. A system described by a Hilbert space of dimension two is called a qubit. The computational basis is defined to be the basis that is constituted by the vectors $|0\rangle$, $|1\rangle$. Using eq. (2.5), an arbitrary state $|q\rangle$ can be written as:

$$|q\rangle = \alpha_1 |0\rangle + \alpha_2 |1\rangle , \tag{2.6}$$

where α_1 and α_2 are two complex numbers which completely identify the state $|q\rangle$ on the computational basis. The normalization condition imposed by eq. (2.2) introduces a constraint relating the coefficients:

$$|\alpha_1|^2 + |\alpha_2|^2 = 1. \tag{2.7}$$

After imposing the normalization condition eq. (2.7), only two real numbers are necessary to describe a generic qubit state. In that way, the arbitrary state $|q\rangle$ in eq. (2.6) can be rewritten in terms of $\theta \in [0, \pi]$ and $\gamma \in [0, 2\pi]$:

$$|q\rangle = \sin\theta |0\rangle + e^{i\gamma} \cos\theta |1\rangle , \tag{2.8}$$

where γ is called the relative phase between the states $|0\rangle$ and $|1\rangle$.

2.2 Linear operators and measurements

Until now, the choice of a particular basis that is used to represent an arbitrary state vector is irrelevant. However, due to the behavior of states upon the action of a measurement, the choice of basis turns out to be guided by what quantity is being measured. The way measurements are modeled in quantum mechanics is by the means of Hermitian operators:

Definition 2.4: Linear Operators

A linear operator is a map between vectors of the same Hilbert space. If a linear operator A maps a ket vector $|\psi\rangle$ into another $|\tilde{\psi}\rangle$ that relation is written as:

$$A\,|\psi\rangle = |\tilde{\psi}\rangle \tag{2.9}$$

Alternatively, the operator A is uniquely related to the "complex conjugate" version of the above eq. (2.9), in which a hermitian conjugate $A^\dagger$ is defined:

$$\langle\psi|\,A^\dagger = \langle\tilde{\psi}|\,. \tag{2.10}$$

If the operator A happens to be invariant under the complex conjugation †, that is $A^\dagger = A$, then A is a **Hermitian operator**.

By fixing a particular basis, we can uniquely identify an operator A in matrix form by calculating its action on the basis. Given that i and k are indexes of the basis elements $|i\rangle$ and $|j\rangle$, the matrix elements A_{ij} are the inner product $\langle i|A|j\rangle$. It's clear from the conjugation property defined in definition 2.1 that the matrix elements of $A^\dagger$ are related by $\overline{\langle i|A|j\rangle} = \langle j|A^\dagger|i\rangle$.

The relation between an operator and a specific basis is elucidated by the question of which vectors have their directions kept invariant under the action of that operator. The existence of such basis vectors for an arbitrary operator is not ensured. However, if we restrict ourselves to Hermitian operators, then a basis can always be constructed:

Theorem 2.1: Spectral Theorem for Hermitian Operators

A Hermitian operator A defined on a Hilbert space $\mathcal{H}$ is related to a set of vectors $\{|a_k\rangle\}$ and real numbers $\{\lambda_k\}$ by the equation:

$$A\,|a_k\rangle = \lambda_k\,|a_k\rangle\,. \tag{2.11}$$

The vectors $|a_k\rangle$ and numbers λ_k are called eigenvectors and eigenvalues of A respectively. The set $\{|a_k\rangle\}$ forms an orthonormal basis for the space $\mathcal{H}$. It follows

that the operator A admits the **spectral decomposition**:

$$A = \sum_{k=0}^{N} \lambda_k P_k, \tag{2.12}$$

where N is the dimension of the space and the operator P_k projects a vector into the direction of $|a_k\rangle$.

The operator P_k defined in eq. (2.12) is called a projector of the vector $|a_k\rangle$. A convenient use of the *bras* and *kets* notation enables us write the projector P_k in terms of a product of a ket with a bra:

$$P_k = |a_k\rangle\langle a_k| \,. \tag{2.13}$$

The operation defined in eq. (2.13) is different from the inner product in the sense that the first produces an operator while the latter results in a complex number. By applying P_k to a vector $|\psi\rangle$, one should first calculate the projection $\langle a_k|\psi\rangle$ and use that to rescale $|a_k\rangle$. Since the vectors $|a_k\rangle$ form an orthonormal basis, it is clear that the projectors exhibit the orthogonality property $P_i P_j = \delta_{ij} P_i$.

A very useful representation of the identity operator $\mathbb{1}$ can be given as a sum projectors. For any orthonormal basis $\{|a_k\rangle\}$ or $\{|b_k\rangle\}$ the identity operator can be written as:

$$\mathbb{1} = \sum_k |a_k\rangle\langle a_k| = \sum_j |b_j\rangle\langle b_j| = \dots \tag{2.14}$$

The language of projectors introduced by eq. (2.13) plays an important role in the definition of measurements:

Postulate 2.2: Projective measurements

Every observable quantity of a system is associated to a Hermitian operator. Consider the measurement of a quantity associated to the operator O of system in the state $|\psi\rangle$. Given that λ_k and P_k are eigenvalues and projectors associated to the spectral decomposition of O (as defined in eq. (2.12)) we make the the following assertions:

- The values λ_k define the possible outcomes of an experiment that measures the observable associated to O.
- The probability $p(\lambda_k)$ of obtaining λ_k in a measurement is given by:

$$p(\lambda_k) = \langle\psi|P_k|\psi\rangle \,. \tag{2.15}$$

- If the outcome of a specific measurement is λ_k, the state of the system just

after the measurement is given by:

$$|\psi_{\text{after}}\rangle = \frac{P_k |\psi\rangle}{\sqrt{\langle\psi|P_k|\psi\rangle}} = \frac{P_k |\psi\rangle}{\sqrt{p(\lambda_k)}}. \tag{2.16}$$

It is important to point out that, although postulate 2.2 covers a wide class of measurements, it is not the most general postulate about measurements of quantum systems. A wider class called *general measurements* [45], which includes projective measurements can be defined, however such generalization will not be necessary for us.

Consider a qubit which is found in the state 2.8

$$|q\rangle = \sin\theta\,|0\rangle + e^{i\gamma}\cos\theta\,|1\rangle\,. \tag{2.17}$$

Because $|\psi\rangle$ is given as a linear combination of the states $|0\rangle$ and $|1\rangle$, it is said to be on a **superposition** of these states. This phenomenon is responsible for major features of data processing using quantum systems [29].

The probabilities of measuring an outcome associated to each state $|0\rangle$ and $|1\rangle$ are given respectively by $\sin^2\theta$ and $\cos^2\theta$. We note that, unless $\theta = 0$ or $\pi/2$, one cannot predict what state the qubit will collapse to. The theory is only deterministic in the sense that the probabilities of such collapse can be predicted.

2.3 Composite systems

So far, only isolated systems were considered. By the postulate 2.1, those systems are described by state vectors of a particular Hilbert space and the measurements of observables are described by postulate 2.2. As no system is completely isolated from the surrounding environment, we expect those rules to generalize without drastic modifications for systems composed of multiple subsystems.

Before introducing the postulate which give us access to the state of the composite system, let us introduce the definition of tensor product:

Definition 2.5: Tensor product

The tensor product of two Hilbert spaces denoted by $\mathcal{H}_1$ and $\mathcal{H}_2$ consists in the Hilbert space generated by all possible tensor products $|\psi_1\rangle \otimes |\psi_2\rangle$ with $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$. This definition can be extended parwise to include an arbitrary but countable number of spaces $\mathcal{H}_1, \mathcal{H}_2, \mathcal{H}_3, \ldots$. The Hilbert space $\mathcal{H}$ generated by the tensor product of such states is written as:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \ldots = \bigotimes_k H_k. \tag{2.18}$$

Given that $|e_i\rangle$ and $|u_i\rangle$ are basis elements of two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ the generic operator A acting on the space $\mathcal{H}_1 \otimes \mathcal{H}_2$ is given by:

$$A = \sum_{ijkl} \alpha_{ijkl}(|e_i\rangle \langle e_j|) \otimes (|u_k\rangle \langle u_l|). \tag{2.19}$$

A generalization of eq. (2.19) to an arbitrary number of spaces is found naturally by considering all possible combinations of operators $|e_i\rangle \langle e_j|$ for each space.

A particular case arises when constructing an operator of $\mathcal{H}$ which reproduces the action of a particular operator A_k of one of the subspaces $\mathcal{H}_k$. This operator A is given by composing A_k with the identities of each space:

$$A = \mathbb{1} \otimes_1 \cdots \otimes A_k \otimes \cdots \otimes \mathbb{1}_n. \tag{2.20}$$

It is clear how the above property 2.20 is useful in separating the application of an operator of a particular subsystem from the rest of the composite system. The postulate connecting the composite system state with the individual ones by tensor products follows immediately from the definition 2.5:

Postulate 2.3: Composite system state

The joint state $|\psi\rangle$ of a system composed by the entities with respective states $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \ldots$ is constructed by the tensor product of the individual states:

$$|\psi\rangle = \bigotimes_k |\psi_k\rangle . \tag{2.21}$$

A basis for the composite system can be defined using all possible combinations of the individual basis elements of each space $\mathcal{H}_k$. An observable of the composite system is also modeled as a Hermitian operator acting on the joint states $|\psi\rangle \in \mathcal{H}$.

To exemplify the property introduced by postulate 2.3, let us consider an experiment involving the preparation of a system with two particles in the joint state $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$. The experiment consists in the measurement of the observable of the first particle described by the operator O_1. The expectation value $\langle O_1 \rangle$ can be calculated as:

$$\begin{aligned} \langle O_1 \rangle &= \langle \psi | (O_1 \otimes \mathbb{1}_2) | \psi \rangle \\ &= (\langle \psi_1 | \otimes \langle \psi_2 |) (O_1 \otimes \mathbb{1}_2) (|\psi_1\rangle \otimes |\psi_2\rangle) \\ &= \langle \psi_1 | O_1 | \psi_1 \rangle \langle \psi_2 | \psi_2 \rangle = \langle \psi_1 | O_1 | \psi_1 \rangle \end{aligned} \tag{2.22}$$

Note that the result obtained is just the same as if we were treating the first particle isolated. In general, such simplification is not possible due to **entanglement**.

2.4 Entanglement

Consider an experiment involving two qubits such that the joint state is prepared to be

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B \right). \tag{2.23}$$

The state described by eq. (2.23) is called a Bell state, and it describes a case where the qubits are maximally entangled. Such entanglement can be observed as a correlation between observables of each qubit. Suppose that a measurement described by the operator M_A is carried out on the qubit A:

$$M_A = \lambda_0 \, |0\rangle\langle 0|_A + \lambda_1 \, |1\rangle\langle 1|_A \, . \tag{2.24}$$

Such measurement projects the state of qubit A in one of the two components $|0\rangle$, $|1\rangle$. Let $|\psi_{\text{after}}\rangle$ be the joint state after the measurement. Each possible outcome is given by the application of postulate 2.2:

$$\begin{aligned} &\text{Measures } \lambda_0 \Rightarrow |\psi_{\text{after}}\rangle = |0\rangle_A \otimes |0\rangle_B \\ &\text{Measures } \lambda_1 \Rightarrow |\psi_{\text{after}}\rangle = |1\rangle_A \otimes |1\rangle_B \end{aligned} \tag{2.25}$$

We consider the subsequent measurement of a quantity on the qubit B described by on operator similar to M_A:

$$M_B = \lambda_0 \, |0\rangle\langle 0|_B + \lambda_1 \, |1\rangle\langle 1|_B \, . \tag{2.26}$$

Because the state of the subsystem B is altered after the measurement of M_A, one observe that the outcomes of both measurements are correlated. Such correlation is originated from the structure of the state 2.23. This feature is called entanglement and can not be explained by classical means.

Entanglement also plays an important role in quantum information transmission, since joint states remain entangled even if they are separated far apart [14].

2.5 Density Matrix

Until now, no uncertainty was introduced when considering the preparation of states. We have assumed that, in some way, the state of our system could be prepared with absolute certainty. This assumption is clearly not realistic, in the general case, assertions about the apparatus used to produce the state would have to include inherent uncertainties. In such situation, the state being prepared could turn out to be a stochastic variable. A similar case arises when studying systems in thermodynamic equilibrium, where the states

are inherently distributed according to a statistical law due to, for example, a known interaction with a thermal reservoir [54].

In these cases, one might consider a statistical ensemble of states in which the system can be found. To each possible state, a preparation probability p_i can be assigned. A convenient way of representing expected values of a physical observable in terms of the preparation probabilities is by using the density matrix associated with that ensemble:

Definition 2.6: Density matrix

The density matrix or density operator ρ is an operator defined on the state space $\mathcal{H}$ of the system which satisfies:

- **Unitary trace**:

$$\operatorname{Tr}\rho = 1. \tag{2.27}$$

- **Positivity**:

$$\langle\psi|\rho|\psi\rangle \geq 0, \quad \text{for every } |\psi\rangle \in \mathcal{H}. \tag{2.28}$$

If $0 \leq p_i \leq 1$ is the probability of the system being prepared in the (normalized) state $|\psi_i\rangle$, then ρ can be written as:

$$\rho = \sum_i p_i \, |\psi_i\rangle\langle\psi_i| \tag{2.29}$$

The density matrix ρ is a completely equivalent way of describing an arbitrary state. The expected values are now given in terms of traces involving the density matrix and the Hermitian operator associated.

Theorem 2.2: Expected values in terms of ρ

If an observable quantity is associated to a Hermitian operator O, then the expected value of that quantity over a state defined by ρ is given by

$$\langle O\rangle = \operatorname{Tr}\rho O. \tag{2.30}$$

Since any transformation described by a linear operator U on a state $|\psi\rangle$ maps its projector $|\psi\rangle\langle\psi|$ to $U\,|\psi\rangle\langle\psi|\,U^\dagger$, the density operator ρ also transforms as $\rho \to U\rho U^\dagger$. In particular, if U describes a measurement operator, we can recover the content of Postulate 2.2:

Theorem 2.3: Projective measurements in terms of ρ

If a projective measurement, defined by the spectral decomposition of an operator $M = \sum_k \lambda_k P_k$, is applied to a system whose initial state is given by ρ, the measurement process produces a state ρ_{after} which is given by:

$$\rho_{\text{after}} = \frac{P_k^\dagger \rho P_k}{p_k}, \tag{2.31}$$

where p_k is the probability of the measurement of λ_k and is given by

$$p_k = \operatorname{Tr} P_k \rho. \tag{2.32}$$

It is important to note that the decomposition in terms of the projectors $|\psi_i\rangle\langle\psi_i|$ in eq. (2.29) is essentially different from the superposition definition in eq. (2.17). In the first case, each projector describes a particular superposition of states. Then, the resulting density matrix is a sum of these projectors each describing a possible way in which the system could be prepared. Such composition of projectors is called an **incoherent mixture**, as it describes a "*classical uncertainty*" of which state a system is in.

It is important to establish a way of differentiating both cases. When a system's state is prepared with certainty, that is with probability $p_k = 1$, then the density matrix is given by a single projector of that state:

$$\rho_{pure} = |\psi\rangle\langle\psi| . \tag{2.33}$$

Every state which can be written as a single projector as in eq. (2.33) is called a **pure state**. In contrast, if the preparation of a system's state cannot be written in the form of eq. (2.33), then its said to be in a **mixed state**. An important quantity for testing the purity of a state is the trace of ρ^2:

Theorem 2.4: Purity of a state

A state described by ρ is said to be a pure state if and only if:

$$\operatorname{Tr} \rho^2 = \operatorname{Tr} \rho = 1. \tag{2.34}$$

Otherwise, $\operatorname{Tr} \rho^2 < 1$ and ρ describes a mixed state.

2.6 Partial trace

Since the density operator is defined as an operator acting on state vectors of a particular Hilbert space, it is natural to guess that the density operator associated with a composite system is obtained by tensor products just as the operators in eq. (2.19). The previous postulate about the space of composite systems may be reformulated as:

Postulate 2.4: Composite system density matrix

Given an arbitrary joint state $|\psi_j\rangle$ constructed by the tensor product of the subsystem states $|j\rangle_l$:

$$|\psi_k\rangle = \sum_{j_1 \cdots j_N} \alpha^{(k)}_{j_1 \ldots j_N} |j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_N\rangle \,. \tag{2.35}$$

The joint density operator is given by a combination of the operators $|\psi_k\rangle\langle\psi_k|$ weighted by the associated probabilities p_k

$$\rho = \sum_k p_k \, |\psi_k\rangle\langle\psi_k| \tag{2.36}$$

Again, the state described by ρ is called pure when only a single p_k is non-zero. An important definition arises when considering the case where all the states $|\psi_k\rangle\langle\psi_k|$ can be written as a product of component projectors. In such case, the state described by ρ is called separable, otherwise it is called entangled [60].

Definition 2.7: Separable and entangled states

Given that $\mathcal{H}_i$ is the Hilbert space of the i-th subsystem, a state $|\psi\rangle$ is called separable if every $|\psi_k\rangle\langle\psi_k|$ in eq. (2.36) can be written as:

$$|\psi_k\rangle\langle\psi_k| = |k_1\rangle\langle k_1| \otimes |k_2\rangle\langle k_2| \otimes |k_3\rangle\langle k_3| \otimes \ldots, \tag{2.37}$$

such that each $|k_i\rangle \in \mathcal{H}_i$. If a state is not separable, it is **entangled**.

By means of definition 2.7 we now have a rigorous definition of entanglement. However, given a generic density matrix ρ, the question whether ρ is separable or not is far from trivial. An operational measure of entanglement will only be provided here for the case of a pure state. We restrict ourselves further to the measure of entanglement between two complementary parts of a system in a pure state.

Consider a system that is divided in two complementary subsystems A and B. It can be showed that an arbitrary state $|\psi_{AB}\rangle$ can be written in terms of two orthonormal basis relative to each partition. This is called the Schmidt decomposition of $|\psi_{AB}\rangle$ [45]:

Theorem 2.5: Schmidt decomposition

Given an arbitrary state $|\psi_{AB}\rangle$ of a bipartite system, there always exists orthonormal bases $\{|i_A\rangle\}_i$ and $\{|i_B\rangle\}_i$ relative to each partition A and B respectively and a set of real coefficients λ_i which can be used to write $|\psi_{AB}\rangle$ as:

$$|\psi_{AB}\rangle = \sum_i \lambda_i \, |i_A\rangle \otimes |i_B\rangle \,. \tag{2.38}$$

The λ_i are called Schmidt coefficients and are non-negative numbers satisfying $\sum_i \lambda_i^2 = 1$.

The number of non-zero Schmidt coefficients is called the Schmidt rank of the system. A system with Schmidt rank equal to one has only one $\lambda_i = 1$. In that case, the density matrix ρ for such state is given by a single term:

$$\begin{aligned}\rho &= |\psi_{AB}\rangle\langle\psi_{AB}| \\ &= (|\psi_A\rangle \otimes |\psi_B\rangle)(\langle\psi_A| \otimes \langle\psi_B|) \\ &= |\psi_A\rangle\langle\psi_A| \otimes |\psi_B\rangle\langle\psi_B|,\end{aligned} \tag{2.39}$$

In this case, the ρ in eq. (2.39) matches the definition of a pure separable state as stated in definition 2.7. The reverse argument can be made, so we conclude that a pure state is only separable when it has Schmidt rank equal to one.

Before establishing an expression for the amount of entanglement of a system in a pure state, let us define a useful tool to study the properties of subsystems. The partial trace of an operator is obtained by averaging the degrees of freedom related to a specific subsystem. The operator left acts only on variables of the complementary subsystem.

Definition 2.8: Partial Trace

The partial trace Tr_A relative to a subsystem labeled A is defined as the trace over the degrees of freedom of A. As a consequence of theorem 2.5, an arbitrary operator for a bipartite system is written as:

$$O = \sum_{ijkl} \alpha_{ijkl} |e_i^A\rangle \langle e_j^A| \otimes |e_l^B\rangle \langle e_k^B|, \tag{2.40}$$

where the states $|e_i^A\rangle$ and $|e_l^B\rangle$ are the Schmidt basis for the subsystems A and B respectively.
The partial trace $\mathrm{Tr}_A O$ is given by [45]:

$$\begin{aligned}\mathrm{Tr}_A O &= \sum_{ijkl} \alpha_{ijkl} \mathrm{Tr}\Big(|e_i^A\rangle \langle e_j^A|\Big) |e_l^B\rangle \langle e_k^B| \\ &= \sum_{kl} \left(\sum_i \alpha_{iikl}\right) |e_l^B\rangle \langle e_k^B| \\ &= \sum_{kl} \alpha'_{kl} |e_l^B\rangle \langle e_k^B|,\end{aligned} \tag{2.41}$$

where on the first line we used the fact that, for an orthonormal basis $|e_i^A\rangle$, we have $\mathrm{Tr}\Big(|e_i^A\rangle \langle e_j^A|\Big) = \delta_{ij}$.

It is convenient to define the quantity $\mathrm{Tr}_A O$ as the reduced operator O_B. An important quantifier of entanglement of pure bipartite systems can be defined in terms

of the reduced density matrix ρ_A (or ρ_B), obtained by taking the partial trace of ρ over B (or A). Given that a system is in the state $|\psi_{AB}\rangle$, the density matrix can be expanded using the Schmidt decomposition defined in eq. (2.38):

$$\begin{aligned}\rho &= |\psi_{AB}\rangle\langle\psi_{AB}| \\ &= \left(\sum_i \lambda_i |i_A\rangle \otimes |i_B\rangle\right)\left(\sum_j \lambda_j \langle j_A| \otimes \langle j_B|\right) \\ &= \sum_{ij} \lambda_i\lambda_j |i_A\rangle \langle j_A| \otimes |i_B\rangle \langle j_B| \,.\end{aligned} \tag{2.42}$$

The last expression for ρ in eq. (2.42) can be used for computing the reduced density matrix ρ_A by taking the partial trace over the states $|\psi_B\rangle$:

$$\begin{aligned}\rho_A &= \mathrm{Tr}_B\, \rho \\ &= \sum_{ij} \lambda_i\lambda_j |i_A\rangle \langle j_A| \,\mathrm{Tr}(|i_B\rangle \langle j_B|) \\ &= \sum_{ij} \lambda_i\lambda_j |i_A\rangle \langle j_A| \langle j_B|i_B\rangle \\ &= \sum_{ij} \lambda_i\lambda_j |i_A\rangle \langle j_A| \,\delta_{ij} \\ &= \sum_i \lambda_i^2 |i_A\rangle\langle i_A| \,.\end{aligned} \tag{2.43}$$

where we used the fact that $\langle j_B|i_B\rangle = \delta_{ij}$. Similarly, the reduced matrix ρ_B can be found by tracing over A:

$$\begin{aligned}\rho_B &= \mathrm{Tr}_A\, \rho \\ &= \sum_i \lambda_i^2 |i_B\rangle\langle i_B| \,,\end{aligned} \tag{2.44}$$

The expressions eq. (2.43) and eq. (2.44) are the spectral decomposition of the operators ρ_A and ρ_B respectively. It is clear that both operators share the same eigenvalues λ_i^2.

It is important to note that, as we saw earlier, if the Schmidt rank of a state is equal to one, that means it is a separable state. In that case, the reduced state of the subsystem, described by ρ_A (ρ_B), also contains a single projector $|i_A\rangle\langle i_A|$ ($|i_B\rangle\langle i_B|$) and it describes a pure state. The reverse also holds, if one of the two reduced density matrices ρ_A or ρ_B describes a pure state that means that only one Schmidt coefficient is non-zero, and the joint state described by eq. (2.42) has only one product state $|i_A\rangle\langle i_A| \otimes |i_B\rangle\langle i_B|$ term.

To summarize, the Schmidt decomposition and the partial trace are important tools for determining the separability of a system in a pure state. If the reduced density matrix of one subsystem describes a mixed state, we can immediately conclude that the joint state is entangled. A quantitative measurement of entanglement can then be developed in terms of how much the reduced state is mixed.

2.7 Entropy of entanglement

A classical measure of "*surprise*", "*unpredictability*" of a discrete random variable X was first given by Shannon [55]:

$$H[X] = -\sum_k P(x_k) \log P(x_k), \tag{2.45}$$

where the logarithm is taken in the base 2, k indexes all the possible outcomes and $P(x_k)$ is the probability associated to the x_k outcome. A measure of entanglement, based on how mixed a state is, can be constructed in a way that it matches the Shannon entropy 2.45 when applied to the Schmidt decomposition of the system in study:

Definition 2.9: Entropy of entanglement

Given that ρ_A and ρ_B are the reduced density matrix of each subsystem A and B respectively, a measure of entanglement between the two subsystems is given by the von Neumann entropy of any of the reduced density matrix [13]:

$$\begin{aligned} S &= -\operatorname{Tr}(\rho_A \log \rho_A) = -\operatorname{Tr}(\rho_B \log \rho_B) \\ &= -\sum_k \lambda_k^2 \log \lambda_k^2, \end{aligned} \tag{2.46}$$

where the λ_k are the Schmidt coefficients of the particular decomposition.

Since the coefficients are positive numbers satisfying $\sum_k \lambda_k^2 = 1$, their square can be interpreted as probabilities and, in that case, the last line shows that the entanglement entropy is the Shannon entropy of the squared Schmidt coefficients. In the special case where ρ is separable, only one of the λ_k is non-zero and it is equal to one. In that case, the entanglement entropy defined in eq. (2.46) vanishes:

$$\rho \text{ is separable (not entangled)} \Leftrightarrow S = 1 \log 1 = 0. \tag{2.47}$$

Under the constraints $\sum_{k=1}^{d} \lambda_k^2 = 1$ and at fixed d, the function S attains it maximum when [45]:

$$\lambda_k^2 = \frac{1}{d} \Rightarrow S = \max_{\{\lambda_k\}_k} S = \log d, \tag{2.48}$$

where d is identified as the Schmidt rank of the state ρ. This result indicates that the entropy S is maximized when the reduced density matrices ρ_A or ρ_B describes a uniform distribution across the subsystem states. Shortly, S is maximized when ρ_A and ρ_B are maximally mixed.

A convenient expression to calculate the entanglement entropy 2.9 was given by Rényi [51] in terms of a family of functions H_α, with $\alpha > 0$, that satisfies a set of postulates characterizing them as different measures of entropy. Each function is called Rényi entropy of order α:

Definition 2.10: Rényi entropy

The Rényi entropy of order α, being α a strict positive real parameter, of a state given by the density matrix ρ is given by:

$$H_\alpha[\rho] = \frac{1}{1-\alpha} \log\left(\mathrm{Tr}(\rho^\alpha)\right). \tag{2.49}$$

The von Neumann entropy S is then obtained by taking the limit $\alpha \to 1$:

$$S[\rho] = \lim_{\alpha\to 1} H_\alpha[\rho] = \lim_{\alpha\to 1} \frac{1}{1-\alpha} \log\left(\mathrm{Tr}(\rho^\alpha)\right) \tag{2.50}$$

Using eq. (2.50), one avoids computing the logarithm of an operator in order to obtain S.

3 Differential Geometry and Curvature

3.1 Manifolds and Tangent Spaces

As a premise of General Relativity's theory, spacetime is not merely a static stage in which physical events occur, instead it is a dynamical object which can be curved by the presence of matter or energy and influence objects as a consequence of its curvature. The presence of curvature calls for a definition of spacetime in terms of a more general object than the pre-relativistic space $\mathbb{R} \times \mathbb{R}^3$. As a starting point for constructing a formal notion of curvature, we define the spacetime to be a **manifold**[59]:

Definition 3.1: Manifold

A C^∞ manifold $\mathcal{M}$ of dimension n is a set with a collection of subsets $\{O_\alpha\} \in \mathcal{M}$ such that:

1. Each point $p \in \mathcal{M}$ is in at least one O_α.
2. For each subset O_α there is a one-to-one map ψ_α from O_α to U_α where U_α is an open subset of $\mathbb{R}^n$. ψ_α is called a coordinate system.
3. If two subsets O_α, O_β overlap ($O_\alpha \cap O_\beta \neq \varnothing$) the mapping $\psi_\alpha \circ \psi_\beta^{-1}$ given by the composition of ψ_α with ψ_β^{-1} is C^∞ (infinitely differentiable) and the sets $\psi_\alpha(O_\alpha \cap O_\beta)$ and $\psi_\beta(O_\alpha \cap O_\beta)$ are open.

It is clear from the first item that by "gluing" all the O_α the starting Manifold $\mathcal{M}$ is restored.

The coordinate maps ψ_α are of great importance since they enable us to define new concepts in terms of tools of regular calculus. For example, a function $f : \mathcal{M} \to \mathcal{M}'$ between two different manifolds $\mathcal{M}$, $\mathcal{M}'$ is said to be C^∞ if for every $\psi_\alpha : \mathcal{M} \to \mathbb{R}^n$ and $\psi'_\beta : \mathcal{M}' \to \mathbb{R}^{n'}$ the mapping $\psi'_\beta \circ f \circ \psi_\alpha^{-1}$, which is a map from R^n to $R^{n\prime}$, is C^∞ in the sense of multivariate calculus [59].

A classic example of a two-dimensional manifold is the two sphere $\mathbb{S}^2$ consisting of all points (x_1, x_2, x_3) such that $x_i \in \mathbb{R}$ and $x_1^2 + x_2^2 + x_3^2 = 1$. Although this can be seen as a unit spherical shell centered on the origin of $\mathbb{R}^3$ such notion of embedding on a space of higher dimension is not necessary. In fact, a formal notion of curvature can be defined without referring to an outer space.

We look further to extend the concept of vectors fields on flat spacetime to curved ones. It is clear that the structure of vector space is lost when we consider, for example, the

displacement vector defined over a sphere $\mathbb{S}^2$. By adding two different displacements, we arrive at a point which is not contained by $\mathbb{S}^2$. Instead, we motivate ourselves to construct a vector space which is point dependent on the manifold, and then transport it, in some way yet to be defined, to another point for further comparison. This vector space defined at each point $p \in \mathcal{M}$ is called the **tangent space $\mathbf{T_p}$**.

Due to the requirement for a pointwise vector space, it is reasonable to consider objects which depend at most on the vicinity of the considered point. It is known that a directional derivative of a function $\mathbb{R}^n \to \mathbb{R}$ evaluated at fixed point of $\mathbb{R}^n$ forms a vector space which is isomorphic to $\mathbb{R}^n$ [59]. The intuition of directional derivatives on $\mathcal{R}^n$ serves then as a motivation for a rigorous definition of T_p:

Definition 3.2: Tangent space

Consider the set $\mathcal{F}$ of functions $f : \mathcal{M} \to \mathbb{R}$ such that $\mathcal{M}$ is a manifold. The tangent space T_p consists of all maps $v : \mathcal{F} \to \mathbb{R}$ which satisfies:

1. **Linearity property:** $v(\alpha f + \beta g) = \alpha v(f) + \beta f(g)$,
2. **Leibniz's rule:** $v(fg) = fv(g) + v(f)g$,

for $f, g \in \mathcal{F}$ and $\alpha, \beta \in \mathbb{R}$.

The fact that this definition of tangent space actually produces a vector space is made clear when we introduce a particular coordinate system $\phi : O \to \mathbb{R}^n$, with O being an open set of $\mathcal{M}$. This choice of ϕ induces a set of maps $X_\mu : \mathcal{F} \to \mathbb{R}$ which spans the space T_p. Such set is called the **coordinate basis for $\mathbf{T_p}$** since it depends on a particular ϕ:

Theorem 3.1: Coordinate Basis for T_p

The set of n mappings $X_\mu : \mathcal{F} \to \mathbb{R}$ given by

$$X_\mu(f) = \frac{\partial}{\partial x^\mu}(f \circ \phi^{-1})\bigg|_{\phi(p)} \tag{3.1}$$

forms a basis for the tangent space T_p at the point p of the n-dimensional manifold $\mathcal{M}$. The basis vector X_μ is often abbreviated as $\frac{\partial}{\partial x^\mu}$.

The proof for theorem 3.1 can be found in [59] and it simply exploits the differentiability of the function $f \circ \phi^{-1} : \mathbb{R}^n \to \mathbb{R}$. It is important to point out that theorem 3.1 implies that T_p has the same dimension of $\mathcal{M}$.

Since X_μ forms a basis for T_p, an arbitrary vector $v \in T_p$ may be written as:

$$v(f) = v^\mu X_\mu(f), \tag{3.2}$$

with $v^\mu \in \mathbb{R}$ and $f \in \mathcal{F}$. It is clear by applying the chain rule on eq. (3.1) that by choosing another coordinate system ϕ' the new components of v are given by

$$v^{\mu'} = \frac{\partial x^{\mu'}}{\partial x^\mu} v^\mu, \tag{3.3}$$

where the function x'^μ is the μ-th component of the map $\phi' \circ \phi^{-1}$. The above eq. (3.3) is called **vector transformation law**.

We might use a vector of each tangent space T_p at each point p to construct a vector field over the manifold.

Definition 3.3: Vector field

A vector field (or tangent field) is an assignment of a tangent vector $v_p \in T_p$ for each point $p \in \mathcal{M}$.
Given a smooth function $f : \mathcal{M} \to \mathbb{R}$, a vector field is said to be smooth if the function $v_p(f) : \mathcal{M} \to \mathbb{R}$ is also smooth.

In the case of adopting a coordinate basis, a vector field is smooth if and only if its basis components $v^\mu(p)$ at eq. (3.2) are smooth functions [59].

3.2 Dual vectors and Tensors

In the last section, a definition of a tangent space T_p has been given as a vector space defined for each point p of a C^∞ n-dimensional manifold. Just as any real valued vector space, a dual vector space can be defined from the linear functionals $\omega : T_p \to \mathbb{R}$. Such a vector space, is called the **dual of $\mathbf{T_p}$** and is denoted as T_p^*.

A one-to-one relation between elements of both vector spaces can be fixed from the choice of a basis on one space. In particular, it can be shown [40] that a basis for T_p^* with elements v^μ can be constructed by demanding that

$$v^\mu(v_\nu) = \delta^\mu_\nu, \tag{3.4}$$

where v_ν is a generic basis element for T_p and δ^μ_ν is the Kronecker delta. Since eq. (3.4) defines an injective relation between two finite basis with the same size, it is clear that it implies that T_p and T_p^* are isomorphic and, therefore, share the same dimension. Another isomorphism which does not depend on a choice of basis can be defined in terms of the metric tensor as will be noted further in this section.

Last section, we defined the coordinate basis as the basis formed by the partial derivatives ∂_μ at a fixed coordinate system $\phi : \mathcal{M} \to \mathbb{R}$. By using the relation eq. (3.4) we define the basis of T_p^* with element dx^μ to be the unique basis satisfying:

$$dx^\mu(\partial_\nu) = \delta^\mu_\nu. \tag{3.5}$$

It is clear that, by exploring the above eq. (3.5) and the vector transformation law in eq. (3.3), that, under a change of coordinate system, the new components $v^{\mu'}$ of a dual vector should relate to the old as:

$$v_{\mu'} = \frac{\partial x^\mu}{\partial x^{\mu'}} v_\mu. \tag{3.6}$$

Because T_p^* is also a vector space, one might consider the dual space $(T_p^*)^*$ which, in the finite dimension case, will correspond to the initial space T_p. The space T_p then can also be viewed as the space of linear functionals $v : T_p^* \to \mathbb{R}$. It should be pointed out however that such association does not necessarily hold when $\dim(V) = \infty$, this is, $(V^*)^* = V$ is not necessarily true.

The fact that vectors and dual vectors can be seen as linear functionals motivate us to consider a multilinear mapping that depends on a collection of k vectors and l dual vectors. Such mapping is called a $(\mathbf{k}, \mathbf{l})$ **tensor** and takes k dual vectors and l vectors as input and returns a real number as output.

Definition 3.4: Tensor

A (k, l) tensor T is a mapping:

$$T : \underbrace{V_p^* \times V_p^* \times \ldots}_{k \text{ times}} \times \underbrace{V_p \times V_p \times \ldots}_{l \text{ times}} \to \mathbb{R}, \tag{3.7}$$

which is linear at each component when all others are kept fixed.
The vector space of all (k, l) tensors is defined as $\mathcal{F}(k, l)$ and has a basis formed by all combinations of k basis elements v_μ of T_p and l basis elements v^ν of T_p^*. A generic (k, l) tensor might be written as:

$$T = \sum_{\substack{\mu_1 \mu_2 \ldots \\ \nu_1 \nu_2 \ldots}} T^{\mu_1 \ldots \mu_k}{}_{\nu_1 \ldots \nu_l} \; v_{\mu_1} \otimes \cdots \otimes v_{\mu_k} \otimes v^{\nu_1} \otimes \cdots \otimes v^{\nu_l}, \tag{3.8}$$

where the operation $\otimes$ is called outer product (or tensor product). The outer product of two arbitrary tensors $A : V \to \mathbb{R}$ and $B : U \to \mathbb{R}$, applied to $x \otimes y$ where $x \in V$ and $y \in U$ is given by

$$(A \otimes B)(x \otimes y) = A(x)B(y). \tag{3.9}$$

It is clear that a $(1, 0)$ tensor is identified as a vector and a $(0, 1)$ tensor as a dual vector. From that identification and the multilinear property of definition 3.4 we can

deduce that [59], under a change of coordinate system, the components of a tensor T transform as

$$T^{\mu'_1\cdots\mu'_k}{}_{\nu'_1\cdots\nu'_l} = \frac{\partial x^{\mu'_1}}{\partial x^{\mu_1}}\cdots\frac{\partial x^{\mu'_k}}{\partial x^{\mu_k}}\frac{\partial x^{\nu_1}}{\partial x^{\nu'_1}}\cdots\frac{\partial x^{\nu_k}}{\partial x^{\nu'_k}}T^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}\,. \tag{3.10}$$

The above eq. (3.10) is known as **tensor transformation law**. Since it is logically reasonable to expect that physical laws are independent of a particular choice of a coordinate system ϕ, we expect them to be manifested by equations relating quantities that behave like a tensor, that is, quantities that follow a transformation law described by eq. (3.10).

3.2.1 The Metric tensor

It is clear from the theorem 3.1 which defines a coordinate basis, that a basis vector $X_\mu(f)$ measures the instant variation of a function $f : \mathcal{M} \to \mathbb{R}$ around a point p with respect to the component x_μ of a coordinate system. Since tangent vectors can be viewed as a *"infinitesimal variation"*, it is then reasonable to guess that a measure of *"infinitesimal distance"* can be computed from them. The mapping from tangent vectors to real numbers which provides such a notion is the **metric tensor**:

Definition 3.5: Metric tensor

The metric tensor g is a $(0,2)$ tensor, this is, a $T_p \times T_p \to \mathbb{R}$ mapping which is:

1. **Symmetric:** $g(v,u) = g(u,v)$,
2. **Non-degenerate:** $g(v,u) = 0$ for any v implies that $u = 0$,

for $u, v \in T_p$.

It can be shown that [18], for each spacetime point p, a basis v_μ can be found such that $g(v_\mu, v_\nu) = \pm\delta_{\mu\nu}$ which we call the **canonical form** of g. The occurrence of each $+1$ or -1 is independent of which basis is chosen to bring g in its canonical form. These sequences of $+1$ and -1 defines the metric's signature. A metric with only plus signs is called **Riemannian**, while a metric with a single negative sign is called **Lorentzian**. Since spacetime has a Lorentzian signature, we will only consider the later case.

By fixing the first argument of $g(v,u)$ one ends up with a $(0,1)$ tensor which is a dual vector. Because of the non-degenerate property in definition 3.5, the resulting functional is uniquely associated with the fixed vector. Furthermore, since both spaces share the same dimension the relation is also surjective. As a consequence, the metric g establishes a unique isomorphism between T_p and T_p^*. The operation of mapping a (k,l) tensor into a $(k+1, l-1)$ (for example, a vector into a dual vector) using the metric is

called index lowering:

$$g_{\mu\lambda}v^{\lambda} = v_{\mu}, \tag{3.11}$$

where $v_{\mu} \in T_p^*$ is identified as the unique correspondent of $v^{\mu} \in T_p$ after lowering indices. Similarly, the inverse metric $g^{\mu\lambda}$ can be used to raise indices back:

$$g^{\mu\lambda}v_{\lambda} = v^{\mu}. \tag{3.12}$$

3.3 Connection and curvature

In the last section we stated the definition of a vector space and its dual which are the basis for working with vectorial (and tensorial) quantities. In the same path, we now aim to extend the notion of differentiation for manifolds. It can be easily checked by direct calculation that, given a tensor $T^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}$, the components of $\partial_\lambda T^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}$ do not follow the tensor transformation law of eq. (3.10). Hence, physical laws involving ∂_λ cannot be written as equations between tensor quantities in a covariant way. For resolving that, a new differential operator is used to replace the partial derivative ∂_μ. Such operator is the **covariant derivative** ∇_μ and is formally defined as:

Definition 3.6: Covariant Derivative

A covariant derivative ∇_μ is a map between (k, l) and $(k+1, l)$ tensors which satisfies the following properties:

1. **Linearity**:

$$\nabla_\mu(\alpha A^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l} + \beta B^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}) = \alpha\nabla_\mu A^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l} + \beta\nabla_\mu B^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}.$$

2. **Leibniz rule:**

$$\nabla_\mu(A^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}C^{\mu'_1\cdots\mu'_k}{}_{\nu'_1\ldots\nu'_l}) = (\nabla_\mu A^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l})C^{\mu'_1\cdots\mu'_k}{}_{\nu'_1\ldots\nu'_l} + A^{\mu_1\cdots\mu_k}{}_{\nu_1\ldots\nu_l}(\nabla_\mu C^{\mu'_1\cdots\mu'_k}{}_{\nu'_1\ldots\nu'_l}).$$

3. **Commutativity with contraction:**

$$\nabla_\mu(A^{\mu_1\ldots\lambda\ldots\mu_k}{}_{\nu_1\ldots\lambda\ldots\nu_l}) = \nabla_\mu A^{\mu_1\ldots\lambda\ldots\mu_k}{}_{\nu_1\ldots\lambda\ldots\nu_l}.$$

4. **Reduction to partial derivative on scalars:**

$$\nabla_\mu(\phi) = \partial_\mu\phi.$$

5. **Torsion free:**

$$\nabla_\mu\nabla_\nu\phi = \nabla_\nu\nabla_\mu\phi.$$

Where for all items, we have that A and B are (k, l) tensors, C is a (k', l') tensor, α and β are real scalars and ϕ is a real field. It can be shown [59] that, given the listed properties, the operator ∇_μ applied to a vector V must be written as:

$$\nabla_\mu V^\nu = \partial_\mu V^\nu + \Gamma^\mu{}_{\nu\lambda} V^\lambda, \tag{3.13}$$

where $\Gamma^\mu{}_{\nu\lambda}$ are called the connection coefficients and its values are yet to be fixed by the introduction of another condition, namely a connection.

If the manifold in question is equipped with a metric $g_{\mu\nu}$ following the definition 3.5, the coefficients $\Gamma^\lambda{}_{\mu\nu}$ can be calculated by imposing an additional condition:

$$\nabla_\alpha g_{\mu\nu} = 0. \tag{3.14}$$

The above eq. (3.14) is called **metric compatibility** and can then be used together with the torsion free property of definition 3.6 to find the particular connection:

$$\Gamma^\lambda{}_{\mu\nu} = \frac{1}{2} g^{\lambda\rho}(\partial_\mu g_{\nu\rho} + \partial_\nu g_{\rho\mu} - \partial_\rho g_{\mu\nu}), \tag{3.15}$$

which is called Christoffel connection and will be used in the rest of the following work. The coefficients $\Gamma^\lambda{}_{\mu\nu}$ given by the above eq. (3.15) are then called Christoffel Symbols.

From the definition 3.6 the covariant derivative ∇_μ is meant to produce a tensorial quantity when applied to an arbitrary tensor. Because of that construction, the quantity $\nabla_\mu V^\nu$, where V is an arbitrary vector, is a well-defined tensor which transforms as eq. (3.10).

The concept of a covariant derivative can be also used to define a relation between tangent vectors of neighboring points in such a way that a vector is transported along a path keeping itself constant.

Definition 3.7: Parallel Transport

A (k, l) tensor T is **paralleled transported** along a curve if the following condition is satisfied:

$$\frac{\partial x^\sigma}{\partial \lambda} \nabla_\sigma T^{\mu_1 \ldots \mu_k}{}_{\nu_1 \ldots \nu_l} = 0, \tag{3.16}$$

where λ is the parametrization of the curve.

By solving eq. (3.16) for an initial value of T one can compare the tensor T at different points at space. It should be pointed however, that the resulting tensor after the transport depends upon the chosen path. Such path dependent property is a direct consequence of the presence of curvature on the manifold in question.

One can give a precise definition of curvature in terms of the change on a vector after being paralleled transported over an infinitesimal closed path. It is possible to show [59], up to second order, that the change in the vector v^μ when paralleled transported over a small parallelogram with sides Δs and Δt is given by

$$\delta(v^\rho) = \Delta t \Delta s v^\sigma T^\mu S^\nu R^\rho{}_{\sigma\mu\nu}, \tag{3.17}$$

where the vectors T^μ and S^ν are parallel to the parallelogram's sides with length Δt and Δs respectively. The tensor R arises from the failure of two successive applications of ∇_μ to commute locally, and is called the Riemann tensor:

Definition 3.8: Riemann curvature tensor

The Riemann curvature tensor is a $(1,3)$ tensor which is defined by its contraction with an arbitrary dual vector ω_ρ:

$$R^\rho{}_{\sigma\mu\nu}\omega_\rho = (\nabla_\mu\nabla_\nu - \nabla_\nu\nabla_\mu)\omega_\sigma, \tag{3.18}$$

or to the arbitrary vector v^σ as:

$$R^\rho{}_{\sigma\mu\nu}v^\sigma = -(\nabla_\mu\nabla_\nu - \nabla_\nu\nabla_\mu)v^\rho. \tag{3.19}$$

It can also be defined explicitly in terms of the connection $\Gamma^\sigma{}_{\mu\nu}$ as:

$$R^\rho{}_{\sigma\mu\nu} = \partial_\mu\Gamma^\rho{}_{\nu\sigma} - \partial_\nu\Gamma^\rho{}_{\mu\sigma} + \Gamma^\rho{}_{\mu\lambda}\Gamma^\lambda{}_{\nu\sigma} - \Gamma^\rho{}_{\nu\lambda}\Gamma^\lambda{}_{\mu\sigma}. \tag{3.20}$$

The following properties follow directly from the definitions of eq. (3.18) and eq. (3.19) as from the properties of the covariant derivative listed in definition 3.6 (a detailed derivation can be found at [18]):

1. $R_{\rho\sigma\mu\nu} = -R_{\sigma\rho\mu\nu}$.
2. $R_{\rho\sigma\mu\nu} = -R_{\rho\sigma\nu\mu}$.
3. $R_{\rho[\sigma\mu\nu]} = 0$.
4. The Bianchi identity:

$$\nabla_{[\lambda}R_{\rho\sigma]\mu\nu} = 0.$$

From eq. (3.20) it is clear that, using a Christoffel connection given by eq. (3.15), the Riemann tensor would vanish for a constant metric. Indeed, it can be shown [18] that having $R^\rho{}_{\sigma\mu\nu} = 0$ everywhere in the manifold, implies that the metric is globally flat.

An important measure of curvature can be derived by contracting the first and third indices of the Riemannian tensor $R^\rho{}_{\sigma\mu\nu}$:

$$R_{\mu\nu} = R^\lambda{}_{\mu\lambda\nu}. \tag{3.21}$$

The resulting tensor $R_{\mu\nu}$ is called **Ricci tensor**. One could also consider other possible contractions of $R^{\rho}{}_{\sigma\mu\nu}$, however, by its anticommuting properties it can be easily shown that these contractions either vanish or are related to $R_{\mu\nu}$. We can further take its trace and obtain a scalar measure of curvature called **Ricci scalar**:

$$R = R_{\lambda\lambda} = g_{\lambda\mu} R^{\mu}{}_{\lambda}. \tag{3.22}$$

The Ricci scalar or scalar curvature is an important measure of curvature since scalar fields are independent of the coordinate system of choice.

4 Quantum Field Theory

In this chapter, we provide the basic tools to work with quantum scalar fields. We start by defining the Lagrangian formalism for a classical field and apply it to derive its equations of motion. Then, the field is submitted to the process of canonical quantization in order to obtain an operator-valued field, which is later decomposed into a continuous set of independent harmonic oscillators. At the end, we consider the extension of the field formalism to the context of a curved spacetime.

4.1 Classical Field Theory

A field is generally a function which maps a point on a space-time manifold to a mathematical object. For example, a real (or complex) scalar field ϕ has the signature $\phi : \mathcal{M} \to \mathbb{R}$ (or $\phi : \mathcal{M} \to \mathbb{C}$). The procedure of finding a realizable configuration for the field is imported from the Lagrangian formalism of classical mechanics. In this formalism, the realizable trajectories $q_i(t)$ of a set of particles are obtained by finding the extrema of a functional S [27], called action:

$$S[q_i] = \int_{t_i}^{t_f} dt\ L(q_i(t), \dot{q}_i(t), t), \tag{4.1}$$

at fixed t_f and t_i, where L is the Lagrangian, defined as the difference between the kinetic and potential energies $L = K - V$. To shorten the notation, we abbreviated the dependency on all $q_1, q_2, \ldots$ by q_i. Each trajectory can be obtained by imposing that S is an extremum, or equivalently $\delta S = 0$, which leads to the Euler-Lagrange equations:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = 0 \quad i = 1, \ldots. \tag{4.2}$$

The above eq. (4.2) can then be solved for $q_i(t)$.

In order to generalize this treatment for a field, one might informally replace the discrete index i by a continuous 4-dimensional coordinate $x = (t, \vec{x})$. The Lagrangian L becomes a functional of the field ϕ and its derivatives $\partial_\mu \phi$:

Definition 4.1: Action and Lagrangian

The action S is the integral in time of the Lagrangian, which is a functional of the field ϕ:

$$S[\phi] = \int_{t_1}^{t_2} dt L[\phi(x), \partial_\mu \phi(x)]. \tag{4.3}$$

The equations of motion, whose solution gives a realizable configuration of ϕ, are obtained by the extremization of S defined in eq. (4.3):

$$\frac{\delta L}{\delta \phi} - \nabla \frac{\delta L}{\delta(\nabla \phi)} - \frac{\partial}{\partial t}\frac{\delta L}{\delta \dot{\phi}} = 0, \tag{4.4}$$

where $\frac{\delta}{\delta \phi}$ denotes the functional derivative with respect to $\phi(x)$, defined as:

Definition 4.2: Functional Derivative

The variation $\delta F[\phi]$ of a functional $F[\phi]$ with respect to a small variation $\delta\phi(x)$ near the function $\phi(x)$ is given by:

$$\begin{aligned} \delta F[\phi] &= F[\phi + \delta\phi] - F[\phi] \\ &= \int dx \frac{\delta F}{\delta \phi(x)} \delta\phi(x), \end{aligned} \tag{4.5}$$

where the quantity $\frac{\delta F}{\delta \phi}(x)$ is defined as the functional derivative of $F[\phi]$ with respect to ϕ.

To calculate the functional derivative $\delta F/\delta\phi$, one can compute the difference $\delta F[\phi + \delta\phi] - F[\phi]$ up to first order in $\delta\phi$ and identify the term multiplying $\delta\phi$ on the integrand of eq. (4.5).

In order to preserve causality, our treatment of the fields will be restricted to allow only local interactions. The Lagrangian L will then be written in terms of a spatial density $\mathcal{L}$,

$$L = \int d^3x \; \mathcal{L}(\phi(x), \partial_\mu \phi(x)), \tag{4.6}$$

which we will also refer as the Lagrangian for simplicity.

An equivalent formulation can be obtained from the Legendre transform of $\mathcal{L}$,

$$H = \int d^3x \left(\frac{\delta \mathcal{L}}{\delta \dot{\phi}} \dot{\phi} - \mathcal{L} \right), \tag{4.7}$$

which allow us to define the density in the integral as the Hamiltonian density:

Definition 4.3: Hamiltonian and conjugate momentum

The conjugate momentum π of a field ϕ is defined as

$$\pi = \frac{\delta L}{\delta \dot{\phi}} = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \; . \tag{4.8}$$

The Hamiltonian $\mathcal{H}$ is defined as the Legendre transform of $\mathcal{L}$:

$$\mathcal{H} = \pi\dot{\phi} - \mathcal{L}. \tag{4.9}$$

The equations of motion (4.4) are then equivalent to the **Hamilton equations of motion**:

$$\dot{\pi} = -\frac{\delta H}{\delta \phi}, \quad \dot{\phi} = \frac{\delta H}{\delta \pi}. \tag{4.10}$$

Or in terms of the **Poisson bracket**:

$$\dot{\phi} = \{\phi, H\}, \quad \dot{\pi} = \{\pi, H\}, \tag{4.11}$$

$$\text{where } \{F, G\} = \int d^3x \left(\frac{\delta F}{\delta \phi(x)} \frac{\delta G}{\delta \pi(x)} - \frac{\delta F}{\delta \pi(x)} \frac{\delta G}{\delta \phi(x)} \right). \tag{4.12}$$

More generally, the temporal evolution of any functional F is given by $\dot{F} = \{F, H\}$.

4.2 Lorentz invariance

We aim to work with theories that satisfy the covariance principle of special relativity. As a consequence, we require L to be invariant under Lorentz transformations. In addition to that, the fields ϕ must belong to an irreducible representation of the Lorentz Group:

Definition 4.4: Lorentz Group

The Lorentz group is the set of linear transformations Λ acting on the coordinates $x = (t, x, y, z)$ which satisfies:

$$\Lambda^T \eta \Lambda = \eta, \tag{4.13}$$

where η is the Minkowski metric:

$$\eta = \text{Diag}(-1, 1, 1, 1). \tag{4.14}$$

A field $\phi(x)$ which is invariant under a Lorentz transformation $x' \to \Lambda x$, satisfies:

$$\phi'(x') = \phi'(\Lambda x) = \phi(x), \tag{4.15}$$

and belongs to the trivial representation. Such field ϕ is called a **scalar field**. The trivial representation is irreducible if and only if it is unidimensional, so it can be described by a single real or complex component.

Other fields ψ that belong to a distinct representation R of the Lorentz Group would in general transform as

$$\psi'(x') = T_R^{-1}(\Lambda) \psi(\Lambda x), \tag{4.16}$$

where $T_R(\Lambda)$ is a linear transformation on R associated to Λ. Some examples of representations R are four-vectors, spinors or tensors made out of such objects. The trivial representation can be recovered by setting $T_\Lambda = \mathbb{1}$ for any Λ.

In addition to Lorentz transformations, one must require invariance under translations by a constant shift vector a^μ:

$$x^\mu \to x^\mu + a^\mu. \tag{4.17}$$

By combining the transformations Λ with the translations one obtains a larger group called the Poincaré Group, which encompasses all the space-time symmetries required by special relativity.

4.3 Canonical Quantization of the Klein-Gordon field

In order to obtain a quantum theory of fields one has to construct a set of field operators which act on a Hilbert space. One of the procedures to obtain such operators is called **canonical quantization**. It consists in first defining a classical Hamiltonian H in terms of a field ϕ and its conjugate momentum π, promoting those fields to operators while imposing the equal time commutation relations:

Definition 4.5: Equal time (bosonic) commutation relations

The equal time commutation relations (ETQC) for the operator valued fields $\phi(\vec{x}, t)$ and $\pi(\vec{x}, t)$ are:

$$\begin{aligned} &[\phi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = i\delta^3(\mathbf{x} - \mathbf{x}'), \\ &[\phi(\mathbf{x}, t), \phi(\mathbf{x}', t)] = [\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = 0. \end{aligned} \tag{4.18}$$

Note that eq. (4.18) says nothing about the commutation of ϕ and π at different times.

More generally, the canonical quantization process maps the Poisson bracket (4.12) to the commutator

$$\{A, B\} \to -i[A, B], \tag{4.19}$$

where A, B in the commutators are the promoted operators originated from the functional in the brackets. By setting A and B to ϕ and π and using the properties of functional derivatives [27], one recovers definition 4.5.

We may now apply the canonical quantization process to a real scalar field ϕ having the following Hamiltonian:

$$\mathcal{H} = \frac{1}{2}\left[\pi^2 + \nabla\phi \cdot \nabla\phi + m^2\phi^2\right]. \tag{4.20}$$

The field satisfying the above Hamiltonian of 4.20 is called the Klein-Gordon field. The equations of motion for such field are obtained by calculating the commutators of ϕ and π

with H:

$$\dot{\phi}(x) = -i[\phi(x), H] = \pi(x), \tag{4.21}$$

$$\dot{\pi}(x) = -i[\pi(x), H] = (\nabla^2 - m^2)\phi(x). \tag{4.22}$$

The first eq. (4.21) can be differentiated with respect to t to obtain $\dot{\pi}$, which can be substituted in the second 4.22 for obtaining:

$$(\nabla^2 - m^2)\phi = \ddot{\phi}. \tag{4.23}$$

We now expand ϕ in Fourier modes, passing the temporal dependency to the operators $b_p(t)$,

$$\phi(x) = \int \frac{d^3p}{\sqrt{2\omega_p(2\pi)^3}} b_p(t) e^{i\vec{p}\cdot\vec{x}}, \tag{4.24}$$

where $\omega_p = \sqrt{|p|^2 + m^2}$. Inserting the expansion into eq. (4.23) and using the hermiticity of ϕ, we obtain $b_p(t) = a_p e^{-i\omega_p t} + a_p^\dagger e^{i\omega_p t}$, and hence:

$$\phi(x) = \int \frac{d^3p}{\sqrt{2\omega_p(2\pi)^3}} (a_p e^{ipx} + a_p^\dagger e^{-ipx}), \tag{4.25}$$

where $px = \vec{p}\cdot\vec{x} - \omega_p t$. Note that the operators a_p and $a_p^\dagger$ are time-independent. The commutation relations for these operators are obtained by substituting the above expansion in the equal time commutation relations, resulting in

$$[a_p, a_{p'}^\dagger] = \delta^3(p - p'). \tag{4.26}$$

When $p' = p$ the commutator is infinite. This behavior can be understood by first considering a finite box of side L. The momenta are then restricted to a discrete set of values depending on L and the normalization of $\delta^3(p)$ implies that the commutator at eq. (4.26) is proportional to $L^3\delta_{pp'}$ [43]. At this point, the commutator for each p is equivalent to the one of a harmonic oscillator in momentum space. Taking the limit $L \to \infty$, one recovers eq. (4.26).

We can then interpret the Klein-Gordon field as a continuum of harmonic oscillators, each associated to a momentum p. Because the excitations of such operators are related to plane waves, we might interpret each of them as a particle with momentum p.

A diagonal basis for H can be constructed in terms of the eigenvectors of the number operators for each mode p:

$$n_p = a_p^\dagger a_p. \tag{4.27}$$

The eigenvalues of each n_p are separated by an integer amount, and it quantifies the number of particles occupying each momentum state. The state which has no occupation for every p is given by:

$$a_p \left|0\right\rangle = 0\,, \quad \text{for all } p, \tag{4.28}$$

and is called the **ground state** of the field ϕ. Because translations and boosts are symmetries of the Minkowski spacetime, every inertial observer may agree in measuring a vanishing number of particles. However, we emphasize that, a general spacetime may not enjoy such symmetries and, in that case, the vacuum state (4.28) for an observer might not correspond to the vacuum for another observer. We will return to this phenomena in detail in the following section.

4.4 Klein-Gordon field in curved spacetime

A generalization of the Klein-Gordon equation for a curved spacetime [16] can be obtained by the introduction of a background metric $g_{\mu\nu}$, which we assume to not be affected by the presence of the field. The partial derivatives ∂_μ are then replaced by covariant ones ∇_μ and the Lagrangian $\mathcal{L}$ is rescaled by $\sqrt{-g}$, since it describes a density. A coupling to the curvature is introduced by a term involving the Ricci scalar R, leading to:

$$\mathcal{L} = \frac{1}{2}\sqrt{-g}\left[g^{\mu\nu}(\partial_\mu\phi)(\partial_\nu\phi) - (m^2 + \xi R)\phi^2\right], \tag{4.29}$$

where ξ is a real coupling constant and we have used the fact that ϕ is a scalar quantity to write $\nabla_\mu\phi = \partial_\mu\phi$. The above Lagrangian 4.29 leads to the following equation of motion:

$$\left(\Box_c + m^2 + \xi R\right)\phi = 0, \tag{4.30}$$

where the D'Alambertian $\Box_c$ is defined as:

$$\Box_c = g^{\mu\nu}\nabla_\mu\nabla_\nu. \tag{4.31}$$

We can find specific values for ξ which makes eq. (4.30) invariant under the conformal transformations:

$$g_{\mu\nu} \to \bar{g}_{\mu\nu} = \Omega^2(x) g_{\mu\nu}, \tag{4.32}$$

where $0 < \Omega(x) < \infty$ is a real function. It can be showed by direct calculation [16] that the following term is invariant:

$$\left(\Box + \frac{1}{4}\frac{(n-2)}{(n-1)}R\right)\phi \to \left(\bar{\Box} + \frac{1}{4}\frac{(n-2)}{(n-1)}\bar{R}\right)\bar{\phi}, \tag{4.33}$$

where $\bar{\phi} = \Omega^{(2-n)/2}\phi$ and n is the dimension of the manifold. We can fix the value of ξ by demanding eq. (4.30) to be invariant under the conformal transformation 4.32. In our case, $n = 4$ gives $\xi = 1/6$ and this situation corresponds to a **conformal coupling** between the field ϕ and the curvature.

The quantization of the field ϕ can be done just as in the case of a Minkowski metric $g_{\mu\nu} = \eta_{\mu\nu}$ by expanding it on a complete set of modes $u_p(x)$, together with creation and annihilation operators a_p which satisfy the commutation relations of eq. (4.26). However, because of the lack of symmetry on a generic spacetime, a particular decomposition (like (4.25) which is based on rectangular coordinates) might not be of physical significance to all inertial observers as in the case of a Minkowski spacetime. The measurement of particles becomes sensitive to observer dependent properties [25].

Another simple example which illustrates this phenomenon involves the creation of particles due to a time-dependent metric which is asymptotically flat at $t = \pm\infty$ [15]. In this case, two inertial observers located respectively at future and past infinity could observe a different number of particles while being on the same state.

5 Entanglement entropy of scalar fields

As we saw earlier in chapter 2, any pure state $|\psi\rangle$ of an arbitrary quantum system can also be characterized by a density operator:

$$\rho = |\psi\rangle\langle\psi| \,. \tag{5.1}$$

We also saw that if we consider two complementary regions A and B of such system, a measure of entanglement can be constructed in terms of the Von Neumann entropy (2.9) of one of the reduced density matrices ρ_A or ρ_B:

$$S = -\operatorname{Tr}\rho_A \log \rho_A = -\operatorname{Tr}\rho_B \log \rho_B. \tag{5.2}$$

In this chapter, the calculation of S is performed for a lattice of coupled harmonic oscillators. The lattice can describe, in particular, the discretization of a scalar field as done in the next chapter. In this case, the entanglement entropy for the system of oscillators provides an approximation for that of the theory in the continuum

5.1 Lattice of harmonic oscillators

The harmonic oscillator is a classical example of a quantum system subjected to a non-vanishing potential which can be solved analytically. A single oscillator, which could for instance describe the position x of a particle subjected to a parabolic potential proportional to x^2, has the simple Hamiltonian given by [53]

$$\hat{H} = \frac{1}{2m}\left(\hat{p}^2 + (\omega_0 m)^2 \hat{x}^2\right), \tag{5.3}$$

where $\hat{p}$ and $\hat{x}$ are the momentum and position operators, given by $-i\partial_x$ (with $\hbar = 1$) and x in the position basis, and m and ω_0 are the mass and the oscillation frequency of the particle, respectively. The energy levels E_k and wave functions $\langle x|\psi_k\rangle$ of such a system are the solutions of the Schrödinger equation $\hat{H}\psi_k(x) = E_k\psi_k(x)$. They are given by [28]:

$$E_k = \left(\frac{1}{2} + k\right)\omega_0, \tag{5.4}$$

$$\psi_k(x) = \left(\frac{m\omega_0}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n k!}} H_k(\sqrt{m\omega_0}x) \exp\left(-\frac{m\omega_0}{2}x^2\right), \tag{5.5}$$

where H_k is the Hermite polynomial of order k. It follows from eq. (5.5) that the ground state is given by

$$E_k = \frac{\omega_0}{2} \quad \text{and} \quad \psi_0(x) = \left(\frac{m\omega_0}{\pi}\right)^{1/4} e^{-\frac{m\omega_0}{2}x^2}. \tag{5.6}$$

In the two subsequent subsections, the calculation of the entanglement entropy between two complementary sets of interacting harmonic oscillators in the ground state [57] is given. In both sections, each oscillator is subjected to a parabolic potential around a fixed point in space in addition to a quadratic potential which depends on the relative displacement of each oscillator.

5.1.1 Two oscilators case

Consider a system of two harmonic oscillators described by the two degrees of freedom x_1 and x_2 which describe the displacement of each oscillator to its lowest potential energy point. The mass of both oscillators is taken to be the same and is absorbed in the coupling constants. It follows that the Hamiltonian H (in the position basis) is given by:

$$H = \frac{1}{2}\left[-\partial_{x_1}^2 - \partial_{x_2}^2 + k_0(x_1^2 + x_2^2) + k_1(x_1 - x_2)^2\right], \tag{5.7}$$

where ∂_{x_k} is an abbreviation for $\frac{\partial}{\partial x_k}$ and k_0 and k_1 are two positive coupling constants. We introduce normal variables x_+ and x_- inspired by their success in decoupling classical coupled harmonic oscillators:

$$\begin{aligned} x_+ &= \frac{1}{\sqrt{2}}(x_1 + x_2) \\ x_- &= \frac{1}{\sqrt{2}}(x_1 - x_2) \end{aligned} \qquad \Rightarrow \qquad \begin{aligned} x_1 &= \frac{\sqrt{2}}{2}(x_+ + x_-) \\ x_2 &= \frac{\sqrt{2}}{2}(x_+ - x_-)\,. \end{aligned} \tag{5.8}$$

The momentum operators in terms of x_+ and x_- can be obtained by applying the chain rule on each variable:

$$\begin{aligned} \partial_{x_1}^2 &= \left(\frac{\partial x_1}{\partial x_+}\partial_{x_+} + \frac{\partial x_1}{\partial x_-}\partial_{x_-}\right)^2 = \frac{1}{2}\left(\partial_{x_+}^2 + \partial_{x_-}^2 + 2\partial_{x_+}\partial_{x_-}\right), \\ \partial_{x_2}^2 &= \left(\frac{\partial x_2}{\partial x_+}\partial_{x_+} + \frac{\partial x_2}{\partial x_-}\partial_{x_-}\right)^2 = \frac{1}{2}\left(\partial_{x_+}^2 + \partial_{x_-}^2 - 2\partial_{x_+}\partial_{x_-}\right), \end{aligned} \tag{5.9}$$

where the derivatives have been evaluated by straight differention of eq. (5.8). Using the new variables, the Schrödinger equation can be written as:

$$\frac{1}{2}\left[-\partial_{x_+}^2 - \partial_{x_-}^2 + k_0 x_+^2 + (k_0 + 2k_1)x_-\right]\psi(x_+, x_-) = E\psi(x_+, x_-). \tag{5.10}$$

The presence of terms on eq. (5.10) depending on x_+ or x_- separately suggests that the solution may take the form of $\psi(x_+, x_-) = \psi_+(x_+)\psi_-(x_-)$. Inserting this guess, one finds that the eq. (5.10) is only satisfied if each of the following equations are satisfied separately:

$$\begin{aligned} \frac{1}{2}\left(-\partial_{x_+}^2 + k_0 x_+^2\right)\psi_+ &= E_+\psi_+, \\ \frac{1}{2}\left(-\partial_{x_-}^2 + (k_0 + 2k_1)x_-^2\right)\psi_- &= E_-\psi_-, \\ E &= E_+ + E_-. \end{aligned} \tag{5.11}$$

Since by the above eq. (5.11), the energy E is additive in both separation variables E_+ and E_-, the minimal energy is given by minimizing both parameters independently. It is clear that both equations for ψ_+ and ψ_- are equations of two independent harmonic oscillators for the variables x_+ and x_-, respectively. The ground state for each of them is given in terms of eq. (5.6). The joint ground state $\psi_0(x_+, x_-)$ is then:

$$\begin{aligned}\psi_0(x_+, x_-) &= \frac{(\omega_+\omega_-)^{1/4}}{\sqrt{\pi}} \exp\left[-\frac{1}{2}(\omega_+ x_+^2 + \omega_- x_-^2)\right], \\ \psi_0(x_1, x_2) &= \frac{(\omega_+\omega_-)^{1/4}}{\sqrt{\pi}} \exp\left[-\frac{1}{4}\left((\omega_+ + \omega_-)(x_1^2 + x_2^2) + 2(\omega_+ - \omega_-)x_1 x_2\right)\right],\end{aligned} \tag{5.12}$$

where $\omega_+^2 = k_0$ and $\omega_-^2 = (k_0 + 2k_1)$.

We now proceed to calculate the entanglement entropy between the two oscillators. By construction, the system is in a pure state, so the matrix elements of ρ in the position basis are given by:

$$\begin{aligned}\rho(x_1, x_1', x_2, x_2') &= (\langle x_1'| \otimes \langle x_2'|)\, |0\rangle\langle 0|\, (|x_1\rangle \otimes |x_2\rangle) \\ &= \langle x_1' x_2'|0\rangle \, \langle 0|x_1 x_2\rangle \\ &= \psi_0^*(x_1', x_2')\psi_0(x_1, x_2).\end{aligned} \tag{5.13}$$

The reduced density matrix ρ_{out} is computed by taking the partial trace of the inside region:

$$\begin{aligned}\rho_{out}(x_2, x_2') &= \langle x_2'| \operatorname{Tr}_{in}(\rho) \, |x_2\rangle \\ &= \int_{-\infty}^{\infty} \psi_0^*(x_1, x_2')\psi_0(x_1, x_2) dx_1 \\ &= \int_{-\infty}^{\infty} dx_1 \frac{(\omega_+\omega_-)^{1/2}}{\pi} \exp\Big[-\frac{1}{4}\Big((\omega_+ + \omega_-)(2x_1^2 + x_2^2 + {x_2'}^2) + \\ &\qquad + 2(\omega_+ - \omega_-)(x_2 + x_2')x_1\Big)\Big]\end{aligned} \tag{5.14}$$

We can complete the square on the exponent to isolate a single term which depends on x_1:

$$\begin{aligned}\rho_{out}(x_2, x_2') = \int_{-\infty}^{\infty} dx_1 \frac{(\omega_+\omega-)^{1/2}}{\pi} \exp\Bigg\{-\frac{(\omega_+ + \omega_-)}{4}\Bigg[\left(x_1 + \frac{1}{2}\frac{\omega_+ - \omega_-}{\omega_+ + \omega_-}(x_2 + x_2')\right)^2 - x_2 x_2' \\ -\frac{1}{4}\left(\frac{\omega_+ - \omega_-}{\omega_+ + \omega_-}\right)^2 (x_2 + x_2')^2 + \left(\frac{x_2 + x_2'}{\sqrt{2}}\right)^2\Bigg]\Bigg\}.\end{aligned} \tag{5.15}$$

The terms on the exponent of eq. (5.15) which do not depend on x_1 can then be factored out as multiplicative constants and the resulting integrand is a Gaussian shifted by $-\frac{1}{2}\frac{\omega_+ - \omega_-}{\omega_+ + \omega_-}(x_2 + x_2')$. The Gaussian integral yields:

$$\begin{aligned}\rho_{out}(x_2, x_2') &= \frac{\sqrt{\omega_+\omega_-}}{\pi}\sqrt{\frac{2\pi}{\omega_+ - \omega_-}} \exp\left[-\frac{(\omega_+ + \omega_-)}{4}(x_2^2 + E{x_2'}^2) - \frac{\beta}{2}(x_2 + x_2')^2\right] \\ &= \sqrt{\frac{(\gamma - \beta)}{\pi}} \exp\left[-\frac{\gamma}{2}(x_2^2 + {x_2'}^2) - \beta x_2 x_2'\right],\end{aligned} \tag{5.16}$$

where the two newly introduced constants γ and β are given by:

$$\beta = \frac{1}{4}\frac{(\omega_+ - \omega_-)^2}{\omega_+ + \omega_-} \quad \text{and} \quad \gamma + \beta = \frac{\omega_+ + \omega_-}{2}. \tag{5.17}$$

By having an expression for $\rho_{out}(x_2, x_2')$, the next step is to compute the entanglement entropy $S = -\operatorname{Tr}(\rho_{out} \ln \rho_{out})$. To evaluate the trace present on S, the position basis is taken and the eigenvalues of $\hat{\rho}_{out}$ are computed by solving:

$$\begin{aligned} \hat{\rho}_{out} \left| f_k \right\rangle &= p_k \left| f_k \right\rangle \\ \left\langle x \right| \hat{\rho}_{out} \left(\int_{-\infty}^{\infty} dx' \left| x' \right\rangle\!\left\langle x' \right| \right) \left| f_k \right\rangle &= \left\langle x \right| p_k \left| f_k \right\rangle \\ \int_{-\infty}^{\infty} dx' \rho_{out}(x, x') f_k(x') &= p_k f_k(x). \end{aligned} \tag{5.18}$$

It can be verified by substitution [57] that the solutions of eq. (5.18) are given by:

$$f_k(x) = H_k(\alpha^{1/2} x) \exp\left(-\frac{\alpha}{2} x^2\right) \quad \text{and} \quad p_k = (1 - \xi)\xi^k \tag{5.19}$$

where $\alpha = (\gamma^2 - \beta^2)^{1/2}$ and $\xi = \beta/(\gamma + \alpha)$.

The substitution of the eigenvalues p_k computed in eq. (5.19) leads to the evaluation of a geometric series and a series of the form $\sum_k k\xi^k$ which is done in appendix A. After evaluating such series, the entropy S is written as:

$$S(\xi) = -\sum_{k=0}^{\infty} p_k \ln(p_k) = -\ln(1 - \xi) - \frac{\xi}{1 - \xi} \ln(\xi) \tag{5.20}$$

5.1.2 N oscillators case

In the general case of N of oscillators, the Hamiltonian is written (in the position basis) as:

$$H = \frac{1}{2}\left(\sum_{i=1}^{N} p_i^2 + \sum_{i,j=1}^{N} x_i k_{ij} x_j \right) = \frac{1}{2}\left(P^T P + X^T K X \right), \tag{5.21}$$

where we have introduced the vectors $P = (-i\partial_{x_1}, \ldots, -i\partial_{x_N})^T$ and $X = (x_1, \ldots, x_N)^T$ ando also the symmetric matrix $(K)_{ij} = k_{ij}$. For a numerical convenience, uppercase symbols, like X, P and K, refer to the one (or two) dimensional array of numbers which determine the components of these objects in a particular basis. This basis in question will be determined by the transition matrix explicitly defined at each step.

Following the same path developed for the case of two oscillators, a suitable choice of basis is made to decouple the oscillators into normal modes. Since K is symmetric, it admits a diagonalization of the form $K_D = U^T K U$ where K_D is diagonal and $U^T = U^{-1}$ [40]. In this case, the positions vector is written as

$$X = U X_D \tag{5.22}$$

and the momenta vector P follows a transformation which is determined by the chain rule:

$$\partial_{x_{D_j}} = \sum_{i=1}^{N} \left(\frac{\partial x_i}{\partial x_{D_j}} \right) \partial_{x_i} = \sum_{i}^{N} u_{ij} \partial_{x_i} \quad \Rightarrow \quad P = U P_D, \tag{5.23}$$

where the partial derivatives in the above eq. (5.23) are obtained by differentiating eq. (5.22). Hence, the Hamiltonian in eq. (5.21) can be rewritten in terms of X_D, P_D and K_D as:

$$H = \frac{1}{2} \left(P_D^T P_D + X_D^T K_D X_D \right), \tag{5.24}$$

where the property $U^T U = U^{-1} U = \mathbb{1}$ has been used.

Since K_D is diagonal, the Schrödinger equation for the time-independent wave function ψ

$$\frac{1}{2} \left(\sum_{i=1}^{N} -\partial_{x_{D_i}}^2 + x_{D_i}^2 k_{D_{ii}} \right) \psi = E \psi, \tag{5.25}$$

is separable in the variables x_{D_i}:

$$\begin{aligned} \frac{1}{2} \left(-\frac{(\partial_{x_{D_i}}^2 \psi_i)}{\psi_i} + x_{D_i}^2 k_{D_{ii}} \right) \psi_i(x_{D_i}) = E_i \psi_i(x_{D_i}), \\ \sum_i E_i = E, \end{aligned} \tag{5.26}$$

where $\psi(x_{D_1}, \dots) = \prod_{i=1}^{N} \psi_i(x_{D_i})$.

Similarly to the case of two oscillators, each equation in eq. (5.26) corresponds to a single harmonic oscillator. The ground state ψ_0 is then given by the product of each individual mode ground state ψ_i. By substituting the state found in eq. (5.6) the resulting joint state is a multivariate Gaussian in the positions X_{D_i}:

$$\begin{aligned} \psi_0 &= \frac{1}{\pi^{N/4}} (\prod_{i=1}^{N} k_{D_i}^{1/2})^{1/4} \exp \left[-\frac{1}{2} \sum_{i=1}^{N} k_{D_i}^{1/2} x_{D_i}^2 \right] \\ &= \frac{1}{\pi^{N/4}} (\det K_D^{1/2})^{1/4} \exp \left[-\frac{1}{2} X_D^T K_D^{1/2} X_D \right]. \end{aligned} \tag{5.27}$$

One can return to the original set of variables by writing $\Omega = U K_D^{1/2} U^T$ and using the inverse of eq. (5.22) and eq. (5.23) into eq. (5.27):

$$\psi_0 = \pi^{-N/4} (\det \Omega)^{1/4} \exp \left[-\frac{1}{2} X^T \Omega X \right]. \tag{5.28}$$

Now that the ground state has been explicitly found, the calculation of ρ_{out} is carried out by tracing out the degrees of freedom inside a region V. To accomplish such task, we partition the quantities in eq. (5.28) according to the region where they belong. If the region V includes the first n degrees of freedom, then the partition follows as:

$$\Omega = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}, \quad X = \begin{bmatrix} X_{in} \\ X_{out} \end{bmatrix}, \tag{5.29}$$

where the matrix A has size $n \times n$, $B : n \times (N-n)$, and $C : (N-n) \times (N-n)$. Since $\Omega = \sqrt{K}$ is symmetric, so are A and C. The vectors X_{in} and X_{out} have sizes n and $N-n$, respectively.

The reduced density matrix ρ_{out} in the position representation can be written as

$$\begin{aligned}\rho_{out}(X_{out}, X'_{out}) = \left(\frac{\det\Omega}{\pi^N}\right)^{1/2} \exp\left[-\frac{1}{2}\left(X_{out}^T C X_{out} + {X'_{out}}^T C X'_{out}\right)\right] \times \\ \times \underbrace{\int dX_{in} \exp\left[-\frac{1}{2}\left(2X_{in}^T A X_{in} + 2X_{in}^T B(X_{out} + X'_{out})\right)\right]}_{(*)},\end{aligned} \tag{5.30}$$

where the terms in the argument of the exponential which are independent of X_{in} were factored out of the integral. We then proceed to a separate calculation of the integral highlighted as $(*)$ in eq. (5.30). By introducing an auxiliary vector $P = A^{-1}B(X_{out} + X'_{out})$ one notes that $(*)$ in eq. (5.30) can be written as

$$(*) = \int dX_{in} \exp\left[-\left(X_{in}^T A X_{in} + X_{in}^T A P\right)\right]. \tag{5.31}$$

To carry out the integration on the X_{in} variables, we may write the exponent in the integrand of eq. (5.31) as a bilinear form. This can be achieved by noticing the following equivalence:

$$X_{in}^T A X_{in} + X_{in}^T A P = \left(X_{in} + \frac{1}{2}P\right)^T A \left(X_{in} + \frac{1}{2}P\right) - \frac{1}{4}P^T A P, \tag{5.32}$$

leading to

$$(*) = \exp\left[\frac{1}{4}P^T A P\right] \int dX_{in} \exp\left[-\left(X_{in} + \frac{1}{2}P\right)^T A \left(X_{in} + \frac{1}{2}P\right)\right]. \tag{5.33}$$

The remaining integral in eq. (5.33) can be computed by choosing a basis in which A is diagonal. Since A is symmetric, its diagonalization takes the form of $A = G^T A_D G$, where A_D is diagonal and G^T is orthogonal. Performing the change of variables $X'_{in} = G^T X_{in}$ would lead to a Jacobian factor of $|\det G|$, but since V is orthonormal we have that $\det G = 1$ and the integral's measure remains unchanged upon this change of variables. The integration of the n variables then yields:

$$(*) = \exp\left[\frac{1}{4}P^T A P\right] \left(\frac{\pi^n}{\det A}\right)^{1/2}. \tag{5.34}$$

Inserting eq. (5.34) back in eq. (5.30), ρ_V is given by:

$$\begin{aligned}\rho_V(X_{out}, X'_{out}) &= \left(\frac{1}{\pi^{(N-n)}}\frac{\det\Omega}{\det A}\right)^{1/2} \exp\left[-\frac{1}{2}\left(X_{out}^T C X_{out} + {X'_{out}}^T C X'_{out}\right) + \frac{1}{4}P^T A P\right] \\ &= \left(\frac{1}{\pi^{(N-n)}}\frac{\det\Omega}{\det A}\right)^{1/2} \exp\left[-\frac{1}{2}\left(X_{out}^T \gamma X_{out} + {X'_{out}}^T \gamma X'_{out}\right) + X_{out}^T \beta X'_{out}\right],\end{aligned} \tag{5.35}$$

where the definition of W has been used and the two new matrices are given by $2\beta = B^T A^{-1} B$ and $\gamma = (C - \beta)$.

The last expression of eq. (5.35) is further developed by diagonalizing $\gamma = V^T \gamma_D V$ and introducing the new coordinates $X = V^T \gamma_D^{-1/2} Y$:

$$\rho_{out}(Y_{out}, Y'_{out}) = \left(\frac{1}{\pi^{(N-n)}} \frac{\det \Omega}{\det A}\right)^{1/2} \exp\left[-\frac{1}{2}\left(Y_{out}^T Y_{out} + Y'_{out}{}^T Y'_{out}\right) + Y_{out}^T \beta' Y'_{out}\right], \tag{5.36}$$

where $\beta' = \gamma_D^{-1/2} V \beta V^T \gamma_D^{-1/2}$. Finally, another variable $Z = W^T Y$ related to the diagonalization of $\beta' = W \beta'_D W^T$ is introduced:

$$\rho_{out}(Z_{out}, Z'_{out}) = \left(\frac{1}{\pi^{(N-n)}} \frac{\det \Omega}{\det A}\right)^{1/2} \prod_{i=n+1}^{N} \exp\left[-\frac{1}{2}\left(z_i^2 + z_i'^2\right) + \beta'_i z_i^2 z_i'^2\right], \tag{5.37}$$

where β'_i is the i-th eigenvalue of β'.

To compute the entanglement entropy associated with ρ_{out} one must find its eigenvalues p_k by solving:

$$\begin{aligned} \langle x_{n+1} \dots x_N | \, \hat{\rho}_{out} \, | f_k \rangle &= p_k \langle x_{n+1} \dots x_N | f_k \rangle \\ \int dX'_{out} \rho_{out}(X_{out}, X'_{out}) f_k(X'_{out}) &= p_k f_k(X_{out}). \end{aligned} \tag{5.38}$$

Note that by performing a change of variables $X_{out} \to Z = G X_{out}$, with $G = W^T \gamma^{1/2} V$, one must account to a factor of $\det G$ rescaling the matrix element in eq. (5.37) which can be easily understood by requiring that $\operatorname{Tr} \rho_{out} = 1$. Such factor however is cancelled by the Jacobian $|\det G|^{-1}$ appearing when changing the integration variables of eq. (5.38), leaving the eigenvalues unchanged.

The integration of $\rho_{out}(Z, Z')$ is carried out in each variable z'_i independently. The solution f_k is clearly given by a product of $N - n$ one dimensional solutions given by eq. (5.19) with $\gamma \to 1$ and $\beta \to \beta'_k$. Since the solution is given in terms of a product of ordinary functions, the entropy is additive:

$$S = \sum_k S(\xi_k), \quad \text{where} \quad \xi_k = \frac{\beta'_k}{1 + (1 - \beta'_k)^{1/2}}, \tag{5.39}$$

and $S(\xi_k)$ is given by eq. (5.20).

5.2 Symplectic diagonalization of quadratic Hamiltonians

Before generalizing the procedure of computing the entanglement entropy for discretized scalar fields, we will develop a general technique for diagonalizing a quadratic Hamiltonian of a system constituted of a discrete set of bosonic variables. The procedure is then used to compute the covariance matrix for a set of coupled harmonic oscillators, which will be of central importance to the entropy calculation motivated by the real time approach. An external reference for the described method can be found in [1, 3, 4, 44].

5.2.1 Symplectic group

Consider the set of N pairs of bosonic variables (ϕ_i, π_i) satisfying the canonical commutation relations eq. (4.18). We will aggregate all these variables in a single vector

$$\xi^T = \left(\phi_1, \dots, \phi_N, \pi_1, \dots, \pi_N\right), \tag{5.40}$$

so the relations (4.18) can be compactly written as:

$$[\xi_i, \xi_j] = iJ_{ij} \quad \text{where} \quad J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}. \tag{5.41}$$

Consider a transformation S which maps ξ into a new set of variables $\xi' = S\xi$. The commutator in terms of the new variables read as:

$$[\xi'_i, \xi'_j] = \sum_{kl} S_{ik} S_{jl} [\xi_k, \xi_l] = \sum_{kl} S_{ik} S_{jl} (iJ_{kl}) = i(SJS^T)_{ij}. \tag{5.42}$$

Note that the commutator is left invariant if we require that $SJS^T = J$. As a consequence, the new set of variables ξ' also satisfy the bosonic commutation relations of eq. (4.18). Matrices which satisfy the described condition are called symplectic.

Definition 5.1: Symplectic Group

The real symplectic group $Sp(2N, \mathbb{R})$ consists of all real $2N \times 2N$ matrices S:

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{5.43}$$

which satisfy the equivalent relations:

$$SJS^T = J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \iff \begin{cases} AD^T - BC^T = \mathbb{1} \\ AB^T, CD^T \text{ are symmetric} \end{cases}. \tag{5.44}$$

where A, B, C, D are $N \times N$ blocks.
If S is a symplectic matrix, so is S^T, $-S$ and S^{-1}.

5.2.2 Complex form of a symplectic matrix

A change of basis can be employed in the variables ϕ'_i, π'_j so that the creation and annihilation operators are recovered:

$$a_i = \frac{1}{\sqrt{2}}(\phi'_i + i\pi'_i), \quad a_i^\dagger = \frac{1}{\sqrt{2}}(\phi'_i - i\pi'_i), \quad [a_i, a_j^\dagger] = \delta_{ij}. \tag{5.45}$$

This transformation can be written in terms of the vector ξ' as

$$\xi'_{(c)} = \begin{pmatrix} a_1 \\ \vdots \\ a_n \\ a_1^\dagger \\ \vdots \\ a_n^\dagger \end{pmatrix} = W \begin{pmatrix} \phi'_1 \\ \vdots \\ \phi'_n \\ \pi'_1 \\ \vdots \\ \pi'_n \end{pmatrix}, \quad \text{where} \quad W = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & i\mathbb{1} \\ \mathbb{1} & -i\mathbb{1} \end{pmatrix}, \tag{5.46}$$

so that, in terms of the unprimed variables, we have:

$$\xi'_{(c)} = W\xi' = WS\xi = (WSW^\dagger)(W\xi) = S_{(c)}\xi_{(c)}. \tag{5.47}$$

We can define a new matrix $S_{(c)}$ which we refer to as the complex form of S. In block structure, $S_{(c)}$ is written as:

$$S_{(c)} = \begin{pmatrix} M & N \\ N^* & M^* \end{pmatrix} = \frac{1}{2} \begin{pmatrix} A + D - i(B - C) & A - D + i(B + C) \\ A - D - i(B + C) & A + D + i(B - C) \end{pmatrix}, \tag{5.48}$$

where the $N \times N$ matrices M and N have complex entries. The constraints (5.44) introduced by the symplectic requirement are written as:

$$\begin{aligned} MM^\dagger - NN^\dagger &= \mathbb{1}, \\ MN^T &\text{ is symmetric.} \end{aligned} \tag{5.49}$$

A particular case which will be of great interest in the following developments consists in taking $B = C = 0$, which is equivalent to imposing the realness of M and N, and $A = D = O$ where O is a real orthogonal matrix. In such case, we have:

$$S = S_{(c)} = O \oplus O, \tag{5.50}$$

and consequently:

$$\begin{aligned} \phi_i &= \sum_{k=0}^{N} \alpha_{ik}(a_k + a_k^\dagger), \\ \pi_i &= i \sum_{k=0}^{N} \beta_{ik}(a_k - a_k^\dagger), \end{aligned} \tag{5.51}$$

where we defined α and β as:

$$\alpha = \frac{1}{\sqrt{2}} O^T, \quad \beta = -\frac{1}{\sqrt{2}} O^T. \tag{5.52}$$

Note that the above definitions give us α and β real and $\alpha\beta^T = -\frac{\mathbb{1}}{2}$.

5.2.3 Symplectic diagonalization

We introduce now a physical problem described by a set of canonical pairs (ϕ_i, π_i) and a Hamiltonianion which is quadratic in these bosonic variables:

$$H = \frac{1}{2}\sum_{ij} K_{ij}\xi_i\xi_j = \frac{1}{2}\xi^T K \xi, \tag{5.53}$$

where K is a symmetric and positive definite matrix ($K^T = K > 0$). The system is assumed to be in the ground state.

In general, K has off-diagonal terms which mixes different variables and turns the calculation of observables a dificult task. If a symplectic transformation S can be used to cast V in a diagonal form, the Hamiltonian in terms of the variables $\xi' = S^{-1}\xi$ can be simply written as:

$$H = \frac{1}{2}\xi^T K \xi = \frac{1}{2}(\xi')^T S^T K S \xi' = \frac{1}{2}(\xi')^T K_D \xi' = \frac{1}{2}\sum_j (K_D)_{jj}(\xi'_j)^2. \tag{5.54}$$

For a generic V, a symplectic diagonalization may not be possible. However, for a symmetric and positive definite V there is always a real symplectic matrix which provides a diagonal form of V. This fact is ensured by the Williamson theorem:

Theorem 5.1: Williamson Theorem

Let M be a $2N \times 2N$ symmetric and positive definite, that is $M^T = M > 0$. Then there exists $S_M \in Sp(2N, \mathbb{R})$ such that:

$$\begin{aligned} S_M M S_M^T &= \Lambda_M \\ \text{where } \Lambda_M &= \text{Diag}(\mu_1, \ldots, \mu_N, \mu_1, \ldots, \mu_N), \end{aligned} \tag{5.55}$$

with each μ_j satisfying:

$$\det(JM \pm i\mu_j I_{2N}) = 0 \quad \text{for} \quad j = 1, \ldots, N. \tag{5.56}$$

The matrix Λ_M is called the **Williamson normal form** of M.

Note that Λ_M has repeated diagonal blocks of size $n \times n$, this enables us to rewrite H as

$$H = \frac{1}{2}\sum_k \mu_k \left((\phi')^2 + (\pi')^2\right), \tag{5.57}$$

or in its complex form as

$$H = \sum_k \mu_k \left(a_k^\dagger a_k + \frac{1}{2}\right). \tag{5.58}$$

The Hamiltonian of eq. (5.58) describes a set of N decoupled harmonic oscillators. Because each oscillator is independent, the total energy is obtained by minimizing each

term separately. As a consequence, the ground state is given by a product of the individual Gaussian states which is also Gaussian in the original variables ϕ_i, π_i.

5.2.4 Covariance matrix for a set of harmonic oscillators

We now focus on computing the covariance matrix of a set of harmonic oscillators using the techniques developed above. The covariance matrix of the system described by the canonical variables ϕ_i, π_i is defined as:

$$\gamma_{ij} = \frac{1}{2}\left(\langle \xi_i \xi_j \rangle + \langle \xi_j \xi_i \rangle\right) = \frac{1}{2}\,\mathrm{Tr}(\rho(\xi_i \xi_j + \xi_j \xi_i)), \tag{5.59}$$

whose $n \times n$ blocks are related to the two-point correlation functions:

$$\gamma = \begin{pmatrix} \langle \phi_k \phi_l \rangle & \frac{1}{2}\left(\langle \phi_k \pi_l \rangle + \langle \pi_l \phi_k \rangle\right) \\ \frac{1}{2}\left(\langle \pi_k \phi_l \rangle + \langle \phi_l \pi_k \rangle\right) & \langle \pi_k \pi_l \rangle \end{pmatrix}, \tag{5.60}$$

with $k, l = 1, \ldots, N$.

Let us consider the following restrictions on the class of systems described by H:

1. H has no terms of the type $\phi_i \pi_j$ or $\pi_i \phi_j$.
2. H has no terms of the type $\pi_i \pi_j$ for $i \neq j$.
3. The kinetic terms π_i^2 have all the same weight, which is k_p.

The absence of cross terms is equivalent to stating that the $N \times N$ off-diagonal blocks of K are zero. The second two conditions, imply that the lower block related to the momentum π_j coupling is proportional to the identity $\mathbb{1}_N$. These conditions enable us to write K as the following direct sum:

$$K = K_x \oplus k_p \mathbb{1}_N = \begin{pmatrix} K_x & 0 \\ 0 & k_p \mathbb{1}_N \end{pmatrix}, \tag{5.61}$$

where K_x is an $N \times N$ block matrix. Since K is symmetric, we also have that $K_x = K_x^T$ so it admits a diagonalization by a $N \times N$ orthogonal matrix S [40]. It can be checked that K can be diagonalized by the orthogonal transformation $S \oplus S$ which is also symplectic:

$$\begin{aligned} (S \oplus S)^T K (S \oplus S) &= (S \oplus S)^T (K_x \oplus K_p)(S \oplus S) \\ &= (S^T K_x S) \oplus (S^T k_p \mathbb{1}_N S) \\ &= (S^T K_x S) \oplus (k_p \mathbb{1}_N), \end{aligned} \tag{5.62}$$

where to obtain the last line we used the orthogonality property $S^T S = \mathbb{1}_N$. Since $S^T K_x S$ is diagonal by assumption, eq. (5.62) shows that $S \oplus S$ in facts diagonalizes K. We note that the symplectic matrix $S \oplus S$ has vanishing off-diagonal blocks. As a consequence,

$B = C = 0$ in eq. (5.48) and the respective transformation $S_{(c)}$ is given by real matrices N and M.

The Hamiltonian in terms of the primed variables is given as:

$$H = \sum_{i=1}^{N} \left(\mu_i \phi_i'^2 + k_p \pi_i'^2 \right), \tag{5.63}$$

where $\phi_i' = \xi_i'$, $\pi_i' = \xi_{(N+i)}'$ for $1 \leq i \leq N$ with $\xi' = (S \oplus S)^T \xi$ and μ_i is the i-th eigenvalue of K_x. Since the oscillators are decoupled, each correlator is computed by considering an individual unidimensional harmonic oscillator with $m = 1/(2k_p)$ and $\omega_i = 2\sqrt{\mu_i k_d}$ [53]:

$$\langle \phi_i'^2 \rangle = \frac{1}{2}\sqrt{\frac{k_p}{\mu_i}}, \qquad \langle \pi_i'^2 \rangle = \frac{1}{2}\sqrt{\frac{\mu_i}{k_p}}, \qquad \langle \phi_i' \pi_i' \rangle = -\langle \pi_i' \phi_i' \rangle = \frac{i}{2}. \tag{5.64}$$

Since $\langle \phi_i' \rangle = \langle \pi_j' \rangle = 0$, correlators with mixed indices are zero and thus, are omitted from eq. (5.64). Note that $(K_x')^{1/2} = \mathrm{Diag}(\mu_1^{1/2}, \dots)$, so γ' can be written as:

$$\gamma' = \frac{1}{2}\left[k_p^{1/2} (K_x')^{-1/2} \oplus k_p^{-1/2} (K_x')^{1/2} \right]. \tag{5.65}$$

Using the inverse transformation $\gamma = (S \oplus S)\gamma'(S \oplus S)^T$, one obtains:

$$\gamma = \frac{1}{2}\left[k_p^{1/2} K_x^{-1/2} \oplus k_p^{-1/2} K_x^{1/2} \right] = \frac{1}{2} \begin{pmatrix} k_p^{1/2} K_x^{-1/2} & 0 \\ 0 & k_p^{-1/2} K_x^{1/2} \end{pmatrix}. \tag{5.66}$$

Note that we can directly compute the cross correlators with the unprimed variables $\langle \phi_i \pi_j \rangle$ by noting that:

$$\begin{aligned} \langle \phi_i \pi_j \rangle &= \sum_{k,l} S_{ik}^T S_{jl}^T \langle \phi_k' \pi_l' \rangle \\ &= \sum_{k,l} S_{ik}^T S_{jl}^T \left(\frac{i}{2} \delta_{kl} \right) \\ &= \frac{i}{2} [S^T S]_{ij} = \frac{i}{2} \delta_{ij}, \end{aligned} \tag{5.67}$$

since $S^T S = \mathbb{1}_N$.

5.3 Real time approach

In the section 5.1, we have computed the entanglement entropy by explicitly integrating the degrees of freedom outside the region of interest in order to obtain a reduced density matrix. We now may search for a way of calculating S for a discretized field ϕ having only knowledge of ϕ inside the region in question.

The reduced density matrix ρ_A of a region A is expected to reproduce the statistics of all the local observables in that region, that is:

$$\langle O_A \rangle = Tr(\rho_A O_A). \tag{5.68}$$

One might take an axiomatic approach to a quantum field theory [61] and define these observable quantities in terms of the correlation functions of the fields ϕ and π inside A. In such case, ρ_A is expected to have the same physical content of these correlation functions. In the case of a Gaussian state, one only needs the knowledge of the two point correlation functions and the expectations $\langle\phi_i\rangle$, $\langle\pi_i\rangle$ in order to characterize the state [1].

Let's consider the case of a discretized bosonic field described by the hermitian variables ϕ_i, π_j, with $i, j = 1, 2, \ldots, N$, and the commutation relations:

$$\begin{aligned} &[\phi_i, \phi_j] = 0, \quad [\pi_i, \pi_j] = 0, \\ &[\phi_i, \pi_j] = i\delta_{ij}. \end{aligned} \tag{5.69}$$

The two point correlators inside an arbitrary region A are listed as two matrices:

$$\begin{aligned} X_{ij} &= \langle\phi_i\phi_j\rangle = tr(\rho_A\phi_i\phi_j) \\ P_{ij} &= \langle\pi_i\pi_j\rangle = tr(\rho_A\pi_i\pi_j). \end{aligned} \tag{5.70}$$

Given that our Hamiltonian does not have mixed terms consisting of the product of ϕ_i and π_j, the mixed correlators of the form $\langle\phi_i\pi_j\rangle$ are given by eq. (5.67) in section 5.2:

$$\langle\phi_i\pi_j\rangle = -\langle\pi_j\phi_i\rangle = \frac{i}{2}\delta_{ij}. \tag{5.71}$$

We now make two assumptions about the current system. First, we assume canonical variables ϕ_i, π_j are related to a set of creation and annihilation operators $a_I, a_I^\dagger$ by the real matrices α, β:

$$\begin{aligned} \phi_i &= \alpha_{iI}(a_I + a_I^\dagger), \\ \pi_i &= i\beta_{iI}(a_I - a_I^\dagger). \end{aligned} \tag{5.72}$$

The use of upper-case letters on the indices $i \leftrightarrow I$ emphasizes the distinction between the original Hilbert space and the Fock space spawned by a_I and $a_I^\dagger$. These operators obey the commutation relations:

$$[a_I, a_J^\dagger] = \delta_{IJ}. \tag{5.73}$$

The α and β matrices have a $N \times N_{\mathcal{F}}$ shape, where $N_{\mathcal{F}}$ is the dimension of the Fock space.

Inserting the above eq. (5.72) into the commutation relations defined in eq. (5.69), we obtain:

$$[\phi_i, \pi_j] = i\sum_{IJ}\alpha_{iI}\beta_{jJ}\left([a_J^\dagger, a_I] + [a_I^\dagger, a_J]\right). \tag{5.74}$$

Substituting the commutators for a_I and $a_J^\dagger$ defined in eq. (5.73), the above eq. (5.74) reads as:

$$[\phi_i, \pi_j] = -2i\sum_{IJ}\alpha_{iI}\beta_{jJ}. \tag{5.75}$$

Since the commutator on the left is defined by eq. (5.69) to be $i\delta_{ij}$, the above eq. (5.75) can be written in matrix form as:

$$\alpha\beta^T = -\frac{\mathbb{1}}{2}. \tag{5.76}$$

The second assumption consists in fixing the form of the modular Hamiltonian on the region A and consequently the reduced density matrix ρ_A. The latter is assumed to be diagonal in the occupation basis:

$$\rho_A = C \exp\left[-\sum_I \epsilon_I a_I^\dagger a_I\right], \tag{5.77}$$

where $C = \prod_I (1 - e^{-\epsilon_I})$ is a normalization constant and the energies ϵ_I are yet to be determined. Due to the relations (5.72), we note that the modular Hamiltonian appearing in eq. (5.77) is quadratic in the fields ϕ and π.

Using this expression, the correlation matrices can be obtained by evaluating the trace in eq. (5.70) on the occupation number basis $|n_K\rangle$. For this, we note that ρ_A is diagonal in this basis, and only terms of the form $a_I^\dagger a_J$ or $a_J a_I^\dagger$ will contribute to the sum:

$$\begin{aligned} X_{ij} &= \sum_{KIJ} \langle n_K| \left[\alpha_{iI}\alpha_{jJ}(a_I + a_I^\dagger)(a_J + a_J^\dagger)\right] |n_K\rangle \\ &= \sum_{KIJ} \alpha_{iI}\alpha_{jJ} \langle n_K| \left(a_I a_J + a_I a_J^\dagger + a_I^\dagger a_J + a_I^\dagger a_J^\dagger\right) |n_K\rangle . \end{aligned} \tag{5.78}$$

Note that a nonzero term in eq. (5.78) will only be produced if an excitation created by $a_I^\dagger$ is annihilated by its conjugate a_I. It follows that only terms consisting of a pair of creation and annihilation with $I = J$ will not vanish:

$$\begin{aligned} X_{ij} &= \sum_{KI} \alpha_{iI}\alpha_{jI} \langle n_K| \left(a_I a_I^\dagger + a_I^\dagger a_I\right) |n_K\rangle \\ &= \sum_{KI} \alpha_{iI}\alpha_{jI} \langle n_K| \left(2a_I^\dagger a_I + [a_I, a_I^\dagger]\right) |n_K\rangle \\ &= \sum_{KI} \alpha_{iI}\alpha_{jI} \langle n_K| (2n_I + 1) |n_K\rangle \end{aligned} \tag{5.79}$$

The other $P_{ij}, \langle\phi_i\pi_j\rangle$ matrix elements can be computed in the same way. In summary, they can be written in matrix form as:

$$X = \alpha(2n + 1)\alpha^T \tag{5.80}$$

$$P = \beta(2n + 1)\beta^T \tag{5.81}$$

$$-\frac{\mathbb{1}}{2} = \alpha\beta^T, \tag{5.82}$$

where n is a $N_\mathcal{F} \times N_\mathcal{F}$ diagonal matrix whose elements are given by $[n]_{II} = \langle n_I\rangle$ we used eq. (5.71) in eq. (5.82).

We will now use the obtained equations to write the spectrum ϵ_k in terms of the local correlators X_{ij} and P_{ij}. By computing the product XP and inverting the relation in eq. (5.82) one obtains:

$$XP = \frac{1}{4}\alpha_r(2n+1)^2\alpha_r^{-1}, \tag{5.83}$$

which shows that XP is similar to $\frac{1}{4}(2n+1)^2$ and, therefore, they share the same eigenvalues. The diagonal elements of n are, by construction, the mean occupation for each mode I, which can be easily computed since ρ_V is already diagonal in the n_I operators:

$$[n]_{II} = \langle a_I^\dagger a_I \rangle = \frac{1}{e^{\epsilon_I} - 1}. \tag{5.84}$$

Therefore, the eigenvalues of the left-hand side of eq. (5.83) can be written as:

$$\frac{1}{4}(2n_{II}+1)^2 = \left(\frac{1}{2}\coth(\epsilon_I/2)\right)^2, \tag{5.85}$$

where $\coth(x) = (e^x+1)/(e^x-1)$.

One can invert the relation between the eigenvalues of ρ and XP in eq. (5.83) by considering the square root of the equation. Let ν_I be the *I-th* eigenvalue of $C = \sqrt{XP}$. By using eq. (5.85), one has:

$$\nu_I = \frac{1}{2}\coth(\epsilon_I/2) \quad \Leftrightarrow \quad \epsilon_I = \ln\left(\frac{\nu_I + \frac{1}{2}}{\nu_I - \frac{1}{2}}\right), \tag{5.86}$$

where we have used the following expression for the inverse hyperbolic cotangent function:

$$\coth^{-1}(x) = \frac{1}{2}\left[\ln\left(1+\frac{1}{2x}\right) - \ln\left(1-\frac{1}{2x}\right)\right]. \tag{5.87}$$

A possible path for computing the entanglement entropy (2.46) is to use eq. (5.86) and the inverse of eq. (5.72) for rewriting eq. (5.77) in terms of the fields ϕ_I, π_J. Then, the resulting problem consists in computing the entropy for a Gaussian state in terms of the N field variables, which was already done in the last section when considering a lattice of N oscillators. Instead of taking this path, one can quickly obtain the entanglement entropy by considering the limit case of a Rényi entropy presented in definition 2.10.

The calculation of $H_r(\rho_V)$ with $r \to 1$ starts by computing the trace of the *r-th*

power of ρ_A:

$$\begin{aligned} tr(\rho_A^r) &= tr\left(C^r \prod_I \exp\left(-r\epsilon_I n_I\right)\right) \\ &= C^r \prod_I \sum_{n_I} (x_I^r)^{n_I}\,, \qquad \text{where} \quad x_I = \exp(-\epsilon_I) = \frac{\nu_I - 1/2}{\nu_I + 1/2} \\ &= \prod_I \left(1 - \frac{\nu_I - 1/2}{\nu_I + 1/2}\right)^r \left[1 - \left(\frac{\nu_I - 1/2}{\nu_I + 1/2}\right)^r\right]^{-1} \\ &= \prod_I \left[\left(\nu_I + \frac{1}{2}\right) - \left(\nu_I - \frac{1}{2}\right)\right]^r \left[\left(\nu_I + \frac{1}{2}\right)^r - \left(\nu_I - \frac{1}{2}\right)^r\right]^{-1} \\ &= \prod_I \left[\left(\nu_I + \frac{1}{2}\right)^r - \left(\nu_I - \frac{1}{2}\right)^r\right]^{-1}. \end{aligned} \tag{5.88}$$

The above expression 5.88 can then be inserted in eq. (2.50):

$$S = \lim_{r\to 1} \frac{1}{r-1} \sum_I \ln\left[\left(\nu_I + \frac{1}{2}\right)^r - \left(\nu_I - \frac{1}{2}\right)^r\right]. \tag{5.89}$$

Note that both numerator and denominator of eq. (5.89) approach 0 when the limit $r \to 1$ is taken resulting in an indetermination $\frac{0}{0}$. This indetermination can be avoided by applying L'Hôpital's rule and differentiating the numerator and denominator with respect to r. Note that:

$$\partial_r \left[\ln\left((x+c)^r - (x-c)^r\right)\right]\Big|_{r=1} = \frac{1}{2c}\left[(x+c)\ln(x+c) - (x-c)\ln(x-c)\right], \tag{5.90}$$

so by setting $c = 1/2$, the derivative of the numerator in eq. (5.89) is obtained. The entropy reads:

$$S = \sum_I \left(\nu_I + \frac{1}{2}\right)\ln\left(\nu_I + \frac{1}{2}\right) - \left(\nu_I - \frac{1}{2}\right)\ln\left(\nu_I - \frac{1}{2}\right), \tag{5.91}$$

or, in terms of the matrix $C = \sqrt{XP}$ whose eigenvalues are ν_I:

$$S = tr\left[\left(C + \frac{1}{2}\right)\ln\left(C + \frac{1}{2}\right) - \left(C - \frac{1}{2}\right)\ln\left(C - \frac{1}{2}\right)\right] \tag{5.92}$$

In summary, for computing the entanglement entropy S between a subregion A and its outside, only the knowledge of the correlation matrices X and P inside A are needed.

6 Numerical calculation of the entanglement entropy

In this chapter, we compute the entanglement entropy of a scalar field in its ground state on a static closed universe. This task is accomplished by implementing a numerical scheme based on the real time approach [21, 46] described in the last chapter. The entanglement entropy is then used to estimate two perturbative coefficients, which encode the dependency of this quantity on the intrinsic and extrinsic geometry of the problem. The contents of this chapter are a description of the work published in [56].

6.1 Model definition

6.1.1 Scalar field in an Einstein universe

We consider a spherically symmetric static universe $\mathbb{R} \times \mathbb{S}^3$ described by the line elements

$$ds^2 = -dt^2 + R^2(d\chi^2 + \sin^2\chi d\Omega^2). \tag{6.1}$$

where the infinitesimal solid angle given by

$$d\Omega^2 = d\theta^2 + \sin^2\theta d\alpha^2. \tag{6.2}$$

The temporal component $t \in \mathbb{R}$ parametrizes a set of 3-spheres of radius R described the parameters $\theta, \chi \in [0, \pi]$ and $\alpha \in [0, 2\pi]$. Using these coordinates, the metric tensor elements $g^{\mu\nu}$ reads

$$g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & R^2 & 0 & 0 \\ 0 & 0 & R^2\sin^2\chi & 0 \\ 0 & 0 & 0 & R^2\sin^2\chi\sin^2\theta \end{pmatrix} \tag{6.3}$$

and the associated volume element is

$$\sqrt{-g} = R^3\sin^2\chi\sin\theta. \tag{6.4}$$

The scalar curvature $\mathcal{R}$ (defined in eq. (3.22)) is given by

$$\mathcal{R} = \frac{6}{R^2}. \tag{6.5}$$

We now consider a real scalar field given by the Klein-Gordon Lagrangian 4.29. Using the particular metric given by eq. (6.3) and integrating by parts, one finds:

$$\begin{aligned} L = \frac{1}{2}\int_{\mathbb{S}^3} d\chi d\theta d\alpha \Bigg\{ & R^3 \sin^2\chi \sin\theta \left[\dot{\Phi}^2 - \left(m^2 + \frac{6\xi}{R^2}\right)\Phi^2\right] \\ & - R\sin\theta\left[\sin^2\chi(\partial_\chi\Phi)^2 - \Phi\Delta_{S^2}\Phi\right]\Bigg\}, \end{aligned} \tag{6.6}$$

where Δ_{S^2} is the Laplace-Beltrami operator in the unit 2-sphere, given by:

$$\Delta_{S^2} = \frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\alpha^2. \tag{6.7}$$

The Hamiltonian formalism can be obtained by directly computing the conjugate momenta Π:

$$\Pi = \frac{\partial L}{\partial(\dot{\Phi})} = R^3\sin^2\chi\sin\theta\dot{\Phi}, \tag{6.8}$$

which, together with Φ, satisfies the Poisson bracket (defined in eq. (4.12)):

$$\begin{aligned} \{\Phi(x), \Pi(y)\} &= \delta(x-y), \\ \{\Phi(x), \Phi(y)\} &= \{\Pi(x), \Pi(y)\} = 0. \end{aligned} \tag{6.9}$$

Using the above expression for Π, one obtains:

$$\begin{aligned} H = \frac{1}{2}\int_{\mathbb{S}^3} d\chi d\theta d\alpha \Bigg[& \frac{\Pi^2}{R^3\sin^2\chi\sin\theta} + R\sin\theta\left(\sin^2\chi(\partial_\chi\Phi)^2 - \Phi\Delta_{\mathbb{S}^2}\Phi\right) + \\ & + R^3\sin^2\chi\sin\theta\left(m^2 + \frac{6\xi}{R^2}\right)\Phi^2\Bigg] \end{aligned} \tag{6.10}$$

The spherical symmetry is exploited by expanding the field Φ in spherical harmonics:

$$\Phi(t,\chi,\theta,\alpha) = \sum_{l=0}^{\infty}\sum_{\mu=-l}^{l}\Phi_{l\mu}(t,\chi)Y_{l\mu}(\theta,\alpha), \tag{6.11}$$

and noting that the spherical harmonics are eigenfunctions of Δ_{S^2}:

$$\Delta_{S^2}Y_{l\mu} = -l(l+1)Y_{l\mu}. \tag{6.12}$$

Using the orthonormality of the $Y_{l\mu}$ functions, one obtains a Lagrangian which is given in terms of the fields $\Phi_{l\mu}$:

$$L = \frac{R^3}{2}\sum_{l\mu}\int_0^\pi d\chi\sin^2\chi\left\{\left[\dot{\Phi}_{l\mu}^2 - \left(m^2 + \frac{6\xi}{R^2}\Phi_{l\mu}^2\right)\right] - \frac{1}{R^2}(\partial_\chi\Phi_{l\mu})^2 + \frac{l(l+1)}{R^2\sin^2\chi}\Phi_{l\mu}^2\right\}. \tag{6.13}$$

6.1.2 Radial discretization

In order to obtain a discrete set of field variables, we need to discretize the only continuous variable left in the Lagrangian of eq. (6.13). The radial component, described by $\chi \in [0, \pi]$, is partitioned into N intervals of the same size, π/N indexed by $j = 1, \ldots, N$. The physical length of each interval is given by:

$$\epsilon = R\frac{\pi}{N}. \tag{6.14}$$

The field $\Phi_{l\mu}(\chi)$ is then approximated by a set of N variables corresponding to its value at the center of each interval. The spatial derivative $\partial_\chi \Phi_{l\mu}(\chi)$ can also be approximated by a finite difference between two adjacent field variables. Together, these approximations are given by the replacements:

$$\begin{aligned} \Phi_{l\mu}(\chi) &\to \Phi_{l\mu j} = \Phi_{l\mu}\left(\left(j - \frac{1}{2}\right)\frac{\pi}{N}\right), \\ \partial_\chi \Phi_{l\mu}(\chi) &\to \frac{\Phi_{l\mu j+1} - \Phi_{l\mu j}}{\pi/N}. \end{aligned} \tag{6.15}$$

With this scheme, the integral in the Lagrangian is replaced by a sum involving $N-1$ terms which contain the discretized space derivative and N terms with no spatial derivatives. Because these terms with spatial derivatives also includes spatial functions (such as $\sin^2\chi$) a choice regarding where these spatial functions should be computed has to be made. In order to preserve the symmetry under a reflection about the equatorial surface $\chi = \pi/2$, we compute such functions on the edge of the two adjacent intervals $\chi = j\pi/N$, thus resulting in a different discretization for terms with and without spatial derivatives:

$$\begin{aligned} \sin^2\chi \Phi_{l\mu}(\chi)^2 &\to \sin^2\chi_{j-1/2}\Phi^2_{l\mu j}, \\ \sin^2\chi (\partial_\chi \Phi_{l\mu}(\chi))^2 &\to \sin^2\chi_j \left(\frac{\Phi_{l\mu j+1} - \Phi_{l\mu j}}{\pi/N}\right)^2. \end{aligned} \tag{6.16}$$

To illustrate the difference between the discretization for each type of terms, we sketched the process for a fixed j in fig. 1.

After replacing the integral by a sum $\int \to \frac{\pi}{N}\sum_j$ and applying the discretization prescription, we obtain the discretized Lagrangian:

$$L = \frac{R^2\epsilon}{2}\sum_{l\mu}\left[\sum_{j=1}^{N}\sin^2\chi_{j-1/2}\dot{\Phi}^2_{l\mu j} - \sum_{i,j=1}^{N+1}\Phi_{l\mu i}\tilde{V}^{(l\mu)}_{ij}\Phi_{l\mu j}\right], \tag{6.17}$$

where the symmetric coupling matrix $\tilde{V}_{ij}$ is given by:

$$\begin{aligned} \tilde{V}^{(l\mu)}_{ij} = \delta_{ij}&\left\{\sin^2\chi_{j-1/2}\left[\frac{l(l+1)}{R^2\sin^2\chi_{j-1/2}} + m^2 + \frac{6\xi}{R^2}\right] + \frac{1}{\epsilon^2}(\sin^2\chi_j + \sin^2\chi_{j-1})\right\} \\ &- \frac{1}{\epsilon^2}(\delta_{i+1,j}\sin^2\chi_i + \delta_{i,j+1}\sin^2\chi_j). \end{aligned} \tag{6.18}$$

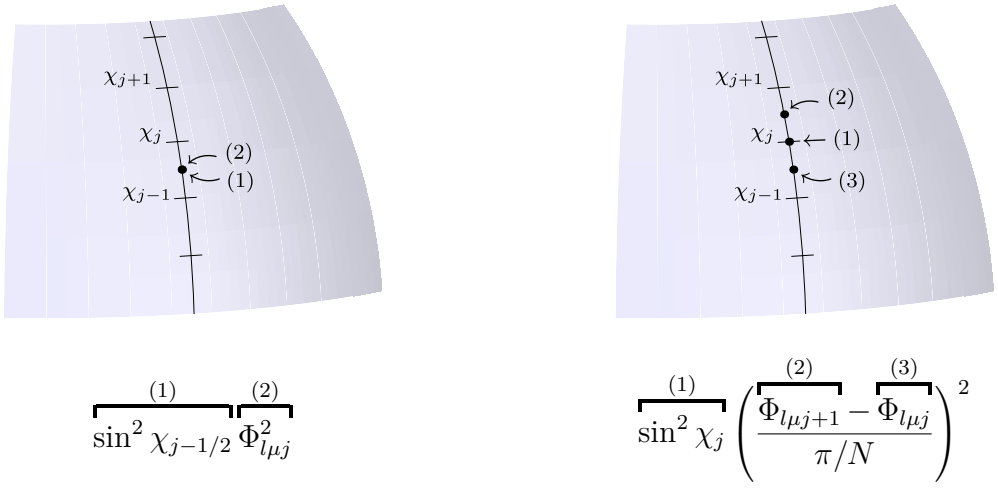

Figure 1 – Sketch of the discretization for a single term. The annotated numbers indicate where each factor is evaluated.

The conjugate momenta for each field variable $\Phi_{l\mu j}$ is given by:

$$\Pi_{l\mu j} = \frac{\partial L}{\partial \dot{\Phi}_{l\mu j}} = \epsilon R^2 \sin^2 \chi_{j-1/2} \dot{\Phi}_{l\mu j} \tag{6.19}$$

which allow us to write the Hamiltonian as:

$$H = \sum_{l\mu} \left(\sum_{j=1}^{N} \frac{1}{2\epsilon R^2 \sin^2 \chi_{j-1/2}} \Pi^2_{l\mu j} + \frac{\epsilon R^2}{2} \sum_{i,j=1}^{N} \Phi_{l\mu i} \tilde{V}^{(l\mu)}_{ij} \Phi_{l\mu j} \right). \tag{6.20}$$

We can further simplify the expression for H by employing a transformation which leaves the bracket in eq. (6.9) invariant, and also the corresponding commutator after quantization. Transformations that follow this property are called canonical, and the one used here simply rescales the fields:

$$\Phi_{l\mu j} \to \frac{\Phi_{l\mu j}}{R \sin \chi_{j-1/2}}, \quad \Pi_{l\mu j} \to \Pi_{l\mu j} R \sin \chi_{j-1/2}, \tag{6.21}$$

leaving the product of $\Phi_{l\mu j}$ and $\Pi_{l\mu j}$ invariant. Then, the Hamiltonian reads as

$$H = \sum_{l\mu} H_{l\mu} \tag{6.22}$$

where

$$H_{l\mu} = \left(\sum_{j=1}^{N} \frac{1}{2\epsilon} \Pi^2_{l\mu j} + \Phi_{l\mu i} V^{(l\mu)}_{ij} \Phi_{l\mu j} \right), \tag{6.23}$$

with the coupling matrix $V^{(l\mu)}_{ij}$ now given by:

$$\begin{aligned} V_{ij} = \frac{\delta_{ij}}{2\epsilon} \Bigg(& \epsilon^2 m^2 \frac{\pi^2 l(l+1)}{N^2 \sin^2 \chi_{i-1/2}} + \frac{\sin^2 \chi_i}{\sin^2 \chi_{i-1/2}} + \frac{\sin^2 \chi_{i-1}}{\sin^2 \chi_{i-1/2}} + \frac{6\pi\xi}{N^2} \Bigg) \\ & - \frac{1}{2\epsilon} \left(\delta_{i+1,j} \frac{\sin^2 \chi_i}{\sin \chi_{i-1/2} \sin \chi_{i+1/2}} + \delta_{i,j+1} \frac{\sin^2 \chi_j}{\sin \chi_{j-1/2} \sin \chi_{j+1/2}} \right) \end{aligned} \tag{6.24}$$

Note that the obtained Hamiltonian (6.23) is given by a sum of independent Hamiltonians $H_{l\mu}$, each one consisting of a lattice of Harmonic oscillators coupled by the matrix $V^{(l\mu)}_{ij}$.

6.2 Entropy calculation

As we saw in the last section, the mode expansion of the field Φ and the subsequent discretization of the radial component χ led us to a Hamiltonian expressed in terms of a set of canonical pairs $\{(\Phi_{l\mu j}, \Pi_{l\mu j})\}$ indexed by the indices l, μ and j. We now aim to apply the real time approach described in the last chapter to compute the entanglement entropy associated to spherical regions.

We note that the full state space $\mathcal{H}$ of the obtained system consists of the tensor product of the Hilbert spaces associated with the canonical pairs indexed by (l, μ, j):

$$\mathcal{H} = \bigotimes_{l\mu j} H_{l\mu j}. \tag{6.25}$$

A decomposition into two complementary regions can be obtained by separating the degrees of freedom as $j < n$ and $j \geq n$, given an integer n associated with a distance $n\pi/N$ along the radial direction χ:

$$\mathcal{H} = \underbrace{\left(\bigotimes_{\substack{l\mu \\ j<n}} H_{l\mu j} \right)}_{\mathcal{H}_A} \otimes \underbrace{\left(\bigotimes_{\substack{l\mu \\ j\geq n}} H_{l\mu j} \right)}_{\mathcal{H}_B} = \mathcal{H}_A \otimes \mathcal{H}_B. \tag{6.26}$$

The distance $n\pi/N$ describes the radius of a 2-sphere that forms the common boundary of the A and B. Such interface has area

$$A_n = 4\pi R^2 \sin^2 \chi_n = 4\pi R^2 \sin^2 \left(\frac{\pi n}{N} \right). \tag{6.27}$$

Note that each mode l, μ corresponds to an independent quadratic term in the Hamiltonian (6.23). As a consequence of (5.2), the ground state of the system is given by a product of independent Gaussian functions. The total entanglement entropy is then additive on the modes:

$$S = \sum_{l\mu} S_{l\mu}, \tag{6.28}$$

where $S_{l\mu}$ corresponds to the entropy associated with the subsystem with Hamiltonian $H_{l\mu}$. We can further exploit a redundancy in this calculation by noting that these Hamiltonian $H_{l\mu}$ are actually independent of μ and, thus, contribute equally to S. Because for each value of l we have a set of $2l + 1$ modes with the same entropy, we can write:

$$S = \sum_{l=0}^{\infty} (2l + 1) S_l, \tag{6.29}$$

where S_l is the entropy of any mode (l, μ).

A single subsystem associated with $H_{l\mu}$ corresponds to a chain of coupled harmonic oscillators. A procedure for computing the entropy contribution S_l is outlined as:

1. Obtain the covariance matrix blocks X and P by employing a symplectic diagonalization of $H_{l\mu}$.

2. Truncate the matrices X_{ij} and P_{ij} by discarding the degrees of freedom outside the 3-sphere determined by $i, j < n$.

3. Use the truncated matrices to determine $\sqrt{X_{red}P_{red}}$ and then compute the entanglement entropy S_l using the real time approach described earlier.

It is easy to see that, for large lm the potential matrix (6.24) takes the form of $l(l+1)J$ where J is diagonal. Then $\sqrt{X_{red}P_{red}}$ simply reduces to $\frac{1}{2}\mathbb{1}$, which gives a vanishing entropy S_l. We can then estimate the total entropy S by truncating the sum in eq. (6.29). This can be accomplished by introducing a finite upper limit l_{max}. The total entanglement entropy between the two spatial regions is then given approximately by:

$$S \approx \sum_{l=0}^{l_{max}} S_l. \tag{6.30}$$

The value l_{max} is tuned in order to produce a stable value for S.

6.3 Universal coefficients

An analytical approach to the computation of the entanglement entropy of massive free scalar fields [39, 56] shows that such quantity is divergent in the continuum limit. It is remarkable that, at non-vanishing ϵ, the entropy is proportional to the interface area. Such constant of proportionality consists in a series of divergent terms when $\epsilon \to 0$ multiplied by numerical constants that are independent of ϵ. The constants multiplying logarithmically divergent terms are called universal coefficients. We aim to obtain a numerical estimative for two of them.

A perturbative analysis of the Rényi entropies of a free massive field on spherical waveguides [39] reveals the dependency of S_α on the curvature of the entangling surface. Using a particular result for a 4-dimensional manifold and a 2-dimensional interface surface found on eq. (2.42) of [39] and setting the spherical waveguide radius to $R\cos(r/R)$ this contribution to the entanglement entropy $S = S_1$ reads:

$$S^{(1)} = \frac{A}{24\pi}\left[\frac{1}{2\epsilon^2} + \left(m^2 + \frac{6\xi - 1}{3R^2\cos^2(r/R)}\right)\log(m\epsilon)\right], \tag{6.31}$$

where A is the area of the entangling surface and r_e is its radius relative to the equator $\chi = \pi/2$.

Another contribution to S can be obtained by a perturbation of the metric of the spherical waveguide, which we quote from our work [56]:

$$S^{(2)} = \frac{A}{360\pi R^2}\left[1 - \tan^2\left(\frac{r_e}{R}\right)\right]\log(m\epsilon). \tag{6.32}$$

Because the metric around the entangling surface in consideration can be approximated by a perturbed spherical waveguide, we expect to observe a contribution to S of the form (6.32).

We now consider the conformal case $\xi = 1/6$ and compute the sum of both contributions for an entangling surface given by fixing $\xi = \pi/2$ ($r_e = 0$), this is, a 2-sphere located at the equator:

$$S \approx S^{(1)} + S^{(2)} = \Big[(\alpha_1 m^2 + \alpha_2)\log(m\epsilon)\Big] A. \tag{6.33}$$

The α_1 and α_2 are universal coefficients that can be calculated by eqs. (6.31) and (6.32):

$$\begin{aligned} \alpha_1 &= \frac{1}{24\pi} \approx 1.32 \times 10^{-2}, \\ \alpha_2 &= \frac{\pi}{360(N\epsilon)^2} \approx \frac{8.73 \times 10^{-3}}{(N\epsilon)^2}, \end{aligned} \tag{6.34}$$

where we substituted the discretization parameters in $R = (N\epsilon)/\pi$.

A numerical estimate for these coefficients can be made by computing the entropy using the real time approach and fitting the α_1 and α_2 to best reproduce the value of S under the model described by eq. (6.33). In particular, we opted to fix a value for N and R which also fix ϵ and vary the mass m over a chosen interval. The motivations for the choice of such interval for m are discussed in the next section.

From the analytical results, the entropy is also expected to include mass dependent terms on the form $(m\epsilon)^p$ with $p \in 2\mathbb{N}$, which are finite in the limit $\epsilon \to 0$. In order to avoid underfitting the data, we can include free parameters associated to those terms. Other terms which are finite but independent of m are effectively included in α_0. A prototype for models which reproduce the computed S is then given by:

$$S(m) = \left[\alpha_0 + (\alpha_1 m^2 + \alpha_2)\log(\epsilon m) + \sum_{\text{even } p}^{p_{max}} \beta_p m^p\right] A, \tag{6.35}$$

where each value of p_{max} results in a different model with $3 + \lfloor p_{\max}/2 \rfloor$ free parameters. In the results sections, we fit the data to a set of models up to $p_{max} = 8$ and compare the estimated values of α_1 and α_2 to the analytical ones listed in eq. (6.34).

6.4 Implementation

6.4.1 Numerical scheme

The recipe outlined above was implemented in Fortran 90 using the OpenBLAS and LAPACK libraries. Because each S_l is independent, its computation was parallelized by using the OpenMPI framework, taking the advantages of its distributed model. The entropy per mode was then aggregated into the total entropy S.

To compute the entropy for a mode l associated to a Hamiltonian $H_l = H_{l\mu}$, one needs to obtain the correlation matrices X and P associated with the field variables ϕ_i, π_j inside the region $i, j < n$. The Hamiltonian H_l satisfies the requirements of the procedure in which we calculated the covariance matrix in section 5.2.4. Following that procedure, the diagonal blocks X and P are obtained by computing the square root of V. Setting $k_p = \epsilon^{-1}$ and $K_x = V$ in eq. (5.66):

$$X = \frac{1}{2}(\epsilon V)^{-1/2}, \quad P = \frac{1}{2}(\epsilon V)^{1/2}. \tag{6.36}$$

The fractional powers of V appearing in eq. (6.36) can be computed in terms of its eigenvalues. Let λ_k be an eigenvalues of V and let M be the matrix which implements its diagonalization, the correlation matrices X and P are then given by:

$$\begin{aligned} X &= \frac{\epsilon^{-1/2}}{2} M \,\mathrm{Diag}(\lambda_1^{-1/2}, \lambda_2^{-1/2}, \ldots) M^T, \\ P &= \frac{\epsilon^{1/2}}{2} M \,\mathrm{Diag}(\lambda_1^{1/2}, \lambda_2^{1/2}, \ldots) M^T. \end{aligned} \tag{6.37}$$

From the explicit expression for V in eq. (6.24) one notes that it is a band matrix, so its diagonalization can be optimized by using a specialized LAPACK's routine designed to solve such task.

The correlations inside A are then obtained by truncating the X and P at the n-th site:

$$[X_{red}]_{ij} = X_{ij}, \quad [P_{red}]_{ij} = P_{ij} \quad \text{for } i, j < n. \tag{6.38}$$

The next step is to apply the real time formalism for obtaining the entanglement entropy using the correlations X_{red} and P_{red}. It follows from eq. (5.91) that S_l is given by:

$$S_l = \sum_i \left(\nu_i + \frac{1}{2}\right) \ln\left(\nu_i + \frac{1}{2}\right) - \left(\nu_i - \frac{1}{2}\right) \ln\left(\nu_i - \frac{1}{2}\right), \tag{6.39}$$

where the ν_i are the eigenvalues of $\sqrt{X_{red} P_{red}}$. These ν_i can be computed by first diagonalizing the product $X_{red} P_{red}$ and then taking the square root of its eigenvalues. We can then use eq. (6.39) to compute the entropy contribution for that mode.

In order to compute the total entanglement entropy, the process described above is repeated for every value $0 \leq l \leq l_{max}$. As noted earlier, the computation of each S_l is independent, so it can be distributed among a set of available CPU cores. A computation of S involves a fixed set of parameters described in table 1.

For the estimation of the universal coefficients, the entropy S has to be calculated under a mass interval $\{m_i\}$. The choice of such interval is detailed in the next subsection. These data points are then fitted into the models described in eq. (6.35). Note that $S(m)$ depends linearly on each coefficient, so the problem of finding α_i and β_i which best

Parameter	**Description**	**Commentary**
R	Universe radius	-
N	Number of radial sites	Determines $\epsilon = R\pi/N$
n	Number of radial sites inside A	-
m	Field mass	-
ξ	Gravity coupling	Fixed at $\xi = 1/6$ (conformal coupling)
l_{max}	Upper bound for the interval $l \in [0, l_{max}]$	-
ϵ_{tol}	Numerical tolerance	Controls $\log(x)$ at $x \approx 0$. (Justified below)

Table 1 – List of parameters necessary for computing S for a free scalar field with a fixed Lagrangian L.

reproduce the generated data is equivalent to a multilinear regression problem. The latter can be solved by employing a QR factorization or SVD decomposition on the matrix formulation of the problem [6].

6.4.2 Choice of parameters

As described above, the discretization procedure introduced an integer variable N which corresponds to the number of radial sites. If the radius of the universe R is fixed, both parameters determine a lattice spacing given by

$$\epsilon = \frac{\pi}{R}\frac{1}{N}. \tag{6.40}$$

To explore the stability of the method under different discretizations, we fixed the universe radius R and increased N. It follows that such increase on N leads to a smaller value of the lattice spacing ϵ which we expect to generate results which are closer to the continuum limit. However, by increasing the number of sites one has to deal with larger matrices, thus significantly increasing the running time required for a single computation of S.

Before discussing the choice of the Hamiltonian parameters, we note that, for a fixed number λ, the transformation $V \to \lambda V$ leaves the $\sqrt{XP}$ product invariant:

$$V \to \lambda V \Rightarrow \begin{cases} X & \to \lambda^{-1/2} X \\ P & \to \lambda^{1/2} P \end{cases} \Rightarrow \sqrt{XP} \to \sqrt{XP}. \tag{6.41}$$

For this reason, we can ignore the leading factors of $(1/2\epsilon)$ on the potential matrix in eq. (6.24), which would correspond to $\lambda = 2\epsilon$. Since the ϵ powers of eq. (6.37) cancel out when the product of both matrices is taken, we are only left with a dependency on the product ϵm.

We are interested in fitting the entropy $S(m)$ with respect to the mass m, so a choice of interval for m has to be made. Because the quantity m^{-1} for a free scalar field is

related to its correlation length $r_{cor} \sim m^{-1}$ [43], it defines a length scale at fixed m. The choice of interval for m is then motivated by the two requirements:

1. The perturbative analysis assumes $r_{cor} \ll R \Rightarrow m^{-1} \ll N\epsilon$.

2. In order to reproduce the continuum limit, the lattice spacing should be much smaller than the typical length scale, given by the correlation length. So $m^{-1} \gg \epsilon$.

   Both inequalities can be written as:

$$\frac{1}{mN\epsilon} \ll 1 \quad \text{and} \quad m\epsilon \ll 1. \tag{6.42}$$

To avoid privileging one of the inequalities, we can set the left-hand sides of eq. (6.42) equal. In that case, both inequalities can be simultaneously satisfied for a sufficiently large N. Therefore, we have:

$$m_{opt}^{-1} = \sqrt{N}\epsilon, \tag{6.43}$$

which is an estimate for an optimal mass that fulfills the required conditions.

6.4.3 Implementation details and optimizations

Since the task of calculating the entropy S for a fixed set of parameters consists in the repetition of an intensive linear algebra for a large interval of l's, the use of an optimized library has a great impact in reducing the running time. To demonstrate the gain in using specialized routines, consider the task of building the X and P matrices in a situation where the eigenvalues λ_i and eigenvectors M of V are already known.

For both cases, we start by noting the fact that the expression for X and P in eq. (6.37) includes a multiplication by a diagonal matrix. We can define an intermediary variable `aux`, which is a $N \times N$ matrix containing the result of $XV_D^{-1/4}$:

```
! Assuming that V_evals(i, i) = λ_i
aux = M
DO i = 1, N
    aux(:, i) = aux(:, i) * V_evals(i, i)**(-0.25)
END DO
```

In this way, the matrix X can be obtained by computing `aux` $\times$ (`aux`)^T. The advantage of this approach is an optimization on data access. Because all the necessary data of the final multiplication operation is explicitly contained in a smaller set of memory, a good compiler would use this fact to avoid cache misses.

We now present two different implementations for the `aux` $\times$ $(\texttt{aux})^T$ operation. An approach using FORTRAN's standard matrix multiplication `MATMUL()` function would read as:

```
1  X = 0.5d0 * MATMUL(aux, TRANSPOSE(aux))
```

which, apart from the ϵ factor that can be ignored, corresponds to the expression in eq. (6.37).

A different implementation uses the `DGEMM()` routine, which solves a general multiplication problem:

```
1  CALL DGEMM("N", "T", N, N, N, 0.5d0, aux, N, aux, N, 0.0d0, X, N)
```

where the transpose operation is specified in the second parameter `"T"`.

In addition to the implementations in our code, a LAPACK library may have different internal implementations. In figure 2 we show a performance test comparing the standard `MATMUL()` with two implementations of the LAPACK library. One based on the OpenBLAS package and the other included by the Intel's MKL library. The results show a massive gain of performance by using a LAPACK specialized routine. In particular, Intel's MKL surpasses OpenBLAS at the cost of working only on Intel processors.

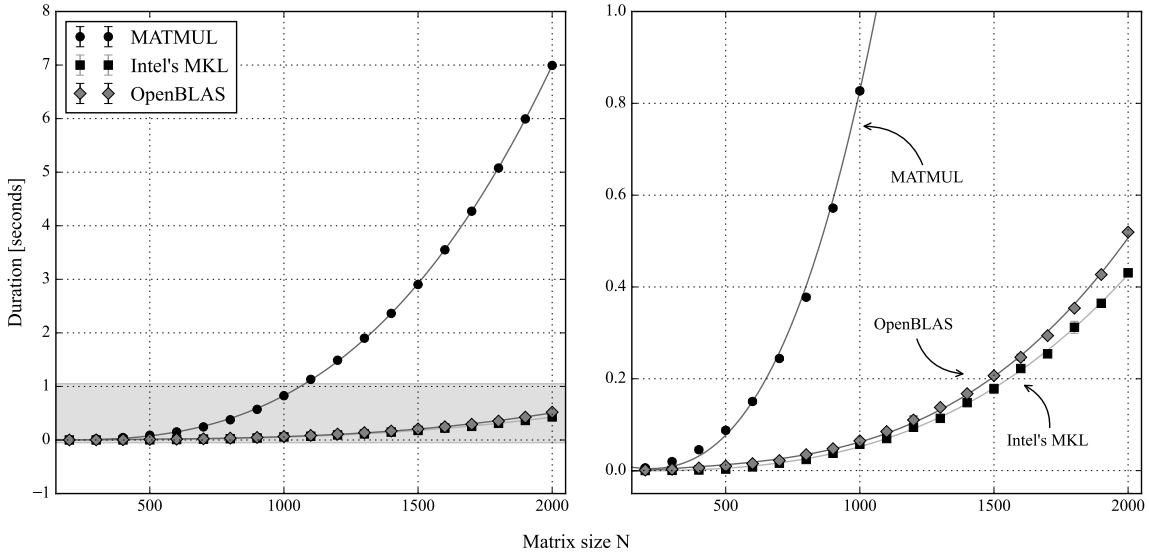

Figure 2 – Performance test comparing the usage of FORTRAN's standard `MATMUL()` against two different implementations of the LAPACK's library. The highlighted area in gray on the left plot is zoomed in the right plot.

The performance increase would be even higher if we consider the case of diagonalizing the band matrix V where the redundancy involving the null entries on the triangular blocks is intentionally avoided. The used LAPACK routines are listed on table 2.

Routine	**Used for**
`DSBEV()`	Diagonalizing V
`DGEMM()`	Calculating X and P matrices
`DSYMM()`	Calculating $X_{red}P_{red}$
`DGEEV()`	Computing the eigenvalues of $X_{red}P_{red}$

Table 2 – Specialized routines used to solve each task of computing the mode entropy S_l. The leading character `D` on each routine's name indicates that it handles double precision floats.

An important detail concerns the calculation of the term $\nu_i \log(\nu_i)$ in the expression for S_l in eq. (6.39) when $\nu_i \approx 0$. Arround this value, the $\log \nu_i$ exhibits a large numerical instability, which can result in erroneous contributions for S. This can be avoided by ignoring the contributions of ν_i's which are lower than a small ϵ_{tol} parameter.

6.5 Results

The results listed in this section were obtained using an implementation of the described scheme in FORTRAN 90. This program makes use of the LAPACK library [2] based on OpenBLAS [62] and the OpenMPI [26] as parallelization framework.

All the results are given for a fixed radius of the universe $R = 1000/\pi$ and with $\xi = 1/6$, corresponding to a conformal coupling. The mass intervals $\mathcal{M} = \{m_i\}$ of each estimation are chosen so adjacent masses are equally spaced $m_i - m_{i+1} = \delta m$. The entangling surface is a 2-sphere located at the equator $\chi = R/2$. The uncertainties included in the estimated coefficients are statistical uncertainties from the multilinear regression.

As a first case of study, we considered a system with $N = 1000$ sites, corresponding to $\epsilon = 1$. These values give an optimal mass of $m_{opt}^{-1} \approx 31.6$ which leads us to choose a set of 48 equidistant masses $\mathcal{M} = (30, 50)$. We then compared the regression models up to $p_{max} = 8$ for different mode bounds $l_{max} = 5 \times 10^3$ and $l_{max} = 10 \times 10^3$. The obtained results are shown in table 3.

We can observe a small relative variation on the estimation of α_1 under an increase of the number of considered modes. Alternatively, the second coefficient α_2 exhibits a relative variation which is much more sensible to a change in $S(m)$. This behavior can be understood by noting that the expected analytical value for α_2 has an order of magnitude much smaller than α_1, as can bee seen in eq. (6.34). In order to observe contributions of α_2 to $S(m)$, one needs a more precise measurement of the latter. We then take $l_{max} = 5 \times 10^3$ as a base parameter to investigate other sources of error.

A better approximation of the continuum limit is expected to be obtained by

p_{max}	$\alpha_1^{(1)}$	$\delta\alpha_1/\alpha_1^{(1)}$	$\alpha_2^{(1)}$	$\delta\alpha_2/\alpha_2^{(1)}$
2	0.0132295(30)	-1.90×10^{-6}	$-2.0(2) \times 10^{-9}$	0.019
4	0.0132595(10)	-7.83×10^{-5}	$8.2(3) \times 10^{-9}$	-0.046
6	0.0132450(60)	-3.27×10^{-4}	$5.0(20) \times 10^{-9}$	0.226
8	0.0133600(700)	8.12×10^{-3}	$2.5(12) \times 10^{-8}$	0.717

Table 3 – Comparison of two estimations of α_1 and α_2 with the input parameters differing only on the maximum summed entropy l_{max}. The variation columns measure the relative difference of both values $\delta\alpha_1 = (\alpha_1^{(1)} - \alpha_1^{(2)})/\alpha_1^{(1)}$. For each run, we have $l_{max}^{(1)} = 5 \times 10^3$ and $l_{max}^{(2)} = 10 \times 10^3$. Other fixed parameters are given by $N = 1000$, $n = 500$, $\epsilon = 1$, $\xi = 1/6$, $\epsilon_{tol} = 10^{-35}$. The mass interval consists in 48 equidistant masses at $m^{-1} \in (30, 50)$.

decreasing the lattice spacing and increasing the number of degrees of freedom N. We then considered different refinements of the lattice under a fixed value of $R\pi = N\epsilon\pi = 1000$ and computed the entropy for the same interval of 48 masses with $m^{-1} \in (30, 50)$. We finally fixed $p_{max} = 4$ to produce the table 4 comparing different lattice refinements. This expression for $S(m)$ is chosen because it gives the model with least number of parameters which still reproduces the computed data with satisfactory stability, as will be explicitly shown when we consider a movable mass interval.

N	α_1	α_2
1000	0.0132595(10)	$8.2(3) \times 10^{-9}$
1250	0.0132615(14)	$8.7(5) \times 10^{-9}$
1500	0.0132625(16)	$8.9(5) \times 10^{-9}$

Table 4 – Estimation of the universal coefficients for $p_{max} = 4$ and different lattices refinements at fixed R.

Because an increase on the density of sites on the lattice results in estimations of α_1 and α_2 which are closer to the analytical values 6.34, we take $N = 1500$ as a base parameter to our next considerations.

As described in section 6.4.2, a fixed mass m introduces a length scale given by the correlation length $r_{cor} \propto m^{-1}$. A poor choice of such quantity can introduce a systematic error originated from the discrete nature of the lattice, as well as break the assumptions made by the perturbative analysis which we are interested to observe. In any case, we might expect a poor estimation for the universal coefficients.

In order to investigate an optimal interval of inverse mass $m^{-1} \in (m_{low}^{-1}, m_{up}^{-1})$, we considered a set of 256 equally spaced inverse masses ranging from $m_{low}^{-1} = 2.45$ to $m_{up}^{-1} = 50.57$, which we denote by $\mathcal{M}$. A subset $\mathcal{M}_i \subset \mathcal{M}$ of W adjacent masses is then chosen so its median equals $m_{med}^{-1} = m_i^{-1}$:

$$\mathcal{M}_i = \{m_{i-W/2}, \ldots, m_i, \ldots, m_{i+W/2}\}. \tag{6.44}$$

We then analyze the regression quality for each subset $\mathcal{M}_i$ by computing the mean squared error $\chi(\mathcal{M}_i)/W$. The values of $\chi(\mathcal{M}_i)/W$ are plotted in figure 3, where the value of m_{med}^{-1} is used in the horizontal axis. The plots clearly show that the regression stabilizes when considering intervals with larger m_{med}^{-1}. As the mass interval $\Delta m^{-1} \propto W$ is increased, a larger median mass m^{-1} is required to obtain the same fitting quality of a lower W. Such behavior can be justified by the fact that a fit with larger W includes masses at a wider range which degrades the regression quality.

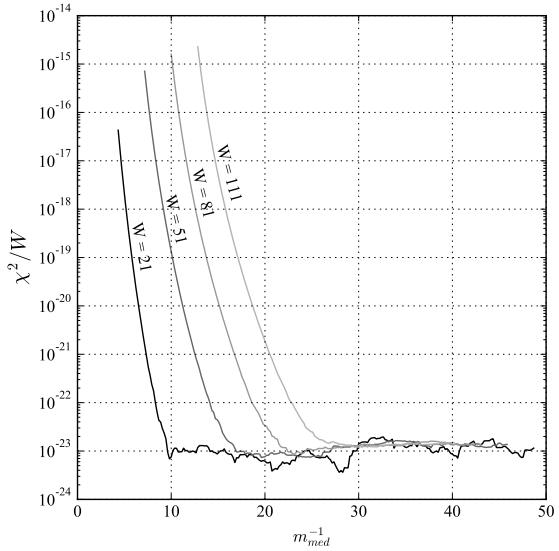

Figure 3 – Mean square error $\chi^2(\mathcal{M}_i)/W$ plotted against the median value m_{med}^{-1} of each interval $\mathcal{M}_i$.

A similar procedure can be employed to verify the stability of the fitted coefficients. In figure 4, we have the values of each universal coefficient, estimated using a mass interval $\mathcal{M}_i$ with $W = 110$, plotted against the median mass of each $\mathcal{M}_i$ on the horizontal axis. We see that the regression stabilizes at $m^{-1} \approx 20$ similarly as indicated by the χ^2/W plot.

An optimal fit which accounts for the parameter analysis done in this section can be made by considering all values of $S(m)$ with $m^{-1} > 30$ for the lattice with $N = 1500$. Under such circumstances, we report the best fit in table 5, which was obtained for $p_{max} = 4$.

	Estimated	Analytical	Relative difference
α_1	$0.0132611(11)$	≈ 0.0132629	-1.4×10^{-4}
α_2	$8.43(36) \times 10^{-9}$	$\approx 8.73 \times 10^{-9}$	-3.4×10^{-2}

Table 5 – Estimates for the universal coefficients obtained by considering all points with $m^{-1} > 30$ and $N = 1500$ is given on the first column. The second column is a reproduction of the perturbative coefficients found in eq. (6.34). The deviation in the third column is relative to the perturbative prediction.

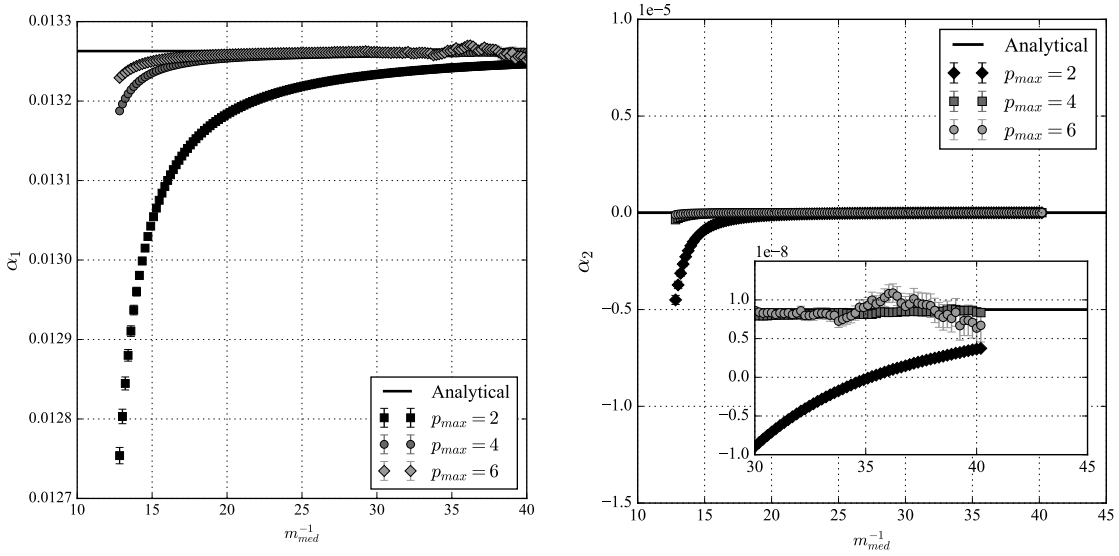

Figure 4 – Graph showing the dependency of the estimated values for each coefficient (α_1 on the left and α_2 on the right) on the chosen mass interval $\mathcal{M}_i$. Each interval includes a set of $W = 110$ masses and is centered at the point represented by m_i.

In order to demonstrate qualitatively the accuracy of the fit, we plot on fig. 5 the values of $S(m^{-1})$ normalized by the area $A(n = N/2)$ used to obtain the results of 5.

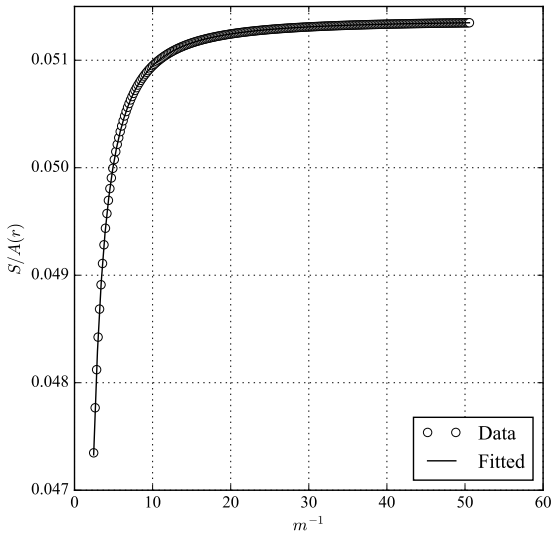

Figure 5 – Graph of the entropy per area $S(m)/A$ for $R = 1500$ and the regression, whose parameters are listed on table 5.

7 Conclusion

7.1 On the geometric entropy

Entanglement is a unique feature of quantum mechanics. Any theory whose degrees of freedom are described by quantum states may exhibit properties which are originated from it. For a quantum field theory, the degrees of freedom are often related to a spacetime coordinate, so the presence of entanglement can be related to geometric properties.

As described on chapter 2, on a pure state, the amount of entanglement between two subsystems can be quantified by the von Neumann entropy S of the reduced density matrix of one of the subsystems. In the particular case where these subsystems are associated to complementary spatial regions, the quantity S becomes a function of the geometric variables which parametrize such regions. For that reason, S is then often referred as geometric entropy.

In the context of free quantum fields, the geometric entropy can reveal the spatial structure of a theory without the necessity of referring to a particular observable. Then, it can be a useful tool for directly probing the fundamental aspects of such theory, as in the case of the study of universal coefficients appearing on the expansion of S.

7.2 On the calculation of the geometric entropy

As reviewed in the introduction 1, the entropy S of a general quantum field theory is divergent on the continuum limit $\epsilon \to 0$. The behavior of such divergence can reveal features of the theory, such as properties of its geometry. In order to compute S numerically, one could opt for fixing a small but non-vanishing ϵ. Despite the numerical convenience, a regularization of the entropy is expected to be motivated by quantum effects on the geometry.

When considering a real scalar free field, taking $\epsilon \neq 0$ results in a lattice of harmonic oscillators coupled by a matrix K. The properties of such systems can be obtained by exploiting the symplectic nature of the commutation relations and the quadratic form of the Hamiltonian 5.2. In particular, the ground state of such system is given by a Gaussian function determined by values of the expectations $\langle \phi_i \rangle , \langle \pi_j \rangle$ and the correlations $\langle \phi_i \phi_j \rangle , \langle \phi_i \pi_j \rangle , \langle \pi_i \pi_j \rangle$.

For computing the entanglement entropy of discrete bosonic systems, the real time formalism provides a robust framework in which only the knowledge of the correlations inside the region of interest V are required to obtain S. However, we emphasize that, for

calculating these correlations, one can not avoid dealing with degrees of freedom outside V. The *brute force* calculation carried on section 5.1 explicitly shows the dependency of the outside reduced density matrix on the inside blocks of the correlation matrix $K^{1/2}$. On our numerical computation, this fact translates to the necessity of calculating the full $N \times N$ matrix $K^{1/2}$ before truncating it to the $n \times n$ matrices X_{red}, P_{red}.

On a general level, one should not expect to avoid dealing with the outside subsystem variables, since the very quantity S we are aiming to compute measures the correlation between the two regions. An exception to this would be the case where the two regions are unentangled and $S = 0$ trivially.

The calculation of S for a free scalar field by employing this formalism also has the advantage of only requiring that $K^T = K > 0$ on the character of the coupling matrix. This restriction includes a variety of systems, defined over a spacetime with arbitrary dimension. In particular, if we assume the presence of a background curvature coupled with the field by a term of the form $\xi\mathcal{R}\phi^2$, this coupling is simply equivalent to the addition of terms in the diagonal entries of K (as showed in eq. (6.24)).

7.3 On the estimation of universal coefficients

On chapter 6 we described a numerical implementation of the real time formalism for a free scalar field defined over a closed universe. Our main task consisted on measuring the contribution of two universal terms on S by statistically estimating the respective universal coefficients.

The contribution of these universal terms is only expected to be observed on the domains of validity of the assumptions used in their derivation. In order to find a set of parameters which reproduce the intended behavior of S, we subdivided the results and analyzed the behavior of the statistical fit in each subset of parameters. The stability of the estimated coefficient under a small variation of the input parameters proved itself as a robust criterion for finding the region of interest.

Using a suitable domain of parameters, a final estimation of the universal coefficients was made. Since one of the coefficients, namely α_2, contributes with a variation of 7 orders of magnitude lower than the typical variation of S, one can conclude that the calculation of S was made with such accuracy that otherwise the contribution of α_2 would not been observed. The further agreement between the estimated and predicted values of the coefficients shows not only the robustness of the real time formalism, but the validity of the perturbative analysis.

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A Appendix 1: $\Sigma_n\, nx^n$ series evaluation

Consider the partial summation S_n of geometric series of ratio $|r| < r$:

$$S_n = 1 + r + r^2 + \cdots + r^n, \tag{A.1}$$

whose limit of $n \to \infty$ is:

$$S_\infty = \frac{1}{1-r}. \tag{A.2}$$

Consider now the partial sum of the series in question as A_n:

$$A_n = 0 + r + 2r^2 + 3r^3 + \cdots + nr^n. \tag{A.3}$$

Note that $A_n - rA_n = A_n(1-r)$ can be related to S_n:

$$A_n(1-r) = r + r^2 + r^3 + \cdots + r^n - nr^{n+1} = S_n - 1 - nr^{n+1}. \tag{A.4}$$

Since, for $|r| < 1$, $nr^{n+1} \to 0$ when $n \to \infty$, the limit A_∞ can be computed by solving for A_n in eq. (A.4) using eq. (A.2):

$$A_\infty = \frac{S_\infty - 1}{1-r} = \frac{r}{(1-r)^2}. \tag{A.5}$$