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Entanglement entropy in quantum field theory

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Abstract

Quantum information has a wealth of applications in quantum field theory stemming from the holographic paradigm. In this dissertation, we review techniques for computing the entanglement entropy of bosonic quantum fields in flat spacetime and extend them to the Einstein universe with uniform spatial curvature.

In the seminal works due to Sorkin et al. [1] and Srednicki [2], space is discretised, thus regularising the theory and rendering the von Neumann entropy finite. An area law for entanglement entropy is found, configuring it as a viable source of entropy for black holes, as proposed by these authors.

Under a characterisation of regularisation-independent contributions to the area law, we sought curvature corrections to this result. We implement numerical calculations in a lattice, based on a more efficient algorithm relying on the covariance matrix description of Gaussian states. We reproduce analytical results expected to hold in any regularisation, thereby providing additional evidence to their universality.

Furthermore, we present a recent approach describing the entanglement entropy of Gaussian states in terms of Kähler structures due to Bianchi et al. [3]. The symplectic geometry of phase space and compatible metric and complex structures therein parametrise the full space of covariance matrices, ultimately allowing for an extension of the algorithm to arbitrary Gaussian states.

Keywords: Entanglement entropy; Quantum Field Theory; Curved Spacetime; Gaussian States; Holography.

Resumo

Informação quântica é rica em aplicações em teoria quântica de campos, derivadas do paradigma holográfico. Nesta dissertação, nós revisamos técnicas para o cálculo da entropia de emaranhamento de campos quânticos bosônicos em espaço-tempo plano e as estendemos para o universo de Einstein de curvatura espacial uniforme.

Nos trabalhos seminais de Sorkin et al. [1] and Srednicki [2], o espaço é discretizado, regularizando a teoria e portanto tornando a entropia de von Neumann finita. Uma lei de área para a entropia de emaranhamento é encontrada, configurando-a como uma fonte viável da entropia de buracos negros, como proposto por esses autores.

Sob uma caracterização de contribuições independentes de regularização para a lei de área, nós buscamos correções de curvatura para esse resultado. Implementamos cálculos numéricos em uma rede baseados no eficiente algoritmo que consiste em usar a matriz de covariância de estados Gaussianos. Reproduzimos assim resultados analíticos esperados em qualquer esquema de regularização, fornecendo evidências adicionais à sua universalidade.

Ademais, apresentamos uma abordagem recente que descreve a entropia de emaranhamento de estados Gaussianos em termos de estruturas de Kähler, introduzida por Bianchi et al. [3]. A geometria simplética do espaço de fase e métrica e estrutura complexas compatíveis parametrizam o espaço de matrizes de covariância, permitindo por conseguinte uma extensão do algoritmo para estados Gaussianos arbitrários.

Palavras-chave: Entropia de Emaranhamento; Teoria Quântica de Campos; Espaço-Tempo Curvo; Estados Gaussianos; Holografia.

Contents

Chapter 1

Introduction

1.1 Entropy and area law

The study of black hole dynamics is a subarea of general relativity. Important hints at new physics concerning quantum gravity come from these studies, and their origins read as a very straightforward story.

The *no-hair theorem* [4, 5, 6, 7] affirms that a stationary black hole has only three parameters defining its configuration: its *mass*, *angular momentum* and *electrical charge*. To an observer which is outside the event horizon, the information contained in a subsystem that falls into the black hole would seem to be lost: the observer has no longer access to it when maintaining her position, because there is no content leaving the event horizon [8]. The state of the infalling system, as complicated as one wants, would be reduced to the three parameters specified by the no-hair property.

This property seemingly contradicts notions of thermodynamics and quantum information: it is fundamental that information should not vanish. A closed physical system can be ever-changing, but we should in principle be able to compute any one state visited at any given time if we know the current state and all physical laws governing the motion of the system. With quantum mechanics in mind, this does not amount to specifying position and momentum of particles, but quantum states. In these terms, the states evolve *unitarily*.

The hint of a new principle then stemmed from a second theorem, possibly resolving this issue. The *area theorem*, proven by Hawking [9], states that the area of a classical black hole should never decrease with time. This goes along intuition, once we know that these objects curve spacetime in such a manner as to set the future of all geodesics from the event horizon inwards, to its central singularity.

Based on this never-decreasing horizon area, it was conjectured by Bekenstein [10, 11, 12, 13] that a more fundamental relation exists between thermodynamics

and general relativity. The behaviour indicated by the area theorem resembles that of entropy, an idea which served as motivation for Bekenstein to propose a *generalised second law* of thermodynamics. Originally, the second law states that the entropy of a closed physical system should never decrease:

$$\Delta\mathcal{S} \geq 0. \tag{1.1}$$

The generalised second law adds a new contribution $\mathcal{S}_{\text{BH}}$ to the total entropy due to the black holes and proportional to the sum of the areas of their horizons. The expression above is replaced with

$$\Delta(\mathcal{S} + \mathcal{S}_{\text{BH}}) \geq 0 \tag{1.2}$$

Further developments added quantum mechanics to the physics of black holes, leading to particle creation. This phenomenon is both quantum mechanical and relativistic: the quantum vacuum fluctuates, and the gravitational field at the horizon induces particle creation, as permitted by $E^2 - \mathbf{p}^2 = m^2$. The particles leaving the black hole to infinity constitute the Hawking radiation [14].

Seen by outside observers, it can be described analogously to the Unruh effect: a change of reference frame leads to different vacua perceived by detectors in such frames and hence different particle content. The appearance of particles is related to an alternative description of the field in terms of normal modes in different coordinate systems. A transformation of modes such as

$$p_\omega = \int \mathrm{d}\omega' \, \alpha_{\omega\omega'} u_{\omega'} + \beta_{\omega\omega'} u^*_{\omega'}, \tag{1.3}$$

for Bogoliubov coefficients α and β, provides a spectrum of particles (bosonic for instance) of the form

$$|\beta_\omega|^2 \approx \frac{1}{\mathrm{e}^{8\pi M\omega} - 1}, \tag{1.4}$$

as seen by the asymptotic observer in the black hole spacetime [15].

A spectrum such as 1.4 has a temperature immediately associated to it [16]. In this case we have

$$T_{\text{BH}} = \frac{1}{8\pi GM}. \tag{1.5}$$

Related to this temperature, and analysing the variation of parameters of black holes in nearby equilibrium configurations [1] an entropy can be cast in terms of the area, as

$$\mathcal{S}_{\text{BH}} = \frac{\mathcal{A}}{4G}, \tag{1.6}$$

[1] If non-rotating and uncharged, the black hole's mass must uniquely define the spacetime around it. Then, it is only natural that a geometrical object such as an area to depend on the black hole's mass.

in such a way that a first law of thermodynamics for these parameters also applies [17].

The black hole shrinks as it evaporates, and therefore its area diminishes and so does any entropy associated to it (recall that this is the case in a regime in which the area theorem does not hold). The particles giving the thermal spectrum we calculated must account for this loss of entropy, in order for the second law of thermodynamics to hold.

The remaining question pertains to the microscopic interpretation of the black hole entropy. Amongst other conjectures, the one on which we are interested was originally proposed by Sorkin et al. in ref. [1] and Srednicki in ref. [2]. The quantum vacuum of any field is highly entangled with respect to spatial degrees of freedom, from which an immediate suggestion is that entanglement entropy might be the origin of black hole entropy. In general relativity, horizons appear as natural *entangling surfaces* of quantum systems. Computing the entanglement entropy for spherical regions in flat space, an entropy-area relation is indeed reproduced.

These studies were the first suggestions that the entropy-area relation holds more generally , in fact one can define entanglement entropy for any spatial separation of quantum degrees of freedom, notwithstanding the existence of black holes or horizons. In addition to the goal of understanding black hole physics, the study of entanglement entropy in curved spaces, from this point onwards, attracted the attention of researchers in the field of quantum gravity by relating geometry to a measure of quantum correlations. In particular, a *holographic principle* was proposed for quantum gravity [18, 19, 20], and the area law was suggested as a probe for semiclassical states in quantum gravity [3].

These properties suggest a mechanism from which spacetime can emerge. The paradigm proposes reconstructing classical spacetime from quantum correlations, taking shape in many formalisms, from loop quantum gravity [21], the AdS/CFT duality [22], to simple quantum theory [23, 24] and thermodynamics [25, 26].

Moreover, the AdS/CFT correspondence [27, 28, 29, 30], first suggested in string theory, which connects an anti-de Sitter geometry to a quantum conformal theory on its boundary, configures a powerful technique for investigating other physical systems (including the Ryu–Takayanagi formula, which computes entanglement entropy on the boundary in terms of minimal surfaces in the bulk [31, 32]).

This dissertation is motivated by the discussion above and concerned with the area law for entanglement entropy. The role that entanglement entropy plays in relation to spacetime is obscured by its divergent behaviour in quantum field theory; it is then expected that quantum gravity provides the means through which this entropy measure is made finite. Since we do not have such a tool yet, we must pick apart the entanglement entropy as it appears in our current theories in order to identify what may be relevant for future investigations of quantum gravity, and

what can be ignored. The aim of the present text is to review this approach and develop it further.

In the first three chapters we summarise general relativity, quantum information and field theory, subjects on which the aforementioned studies are founded. In the first subsections, we give a straightforward introduction to the basics in order to fix notation and emphasize the tools that will be subsequently used. The purpose of the following subsections therein is to discuss more important aspects that will be evidently relevant throughout the text, starting from discussions of symmetry and maximally symmetric spaces in section 2.2, the von Neumann entropy in section 3.2 and canonical quantisation of fields in section 4.2 and the Unruh effect in section 4.4.

In chapter 5 we apply some principles of the preceding chapters in flat spacetime, discussing quantum correlations of scalar fields, the entanglement content of the vacuum state, and the lattice regularisation of the theory, allowing for computations of the entanglement entropy in terms of state operators.

Chapter 6 elaborates on symplectic geometry and its use in describing Gaussian quantum states in terms of canonical variables and Kähler structures. The covariance matrix is studied in this context and used in an algorithm for entanglement entropy computation, improved from the one in the previous chapter.

We conclude the dissertation after chapter 7, in which the techniques already examined coalesce in an analysis of entanglement entropy of the scalar vacuum state in the Einstein universe. Vacuum two-point functions are first studied, and then we obtain results concerning curvature and universal contributions to the area law of entanglement entropy in this geometry.

Chapter 2

General relativity

General relativity formulates the physics of spacetime in a dynamical manner. It is especially fundamental in the sense that, to our current understanding of nature, spacetime is a structure of which one cannot dismiss. Notwithstanding the necessary appearance of spacetime in describing physics, its dynamical nature indicates that it cannot be taken for granted, and in specifying the configuration or state of a system, one is led to consider spacetime.

In this section the mathematical formalism for treating spacetime is introduced, with basic definitions of physical objects stemming from mathematical ones. These constructions will serve primarily as foundation to following sections, alongside the next two introductory sections. The content introduced hereafter is based on [33, 34] for general relativity. The topics referring more specifically to differential geometry can be found in refs. [35, 36].

2.1 Differential geometry

Spacetime is modelled using the language of smooth manifolds. A physical *event* $\mathsf{e} \in O \subset \mathbb{M}$, is mapped by a local system of coordinates to a d-tuple in an open subset O' of $\mathbb{R}^d$ as

$$\begin{aligned} \text{coord}\colon \mathbb{M} \supset O &\to O' \subset \mathbb{R}^d \\ \mathsf{e} &\mapsto \text{coord}(\mathsf{e}) = \left(x^0(\mathsf{e}), \ldots, x^{d-1}(\mathsf{e})\right). \end{aligned} \tag{2.1}$$

In the definition of a manifold, one considers O as part of collection of open sets, together with coordinate homeomorphisms satisfying the above condition (each constituting a coordinate system). These sets cover the whole manifold and are required to be compatible, in the sense that transitioning between two coordinate systems is a smooth operation.

Being smooth functions of points in the spacetime manifold, the fields $\Phi\colon \mathbb{M} \to \mathbb{V}$ have a smooth representation in local coordinates. In the example of a scalar field, when $\Phi(x^\mu)$ is written, ones actually means $\Phi(\mathsf{e})$, as in

$$\Phi(x^\mu) \equiv \Phi \circ \mathrm{coord}^{-1}(x^\mu)\colon \mathbb{R} \supset O' \to \mathbb{R}, \tag{2.2}$$

where (x^μ) is the d-tuple in eq. (2.1), after collapsing each coordinate component to an indexed ordered family $\mu = \{0, \ldots, d-1\}$.

A natural structure on differentiable manifolds is that of tangent spaces. Elements of these tangent spaces are vectors, and in this sense the manifold is linear at any point. Vectors are defined as directional derivatives at the point they are defined; given a coordinate system and a smooth function, a vector V maps functions to functions,

$$\begin{aligned} V_{\mathsf{e}}(f) &\equiv V^\mu \left(\frac{\partial}{\partial x^\mu}\right)_{\mathsf{e}} (f \circ \mathrm{coord}^{-1}) \\ &= \frac{\partial (f \circ \mathrm{coord}^{-1})}{\partial x^\mu}\bigg|_{x=x(\mathsf{e})}. \end{aligned} \tag{2.3}$$

By extracting the f from this definition, one recognises ∂_μ as a basis for the tangent space of vectors at a point, $\mathbf{T}_{\mathsf{e}}\mathbb{M}$.

Likewise, there is a dual concept, that of covector in cotangent spaces, of linear functionals of vectors $\Theta\colon \mathbf{T}_{\mathsf{e}}\mathbb{M} \to \mathbb{R}$. The basis dual to the coordinate basis is defined as

$$\mathrm{d}x^\nu(\partial_\mu) = \delta^\nu_\mu. \tag{2.4}$$

General tensors can be ascribed a classification (m, n), given how many copies of the coordinate basis (m) and copies of the dual basis (n) are needed to describe them. Furthermore, a tensor fields is an assignment of a tensor to all points of the manifold, smoothly.

The geometry of spacetime is described by the metric field $g_{\mu\nu}$. It is a (0,2)-tensor, therefore it has components with respect to the coordinate basis of $\mathbf{T}^*_{\mathsf{e}}\mathbb{M} \otimes \mathbf{T}^*_{\mathsf{e}}\mathbb{M}$, for every e,

$$g_{\mu\nu}\mathrm{d}x^\mu\mathrm{d}x^\nu. \tag{2.5}$$

This is the *line element*, interpreted as the notion of infinitesimal displacement at the coordinate directions.

At the same time, $g_{\mu\nu}$ is a *tensor field* on $\mathbb{M}$, which means its components are smooth functions in their own right, thus having the form

$$g_{\mu\nu}(x^\sigma) \equiv g_{\mu\nu} \circ \mathrm{coord}^{-1}(x^\sigma)\colon \mathbb{R}^d \supset O' \to \mathbf{T}^*_{\mathsf{e}}\mathbb{M} \otimes \mathbf{T}^*_{\mathsf{e}}\mathbb{M}, \tag{2.6}$$

analogous to eq. (2.2). The metric tensor satisfies the properties of nondegeneracy and symmetry; the former implying that it has an inverse: a $(2,0)$-tensor $g^{\mu\nu}$ such that $g^{\mu\rho}g_{\rho\nu} = \delta^{\mu}_{\nu}$, in which δ^{μ}_{ν} is the Kronecker delta.

By providing this notion of length, the metric is paramount for defining integration of functions on $\mathbb{M}$ through the volume form dvol. In coordinate representation and to our purposes it suffices to express the volume form as[1]

$$\mathrm{dvol} = \sqrt{-\det(g_{\mu\nu})}\overbrace{\mathrm{d}x^0 \dots \mathrm{d}x^{d-1}}^{\text{volume element}}, \tag{2.7}$$

which will be abbreviated hereafter by writing $\det(g_{\mu\nu}) \equiv g$, and the minus sign appears because of the Lorentzian signature of spacetime.

Tensors of any rank are fundamental objects in spacetime, preserving their nature under general changes of coordinate. This means that, given a coordinate chart leading to the construction laid out above, the associated basis vectors (and covectors) change in the opposite way to the components of the tensors themselves. Scalar fields do not change under a change of coordinates. For higher rank tensors, whose coordinate components are $T^{\mu_1\cdots\mu_n}{}_{\nu_1\dots\nu_m}$, the universal law for change of coordinates is the following:

$$\begin{aligned} T &= T^{\mu_1\cdots\mu_m}{}_{\nu_1\dots\nu_n}\, \partial_{\mu_1}\dots\partial_{\mu_m}\mathrm{d}x^{\nu_1}\dots\mathrm{d}x^{\nu_n} \\ &= T^{\mu_1\cdots\mu_m}{}_{\nu_1\dots\nu_n} \left(\frac{\partial x^{\mu'_1}}{\partial x^{\mu_1}}\right)\dots\left(\frac{\partial x^{\mu'_m}}{\partial x^{\mu_m}}\right)\left(\frac{\partial x^{\nu'_1}}{\partial x^{\nu_1}}\right)\dots\left(\frac{\partial x^{\nu'_n}}{\partial x^{\nu_n}}\right) \\ &\quad\times\left(\frac{\partial x^{\mu_1}}{\partial x^{\mu'_1}}\right)\dots\left(\frac{\partial x^{\mu_m}}{\partial x^{\mu'_m}}\right)\partial_{\mu_1}\dots\partial_{\mu_m} \\ &\quad\times\left(\frac{\partial x^{\nu_1}}{\partial x^{\nu'_1}}\right)\dots\left(\frac{\partial x^{\nu_n}}{\partial x^{\nu'_n}}\right)\mathrm{d}x^{\nu_1}\dots\mathrm{d}x^{\nu_n}. \end{aligned} \tag{2.8}$$

for which one recognises the new components and bases, codified through a new, primed set of indices, as

$$T^{\mu'_1\cdots\mu'_m}{}_{\nu'_1\dots\nu'_n} \equiv T^{\mu_1\cdots\mu_m}{}_{\nu_1\dots\nu_n} \left(\frac{\partial x^{\mu'_1}}{\partial x^{\mu_1}}\right)\dots\left(\frac{\partial x^{\mu'_m}}{\partial x^{\mu_m}}\right)\left(\frac{\partial x^{\nu'_1}}{\partial x^{\nu_1}}\right)\dots\left(\frac{\partial x^{\nu'_n}}{\partial x^{\nu_n}}\right) \tag{2.9}$$

$$\partial_{\mu'_m} \equiv \left(\frac{\partial x^{\mu_m}}{\partial x^{\mu'_m}}\right)\partial_{\mu_m} \tag{2.10}$$

$$\mathrm{d}x^{\nu'_n} \equiv \left(\frac{\partial x^{\nu_n}}{\partial x^{\nu'_n}}\right)\mathrm{d}x^{\nu_n}. \tag{2.11}$$

[1] Rigorously, dvol is a d-form. The ellipsis … should stand for a string of exterior products $\mathrm{d}x^0 \wedge \mathrm{d}x^1 \cdots \wedge \mathrm{d}x^{d-1}$.

The tensor T itself remains unchanged, for the transformation of components and bases are inverse to one another:

$$\left(\frac{\partial x^{\mu'_m}}{\partial x^{\mu_m}}\right)\left(\frac{\partial x^{\mu_m}}{\partial x^{\mu'_m}}\right) = 1. \tag{2.12}$$

Coordinate-independence of general relativity is important to bear in mind, but when doing explicit calculations, we will work under a choice of coordinates. The language of differential forms and exterior algebra (as hinted in 2.7) is a powerful tool for working in coordinate-free problems, and it carries the information needed for vector calculus (as it will appear later in this dissertation). We now expose some of their use to us in this dissertation, again in coordinate form.

The gradient and the divergent are examples of operators with correspondents in our treatment of differential geometry. Given a smooth function f of the manifold (such as a scalar field), its differential is

$$\mathrm{d}f = \partial_\mu f \mathrm{d}x^\mu; \tag{2.13}$$

one can notice that its components are the familiar components of the gradient of a function in vector calculus, ∇f.

Our exposition of the divergence operator, on the other hand, relies on the metric structure and the notion of *covariant derivative*. It is introduced to correct the non-covariant nature of the regular derivative of components of tensor fields and, by doing so, is a proper physical object according to general relativity. Its coordinate expression, as it acts on vector and covector fields is

$$\nabla_\mu F^\nu = \partial_\mu F^\nu + \Gamma^\nu_{\mu\sigma} F^\sigma \tag{2.14a}$$

$$\nabla_\mu F_\nu = \partial_\mu F^\nu - \Gamma^\sigma_{\mu\nu} F_\sigma; \tag{2.14b}$$

for higher-order tensors, one has one Γ symbol for each index, with respective match as in the expressions above. Because there is nothing to correct when taking derivatives of scalars ($\partial_\mu f$ already transforms correctly), one adds that

$$\nabla_\mu f = \partial_\mu f. \tag{2.14c}$$

The *Christoffel symbols* Γ are introduced to cancel the extra terms appearing in transforming coordinates that spoil the covariance of tensor derivatives. It gives the unique torsion-free ($\nabla_\mu \nabla_\nu f = \nabla_\nu \nabla_\mu f$, for any function f), metric-compatible ($\nabla_\sigma g_{\mu\nu} = 0$) derivative operator of (semi-)Riemannian manifolds, determined by these properties as

$$\Gamma^\sigma_{\mu\nu} = \frac{1}{2} g^{\sigma\rho} \left(\partial_\nu g_{\rho\mu} + \partial_\mu g_{\rho\nu} - \partial_\rho g_{\mu\nu}\right). \tag{2.15}$$

From this explicit expression, one can see that Γ is symmetric under exchange of μ and ν indices. It is important to notice that, from these constructions, ∇_μ, in spite of the index, is not the component of a one-form; it does not constitute a tensor, it is merely a tool (an operator) that constructs tensors.

The contraction of the covariant derivative with a vector field will yield the divergence. Starting from the definition, we have

$$\begin{aligned}\nabla_\mu F^\mu &= \partial_\mu F^\mu + \Gamma^\mu_{\mu\nu} F^\nu \\ &= \partial_\mu F^\mu + \frac{1}{2} g^{\mu\rho} \left(\partial_\nu g_{\mu\rho} + \partial_\mu g_{\rho\nu} - \partial_\rho g_{\mu\nu}\right) F^\nu .\end{aligned} \tag{2.16}$$

This expression can be simplified by renaming dummy indices in either one of the last two factors, e.g. changing μ to ρ in the last one leads to $g^{\mu\rho}\partial_\mu g_{\rho\nu} - g^{\rho\mu}\partial_\mu g_{\rho\nu} = 0$, which vanishes because the metric components form a symmetric matrix, i.e.

$$\nabla_\mu F^\mu = \partial_\mu F^\mu + \frac{1}{2} g^{\mu\rho} \partial_\nu g_{\mu\rho} F^\nu . \tag{2.17}$$

Exploiting the logarithm function of matrices, mapping sums to products, one can recognise the remaining term as

$$\underbrace{g^{\mu\rho}\partial_\nu g_{\mu\rho}}_{\operatorname{tr} A^{-1}\frac{\mathrm{d}A}{\mathrm{d}x}} = \underbrace{\partial_\nu \ln\left|\det(g^{\mu\rho})\right|}_{\frac{\mathrm{d}}{\mathrm{d}x}\ln\det A} . \tag{2.18}$$

It follows that the covariant derivative takes the form

$$\nabla_\mu F^\mu = \partial_\mu F^\mu + \partial_\nu \left(\ln \sqrt{\left|\det g_{\mu\rho}\right|} \right) F^\nu , \tag{2.19}$$

which is a simple product rule. We thus have

$$\begin{aligned}\nabla_\mu F^\mu &= \partial_\mu F^\mu + \partial_\mu \Big(\ln \sqrt{|g|} \Big) F^\mu \\ &= \partial_\mu F^\mu + \frac{1}{\sqrt{|g|}} \partial_\mu \Big(\sqrt{|g|} \Big) F^\mu \\ &= \partial_\mu F^\mu + \frac{1}{\sqrt{|g|}} \partial_\mu \Big(\sqrt{|g|} F^\mu \Big) - \partial_\mu F^\mu \\ &= \frac{1}{\sqrt{|g|}} \partial_\mu \Big(\sqrt{|g|} F^\mu \Big) .\end{aligned} \tag{2.20}$$

With the divergent and the gradient at hands, it is straightforward to state the form of the Laplacian of a function (in vector calculus notation, $\nabla^2 f \equiv \nabla \cdot \nabla f$), viz.

$$\nabla_\mu \partial^\mu f = \frac{1}{\sqrt{|g|}} \partial_\mu \Big(\sqrt{|g|} g^{\mu\nu} \partial_\nu f \Big) . \tag{2.21}$$

Solutions to differential equations involving operators of this nature are well-understood and will play an important role when we explicit fields in terms of a basis of functions which solve these equations, and use them even in the quantum theory. The shape this differential operator takes relies on the structure of spacetime.

Another important concept linked to the covariant derivative (that will not be elaborated further in this dissertation) is the equation of motion of particles in curved spacetime:

$$\begin{aligned} p^\mu \nabla_\mu p^\nu &= \frac{\mathrm{d}^2 x^\nu}{\mathrm{d}\tau^2} + \Gamma^\nu_{\rho\sigma} \frac{\mathrm{d}x^\rho}{\mathrm{d}\tau} \frac{\mathrm{d}x^\sigma}{\mathrm{d}\tau} \\ &= 0, \end{aligned} \tag{2.22}$$

for a trajectory $x^\mu(\tau)$ of a particle with proper time τ, and whose momentum is p^ν.

The expression on the left-hand side is what defines the *parallel transport* of a vector (the one being differentiated) along a curve (whose tangent contracts with the covariant derivative). A tangent vector that is transported in a parallel manner along its curve, defines the curve as a geodesic. We are saying that particles under influence of no force move along geodesics of spacetime.

One of the most important features of general relativity is the intrinsic curvature of the manifold chosen to represent spacetime. This is how gravity manifests itself; one rephrases trajectory of particles in a gravitational potentials as timelike geodesic trajectories on curved spacetime.

In geometry, this curvature appears as the *Riemann tensor* $\mathcal{R}^\rho{}_{\sigma\mu\nu}$. In a manifolds with metric, such as our case, it is closely related to it and to the covariant derivative.

Because spacetime is not embedded in anything higher-dimensional, a concept of curvature which is intrinsic is demanded. It can be seen arising from the failure of the parallel transport of a vector along distinct paths to have equal results. Infinitesimally, this is a statement that the covariant derivative of vector fields is noncommuting. At each iteration of the covariant derivative the vector is carried to a point in its immediate neighbourhood, and the difference between acting on it twice in a different order evaluates to the difference of the result of parallel-transporting.

The failure of covariant derivatives to commute can be measured by

$$\left(\nabla_\mu \nabla_\nu - \nabla_\nu \nabla_\mu\right) F^\sigma, \tag{2.23}$$

with each of these double derivatives having the form

$$\nabla_\mu \nabla_\nu F^\sigma = \partial_\mu \nabla_\nu F^\sigma - \Gamma^\rho_{\mu\nu} \nabla_\rho F^\sigma + \Gamma^\sigma_{\mu\rho} \nabla_\nu F^\rho. \tag{2.24}$$

A few terms will cancel because of this: $\partial_\mu \nabla_\nu F^\mu$ and its counterpart both contain a second-order partial derivative, which is invariant under exchange of indices,

and appear twice with a sign flip; the same happens for those terms containing two Christoffel symbols, whose $\mu\nu$ index the same symbol ($\Gamma^{\rho}_{\mu\nu}\Gamma^{\sigma}_{\rho\eta}F^{\eta}$). After these simplifications,

$$\left(\nabla_\mu\nabla_\nu - \nabla_\nu\nabla_\mu\right)F^\sigma = \left(\partial_\mu\Gamma^\sigma_{\nu\rho} - \partial_\nu\Gamma^\sigma_{\mu\rho} + \Gamma^\sigma_{\mu\eta}\Gamma^\eta_{\nu\rho} - \Gamma^\sigma_{\nu\eta}\Gamma^\eta_{\mu\rho}\right)F^\rho. \tag{2.25}$$

We proceed to *define* the Riemann tensor as this result in terms of the symbols, its components are

$$\mathcal{R}^\rho{}_{\sigma\mu\nu} \equiv \partial_\mu\Gamma^\rho_{\nu\sigma} - \partial_\nu\Gamma^\rho_{\mu\sigma} + \Gamma^\rho_{\mu\eta}\Gamma^\eta_{\nu\sigma} - \Gamma^\rho_{\nu\eta}\Gamma^\eta_{\mu\sigma}. \tag{2.26}$$

Other mathematical objects containing information about curvature are the *Ricci tensor* and *Ricci scalar*, or curvature scalar, obtained by contraction of indices:

$$\mathcal{R}_{\sigma\nu} \equiv \mathcal{R}^\mu{}_{\sigma\mu\nu} \tag{2.27}$$

$$\mathcal{R} \equiv g^{\sigma\nu}\mathcal{R}_{\sigma\nu}, \tag{2.28}$$

respectively.

For completeness, we state the field equations for gravity, connecting the energy content in spacetime with its curvature:

$$\mathcal{R}_{\mu\nu} - \frac{1}{2}\mathcal{R}g_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi G\, T_{\mu\nu}, \tag{2.29}$$

for the cosmological constant Λ, energy-momentum tensor $T_{\mu\nu}$, and Newton's constant G. As already mentioned, we shall not be concerned with the dynamical nature of spacetime. The next section is then dedicated to the introduction of the manifold that will be taken to be the fixed background of forthcoming developments.

2.2 Maximally symmetric spacetimes

The symmetries of spacetime are accounted by *Killing vectors*. These vector fields define the isometries of the metric, that is, transformations of $g_{\mu\nu}$ leaving it invariant. Such symmetries imply conserved quantities, akin to energy, linear or angular momenta, etc. One may refer to these symmetries as directions on the manifold on which a (regular) derivative of the metric vanishes, creating a notion of change of tensors along integral curves defined by a vector field.

Consider a particular coordinate $x^\star$, part of a coordinate chart $(x^{\mu'})$, such that $\partial_\star g_{\mu'\nu'} = 0$. The expression $\partial_\star g_{\mu'\nu'}$ is not covariant, hence it does not define the components of a tensor. We wish to determine the covariant expression of this symmetry condition.

$\partial_\star g_{\mu'\nu'}$ can be made into a tensor. In order to do this, let us first consider a vector field. We start by introducing a second coordinate system indexed by

unprimed letters, (x^μ), and studying the action of $\partial_\star \equiv K^\mu \partial_\mu$ on the function $V(f)$, for V another vector field:

$$\begin{aligned} \partial_\star(V(f)) &= K^\sigma \partial_\sigma (V^\mu \partial_\mu f) \\ &= K^\sigma (\partial_\sigma V^\mu) \partial_\mu f + K^\sigma V^\mu \partial_\sigma \partial_\mu f. \end{aligned} \tag{2.30}$$

By extracting the function f, which was arbitrary in the first place, one could hope that the operator $\partial_\star$ acting on a vector field would produce a vector field, but that is not the case because of the second term in the equation above ($\partial_\sigma \partial_\mu$ does not make sense as a vector).

What we can construct from $\partial_\star$ that is in indeed a vector field is the *commutator* of $\partial_\star$ and a vector field. That is,

$$\begin{aligned} \partial_\star(V(f)) - V(\partial_\star f) &= K^\sigma \partial_\sigma (V^\mu \partial_\mu f) - V^\sigma \partial_\sigma (K^\mu \partial_\mu f) \\ &= K^\sigma (\partial_\sigma V^\mu) \partial_\mu f + K^\sigma V^\mu \partial_\sigma \partial_\mu f \\ &\quad - V^\sigma (\partial_\sigma K^\mu) \partial_\mu f - V^\sigma K^\mu \partial_\sigma \partial_\mu f. \end{aligned} \tag{2.31}$$

The non-vectorial term now vanishes from commutativity of second partial derivatives. Extracting the function leads to a new vector that we shall denote as $\pounds_\star V$ (and whose components are *not* $\partial_\star V^\mu$). By means of the commutator expression, that is

$$\begin{aligned} \pounds_\star V &\equiv \partial_\star(V(f)) - V(\partial_\star f) \\ &= \left(K^\sigma \partial_\sigma V^\mu - V^\sigma \partial_\sigma K^\mu\right) \partial_\mu. \end{aligned} \tag{2.32}$$

Now that we have a tool for comparing vectors along the flow based on $\partial_\star$, we want to extend it to higher-order tensors, particularly to the metric tensor, i.e. a notion of derivative taking metric to metric along the coordinate grid. Consider acting on the function $g_{\mu\nu} V^\mu F^\nu$ with $\partial_\star$, for arbitrary vector fields V and F. We can do that in two ways: first, simply using the product rule on functions,

$$\partial_\star(g_{\mu\nu} V^\mu F^\nu) = K^\rho (\partial_\rho g_{\mu\nu}) V^\mu F^\nu + g_{\mu\nu} K^\rho (\partial_\rho V^\mu) F^\nu + g_{\mu\nu} V^\mu K^\rho (\partial_\rho F^\nu); \tag{2.33}$$

and second in a coordinate-independent way. We now assume a notion of the product rule, which applies to tensors:

$$\pounds_\star(g(V,F)) = \pounds_\star g(V,F) + g(\pounds_\star V, F) + g(V, \pounds_\star F). \tag{2.34}$$

What we want to find is $\pounds_\star g$, as a metric with components $(\pounds_\star g)_{\mu\nu}$. The coordinate expression of the RHS of eq. (2.34) is

$$\begin{aligned} \pounds_\star(g(V,F)) = (\pounds_\star g)_{\mu\nu} V^\mu F^\nu &+ g_{\mu\nu} \left(K^\rho \partial_\rho V^\mu - V^\rho \partial_\rho K^\mu\right) F^\nu \\ &+ g_{\mu\nu} V^\mu \left(K^\rho \partial_\rho F^\nu - F^\rho \partial_\rho K^\nu\right). \end{aligned} \tag{2.35}$$

Equating eq. (2.33) to eq. (2.34) and isolating $\pounds_\star g$ gives

$$(\pounds_\star g)_{\mu\nu}V^\mu F^\nu = g_{\mu\nu}V^\rho(\partial_\rho K^\mu)F^\nu + g_{\mu\nu}V^\mu F^\rho(\partial_\rho K^\nu) + K^\rho(\partial_\rho g_{\mu\nu})V^\mu F^\nu. \quad (2.36)$$

We have left both V and F as arbitrary vector fields, implying that the expression above is independent of them. Correcting for a few indices leads to

$$(\pounds_\star g)_{\mu\nu} = K^\rho\partial_\rho g_{\mu\nu} + g_{\rho\nu}(\partial_\mu K^\rho) + g_{\mu\rho}(\partial_\nu K^\rho). \quad (2.37)$$

Notice that, in the especial case of $x^\star$ being one of the (x^μ) coordinates, then $K^\mu = \delta^\mu_\star$. It follows that $(\pounds_\star g)_{\mu\nu} = \partial_\star g_{\mu\nu}$.

We can ameliorate this expression using the covariant derivative. First, summing $0 = K^\rho(\partial_\mu g_{\rho\nu}) - K^\rho(\partial_\mu g_{\rho\nu})$ twice to this expression and recognising that the positive term can be combined with $g_{\rho\nu}(\partial_\mu K^\rho)$ yields

$$(\pounds_\star g)_{\mu\nu} = K^\rho\partial_\rho g_{\mu\nu} + \partial_\mu(K^\rho g_{\rho\nu}) + \partial_\nu(K^\rho g_{\mu\rho}) - K^\rho(\partial_\mu g_{\rho\nu}) - K^\rho(\partial_\nu g_{\mu\rho}). \quad (2.38)$$

Now we can identify the three last terms as twice the contribution of some component of $-\Gamma^\sigma_{\mu\nu}K_\sigma$,

$$(\pounds_\star g)_{\mu\nu} = \partial_\mu K_\nu + \partial_\nu K_\mu + K^\rho(\partial_\rho g_{\mu\nu}) - K^\rho(\partial_\mu g_{\rho\nu}) - K^\rho(\partial_\nu g_{\mu\rho}) \quad (2.39)$$

$$= \partial_\mu K_\nu + \partial_\nu K_\mu - \frac{1}{2}K_\sigma g^{\sigma\rho}\left(-\partial_\rho g_{\mu\nu} + \partial_\mu g_{\rho\nu} + \partial_\nu g_{\mu\rho}\right) \quad (2.40)$$

$$- \frac{1}{2}K_\sigma g^{\sigma\rho}\left(-\partial_\rho g_{\mu\nu} + \partial_\mu g_{\rho\nu} + \partial_\nu g_{\mu\rho}\right), \quad (2.41)$$

which is recognised as

$$(\pounds_\star g)_{\mu\nu} = \nabla_\mu K_\nu + \nabla_\nu K_\mu. \quad (2.42)$$

We were interested in deriving a notion of derivative of tensors along directions in spacetime, consequently providing the notion of isometry: a symmetry of the metric. Whenever this derivative of the metric vanishes, it is implied that this tensor is the same for all points in that specified direction. Therefore we require the *Killing equation* to be satisfied:

$$\nabla_\mu K_\nu + \nabla_\nu K_\mu = 0, \quad (2.43)$$

for K^μ the components of the vector field defining the direction of isometry.

How does this concept of derivative differs from that of the covariant derivative introduced earlier? The $\pounds_\star$ derivative computes how a tensor field changes, compared to itself, along the flow of a given vector field. The ∇ derivative, on the other hand, dictates how a tensor changes along a path (e.g. $T^\mu\nabla_\mu$, for T^μ

the vector components of the tangent) in comparison to its parallel transport as determined by the Christoffel symbols.

The reader is referred to a more comprehensive discussion of this topic in [33, 34]. A rigorous approach introduces the *Lie derivative* (our $\pounds_\star$) as a more primitive concept, not relying on covariant derivatives or metrics. All of this comes into context when considering the general gauge group of gravity: diffeomorphisms, an active way of expressing the coordinate transformations under which spacetime is invariant (i.e. instead of changing the labels one uses to identify events in spacetime, one consider different manifolds representing the same physical spacetime).

Example 1. Let spacetime be flat, $\mathbb{M} = \mathbb{R}^4$, with metric interval $\mathrm{d}t^2 - \mathrm{d}x^2 - \mathrm{d}y^2 - \mathrm{d}z^2$ written in Cartesian coordinates $(x^\mu) = (t, x, y, z)$ and; it has ten Killing vectors, corresponding to the ten possible Poincaré symmetry transformations: four translations (three in space, one in time), three rotations and three boosts. The Killing vector generating boosts along the x coordinate in the positive sense is

$$K^\mu \partial_\mu = -x\frac{\partial}{\partial t} - t\frac{\partial}{\partial x}, \tag{2.44}$$

as plotted in fig. 2.1. In fact, consider applying this vector field on the coordinate t and x:

$$-\left(x\frac{\partial}{\partial t} + t\frac{\partial}{\partial x}\right) t = -x \tag{2.45}$$

$$-\left(x\frac{\partial}{\partial t} + t\frac{\partial}{\partial x}\right) x = -t. \tag{2.46}$$

The theory of Lie derivatives dictate that the exponential of this operation generates the *finite* (as opposed to infinitesimal) symmetry transformation. This leads to

$$\exp\left[-\eta\left(x\frac{\partial}{\partial t} + t\frac{\partial}{\partial x}\right)\right] t = t + \sum_{n=1}^{\infty} \frac{(-1)^n \eta^n}{n!}\left(x\frac{\partial}{\partial t} + t\frac{\partial}{\partial x}\right)^n t, \tag{2.47}$$

and similarly for the action on x. From the alternating results of acting with the Killing vector, one can see that there is a splitting into infinite sums for odd and even n,

$$\exp\left[-\eta\left(x\frac{\partial}{\partial t} + t\frac{\partial}{\partial x}\right)\right] t = \left(1 + \sum_{\text{even } n>0}^{\infty} \frac{\eta^n}{n!}\right) t - \left(\sum_{\text{odd } n>0}^{\infty} \frac{\eta^n}{n!}\right) x, \tag{2.48}$$

resulting in

$$t' = t\cosh\eta - x\sinh\eta. \tag{2.49}$$

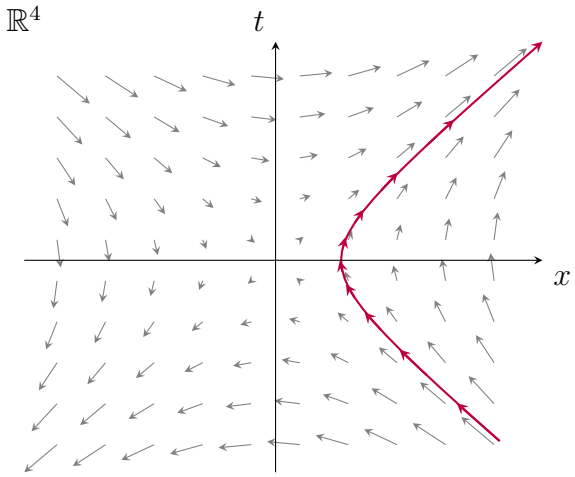

Figure 2.1: Killing vector field for boosts along x, in a two-dimensional slice of $\mathbb{R}^4$. The hyperbola to the right is an integral curve.

A similar calculation for x gives

$$x' = -t\sinh\eta + x\cosh\eta. \tag{2.50}$$

This is a Lorentz boost of rapidity η defining new coordinates (t', x'). With the remaining, unchanged coordinates $y' = y$ and $z' = z$, the transformation is summarised in $x^{\mu'} = \Lambda^{\mu'}{}_{\nu} x^{\nu}$. This is one of the linear transformations between inertial frames at the core of special relativity.

Given an arbitrary spacetime, there could be any number of Killing vectors. In most manifolds, none exist at all. We are interested, however, in spaces bearing a maximal number of these vector fields.

Due to local resemblance of $\mathbb{M}$ to $\mathbb{R}^4$, the counting of independent possible Killing vectors can be made in the flat case, for if any property of the curved manifold changes the counting, it results in a loss of Killing vectors, and not the addition of more. Therefore, in d Euclidean dimensions, one has d directions for translations, and some rotations (or analogous in different signatures).

For rotations, one finds d directions around which to rotate. This operation can be made in any of the remaining $d-1$ senses (e.g. x^i rotated in the x^j sense). The situation is symmetric for the second choice, diminishing the total number by a factor of two. That is a permutation of the d choices into arrangements of two,

divided by two to account for the redundancy between second choices:

$$\frac{1}{2}\frac{d!}{(d-2)!} = \frac{1}{2}d(d-1), \tag{2.51}$$

totalling

$$d + \frac{1}{2}d(d-1) = \frac{1}{2}d(d+1) \tag{2.52}$$

Killing vectors for a manifold of dimension d. Then, for spacetime, the maximal number of symmetries is 10.

Spacetimes of maximal symmetry are classified by their curvature. There are three: the flat case of Minkowski spacetime, the de Sitter spacetime of positive curvature, and the anti-de Sitter spacetime of negative curvature. The classification with respect to curvature stems from the fact that, given their maximum symmetry, the curvature is always the same throughout the manifold. It can be shown that it takes the form

$$g_{\rho\lambda}\mathcal{R}^{\lambda}{}_{\sigma\mu\nu} = \frac{\mathcal{R}}{d(d-1)}(g_{\rho\mu}g_{\sigma\nu} - g_{\rho\nu}g_{\sigma\mu}), \tag{2.53}$$

with the curvature scalar $\mathcal{R}$ being constant over the manifold. The sign of the curvature scalar is the parameter used to classify the maximally symmetric spacetimes.

With cosmological considerations in mind, we will not consider maximally symmetric space*times*, but rather maximally symmetric *spaces*, which does not substantially change our discussion. Assumptions of (spatial) *homogeneity* and *isotropy* are important for cosmology, and in fact they are an expression of the mathematics of isometry as just laid out, determining the existence of three spatial translation and spatial rotation symmetries, respectively.

With further arguments, one is able to find general expressions for the metric in the three cases, known as FLRW models, of $\mathbb{M} = \mathbb{D} \times \mathbb{R}$ type:

$$\mathrm{d}t^2 - R^2(t)\begin{cases} \mathrm{d}\chi^2 + \sin^2\chi(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\alpha^2), \\ \mathrm{d}\chi^2 + \chi^2(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\alpha^2), \\ \mathrm{d}\chi^2 + \sinh^2\chi(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\alpha^2), \end{cases} \tag{2.54}$$

for $\mathbb{D}$ representing the three-dimensional spatial geometry. These are the *closed*, flat and *open* cases, of positive, null and negative curvatures in *comoving coordinates* (with the flat case in polar coordinates). The $R(t)$ function in front of the spatial part is the scale factor, accounting for cosmic evolution (what is the size of a spatial slice $\mathbb{D}$ at instant t).

The curvature tensors can be easily computed from their Christoffel symbols expressions. The curvature scalar in particular is

$$\mathcal{R} = 6\left[\frac{1}{R}\frac{\mathrm{d}^2 R}{\mathrm{d}t^2} + \frac{1}{R^2}\left(\frac{\mathrm{d}R}{\mathrm{d}t}\right)^2 + \frac{k}{R^2}\right]. \tag{2.55}$$

We shall not study all these three cases. We will be mainly interested in the first one, wherein the scale factor is in fact *constant* $R(t) = r$. This configures the Einstein spacetime $\mathbb{M}^4_{\mathrm{E}} \equiv \mathbb{S}^3 \times \mathbb{R}$, with spherical spatial slices. We will supply more details in section 7.2.

The Einstein spacetime is *stationary*, in the sense that it has a Killing vector generating a timelike isometry, and therefore a coordinate system in which it assumes the ∂_0 form, and it is also *static*, implying that it has a coordinate system wherein there are no mixed time-space terms in the metric, $g_{0i} = 0$. The static condition says that there is a spacelike hypersurface of codimension 1 (space) which is perpendicular to the ∂_0 vector field at any point. It is possible to endow static spacetimes with metrics such as those in eq. (2.54), by considering the restriction of $g_{\mu\nu}$ to vectors tangent to $\mathbb{D}$, in which case it takes the form $\mathrm{d}t^2 - \boldsymbol{g}_{ij}\mathrm{d}x^i\mathrm{d}x^j$. This property motivates the studies of causal structures in the following section.

2.2.1 Globally hyperbolic spacetimes

The existence of a foliation in spacelike hypersurfaces, such as those for static spacetimes, is related to the causal structure, and will be further applied to the discussion of quantum fields later on in this dissertation. To better discuss this property, we define a few concepts regarding sets of points in spacetime, assuming that our spacetimes are *time-orientable* (i.e. there is a continuous designation of past and future, and one cannot run into issues such as closed timelike curves) [34].

The tangent vector spaces to a point in a manifold are isomorphic to Minkowski space, $\mathbf{T}_{\mathsf{e}}\mathbb{M} \cong \mathbb{R}^4$. One considers the past and future regions of an event in spacetime $\mathbb{M}$ as inherited from the past and future light cones of the tangent Minkowski spacetime. Although the causal structure of these cases can differ enormously in a global sense, we use this distinction to talk about tangent vectors pointing to the past or the future of an event:

Definition 1. Let

$$\begin{aligned} \gamma\colon \mathbb{R} &\to \mathbb{M} \\ \tau &\mapsto \gamma(\tau) \end{aligned} \tag{2.56}$$

be a smooth curve in spacetime. It is

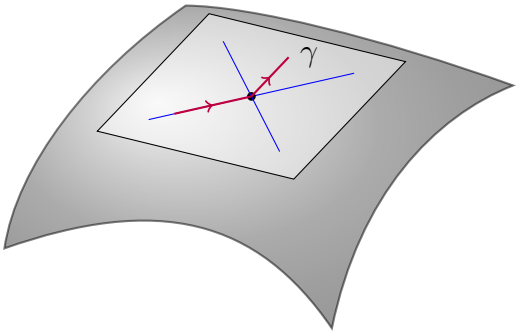

Figure 2.2: A manifold $\mathbb{M}$, its tangent space at a point and the corresponding local light cone. Shown is also a future-point curve γ which is lightlike first and then timelike; consider for instance joining the path of a photon, annihilated at the point, to the path of an electron it helped create at that same point.

- *chronological* if all vectors tangent to it are timelike, either to the past or future;
- *causal* if all vectors tangent to it are either timelike or lightlike, either to the past or future;
- *past (future) inextendible* if there does not exist an event $\mathtt{e}$ (called the endpoint) for which *every* neighbourhood O of it admits τ_{past} (τ_{future}) such that $\tau < \tau_{\text{past}}$ ($\tau > \tau_{\text{future}}$) implies $\gamma(\tau) \in O$.

From the point of view of causality, we can model important physical concepts by defining regions of the manifold which satisfy a some conditions.

Definition 2. Let $\mathtt{e} \in \mathbb{M}$ be an event of spacetime, its *chronological future* $\mathrm{I}^+(\mathtt{e})$ is all other events $\mathtt{p}$ connected to $\mathtt{e}$ by some chronological curve $\gamma(\tau)$ whose tangents are future directed:

$$\mathrm{I}^+(\mathtt{e}) \equiv \{\mathtt{p} \in \mathbb{M} \mid \text{there exists } \gamma \text{ such that } \gamma(0) = \mathtt{e} \text{ and } \gamma(1) = \mathtt{p}\}, \qquad (2.57)$$

such that the tangent vectors $\dot{\gamma}^\mu$ belong to the future light cone, as it is chosen. The same can be said about the *chronological past* $\mathrm{I}^-(\mathtt{e})$ after inverting the order of parameters $\tau = 0$ and 1 in the definition, and the direction of tangent vectors to the curve.

Let $\mathbb{D} \subset \mathbb{M}$ be a hypersurface in spacetime, its *chronological past (future)*

$\mathrm{I}^{-(+)}(\mathbb{D})$ is the union of chronological pasts (futures) of its points, $\mathrm{I}^{-(+)}(\mathbb{D}) \equiv \bigcup_{\mathsf{e}} \mathrm{I}^{-(+)}(\mathsf{e})$.

A particular class of hypersurfaces are what interests us, as they are defined:

Definition 3. Let $\mathbb{D} \subset \mathbb{M}$ be a hypersurface in spacetime. $\mathbb{D}$ is *achronal* if, for every two points, neither is in the chronological future of the other,

$$\mathbb{D} \cap \mathrm{I}^{+}(\mathbb{D}) = \emptyset. \tag{2.58}$$

In addition, if every curve such that $\gamma(0) \in \mathrm{I}^{-}(\mathbb{D})$ and $\gamma(1) \in \mathrm{I}^{+}(\mathbb{D})$ imply that $\gamma(\tau) \in \mathbb{D}$ for some τ, then $\mathbb{D}$ is an achronal *slice*.

An achronal condition is more restricting than a spacelike one. A spacelike hypersurface can be defined as that for which nearby points cannot be connected by timelike curves, whereas an achronal one guarantees that *any* two points, however far from each other, are not related in this way. One could imagine a spacetime with non-trivial topologies or with its collection of light cones bending in a way so as to connect points of the surface by timelike curves.

Finally, we arrive at the concept of interest.

Definition 4. Let $\mathbb{D} \subset \mathbb{M}$ be an achronal hypersurface in spacetime. Its *future domain of dependence* $\mathrm{D}^{+}(\mathbb{D})$is the set of events in spacetime for which every past inextendible causal curve $\gamma(\tau)$ passes through $\mathbb{D}$,

$$\mathrm{D}^{+}(\mathbb{D}) \equiv \{\mathsf{e} \in \mathbb{M} \mid \text{for all } \gamma(1) = \mathsf{e} \text{ there exists } \gamma(0) \in \mathbb{D}\}. \tag{2.59}$$

Similarly for the *past domain of dependence* $\mathrm{D}^{-}(\mathbb{D})$, when interchanging the parameters in the definition and the time direction of the curve. The full domain of dependence is the union of its past and future version.

We are interested in *Cauchy surfaces* $\mathbb{D}$, for which the domain of dependence is all of spacetime: $\mathrm{D}(\mathbb{D}) = \mathbb{M}$. The physical motivation behind this is to allow discernment of when the physical content in a region of spacetime is determined by physical content in a related region. These surfaces can be taken to define "space" as suitable for proper initial-value problems.

Spacetimes which admit a "slicing" into Cauchy surfaces are those for which determining initial conditions at an instant in time implies knowledge about the system at any later or earlier time, everywhere in space; these are *globally hyperbolic*

spacetimes. Dynamical evolution, decoded when one solves the field equations, is therefore a well-posed problem of differential equations.

When treating quantum fields, we will formulate the problem in the Hamiltonian formalism, in which case there are two first order differential equations whose solutions are parametrised by a pair of initial conditions. The consideration of globally hyperbolic spacetimes enables this treatment.

Chapter 3

Quantum theory

The subject under study in this thesis are fields. Having introduced in last section the background where they live, it remains to explain their mechanics. As with the metric field of general relativity, matter and interaction fields are well-understood classically. Our approach to treating quantum fields will pass through the lenses of canonical quantisation.

As it will be introduced in section 4.2, we may look at quantum mechanics by starting with a well-known classical system, and then constructing its quantum counterpart to understand more fine-grained details of its behaviour. It looks rather inconsistent to start from classical physics and, through a procedure, "recover" quantum physics, but clearly one should not expect that quantum mechanics branches out of classical mechanics; our current comprehension dictates that classical mechanics instead is emergent. Quantum mechanics can be formulated independently of quantisation.

In the present section we refrain from relying on classical intuitions and instead directly describe the principles of quantum mechanics. The ability of constructing Hilbert spaces and algebras of operators is essential when dealing with intrinsic quantum phenomena, such as the presence of spin or entanglement. In this part we review foundational aspects of quantum theory to introduce notation and the main ideas to follow in the next sections, based on ref. [37] and [38, 35, 39] for mathematical aspects. The study of entanglement entropy follows discussions in ref. [40].

3.1 Axioms of quantum mechanics

We will refer to vectors in a Hilbert space $\mathbf{H}$ as $|\psi\rangle$, with its dual vector $\langle\psi|$; the inner product then is just the action of any covector $\langle\psi'|$, on any vector $|\psi\rangle$: $\langle\psi'|\psi\rangle$. Basis vectors are often written as $|\lambda\rangle$, for λ indexing the elements of this set.

For simplicity, we will take an axiomatic approach, followed by a brief discussion of why they capture the physics of interest.

Axiom 1 (of systems and states). A *quantum system* is a *separable* Hilbert space $\mathbf{H}$ over the complex numbers $\mathbb{C}$, with an inner product which is

1. Hermitian: $\langle\psi|\psi'\rangle = \overline{\langle\psi'|\psi\rangle}$.
2. Sesquilinear: if $|\psi\rangle = a\,|v\rangle + |v'\rangle$ and $|\psi'\rangle = b\,|u\rangle$, then $\langle\psi|\psi'\rangle = \overline{a}b\,\langle v|u\rangle + b\,\langle v'|u\rangle$.
3. Positive-definite: $\langle\psi|\psi\rangle = 0 \iff |\psi\rangle = 0$, and $\langle\psi|\psi\rangle > 0$ otherwise.

States are *density operators*: linear operators

$$\varrho\colon \mathbf{H} \to \mathbf{H}, \tag{3.1}$$

conditioned to be

1. Positive semi-definite, i.e. $\forall\,|\psi\rangle \in \mathbf{H}$, $\langle\psi|\varrho|\psi\rangle \geq 0$.
2. Trace-class, i.e. $\sum_\lambda \langle\lambda|\varrho|\lambda\rangle < \infty$, for an orthonormal basis $\{|\lambda\rangle\}$.

From the last condition it is possible to require that $\sum_\lambda \langle\lambda|\varrho|\lambda\rangle = 1$, which will be assumed from hereafter.

A bipartite system is such that

$$\mathbf{H} = \mathbf{H}_{\mathtt{A}} \otimes \mathbf{H}_{\mathtt{B}}, \tag{3.2}$$

given that we identify a basis for each subspace, and an isomorphism between the tensor product of such basis elements and the basis $\{|\lambda\rangle\}$. Bipartition is necessary for the study of subsystems: the subspaces in the tensor product of eq. (3.2).

There is a class of important states in a quantum system which are completely defined by vectors of the Hilbert space. The following statement defines them.

Definition 5. *Pure states* are equivalence classes

$$[|\psi\rangle] = \{|u\rangle \in \mathbf{H} \mid |u\rangle \propto |\psi\rangle\}, \tag{3.3}$$

referred to as *rays*. We often choose the representative $|\psi\rangle$ to denote the state. In terms of the density operator the state assumes the form $\varrho = |\psi\rangle\langle\psi|$ for $\||\psi\|\|^2 = 1$.

Any element $|u\rangle$ of $[|\psi\rangle]$ is regarded as the same state; we only pick the representative $|\psi\rangle$ to emphasize its role as a special vector of interest (possibly relying on computational simplicity, e.g. it is normalised). The pure state projects any other vector of the Hilbert space onto its associated ray,

$$\varrho\,|v\rangle = \langle\psi|v\rangle\,|\psi\rangle\,. \tag{3.4}$$

Operators have other roles in quantum mechanics as well, as the following axiom dictates.

Axiom 2 (of observables and spectra). An *observable* is a self-adjoint linear operator

$$\mathcal{O}\colon \mathrm{Dom}(\mathcal{O}) \to \mathbf{H}. \tag{3.5}$$

The possible *measurement outcomes* consist of values in the spectrum of the observable.

In finite-dimensional cases, the spectrum of an operator is the set of eigenvalues of $\mathcal{O}$,

$$\mathrm{EV}(\mathcal{O}) = \{\lambda \in \mathbb{R} \mid \mathcal{O}\,|\psi\rangle = \lambda\,|\psi\rangle\}. \tag{3.6}$$

Eigenvalues can even be part of countably infinite set, such as the case for the harmonic oscillator, although in general the spectrum of $\mathcal{O}$ will consist of more than its eigenvalues. We make the following distinction.

Eigenvalues: If $(\mathcal{O} - \lambda I_{\mathbf{H}})$ is not injective, then λ is said to be an eigenvalue, part of the discrete spectrum.

Continuum: If the range of $\mathcal{O} - \lambda I_{\mathbf{H}}$ is not dense in $\mathbf{H}$, then λ is an element of the continuous spectrum of $\mathcal{O}$.

Of course, $\mathcal{O}$ can lead to neither injective or surjective operators. Then $\mathrm{Spectr}(\mathcal{O})$ consists of these two types of values.

The eigenvalue set then composes the discrete part, whilst there exists a continuous contribution; such is the case of unbounded energy states predicted in the study of the hydrogen atom. To illustrate, fig. 3.1 indicates ticks as eigenvalues, and shaded area as the continuous set of the energy spectrum of hydrogen.

Figure 3.1: Energy of electrons in orbitals of the hydrogen atom.

Much of the essence of quantum theory relies on what information one can possibly acquire about *which* numbers in the spectrum of operators are expected after successive measurements. This pertains to the axiom on measurements.

Axiom 3 (of measurements and probabilities). Let $\mathrm{pr}_\lambda \equiv |\lambda\rangle\langle\lambda|$ be the projection operator onto the subspace of $\mathbf{H}$ spanned by $|\lambda\rangle$. The probability that a system will be found in a state $|\lambda\rangle\langle\lambda|$ is

$$\mathrm{prob}(\lambda) \equiv \mathrm{tr}(\mathrm{pr}_\lambda\, \varrho). \tag{3.7}$$

Furthermore, the expectation value of an observable is

$$\langle \mathcal{O} \rangle \equiv \mathrm{tr}(\mathcal{O}\varrho). \tag{3.8}$$

This can be verified after successive observations, as no one measurement can single-handedly reproduce it due to its probabilistic nature.

Projection operators are idempotent, i.e. satisfy $\mathrm{pr}^2 = \mathrm{pr}$. This is valid, for instance, for pure states: $\varrho^2 = \varrho$.

The second part of axiom 3 is actually a consequence of the first given the spectral decomposition of self-adjoint operators. Let $\mathrm{d}\mu_\lambda$ be a measure in the spectral set of an operator. Through eq. (3.8) one sees that $\langle \mathcal{O} \rangle$ truly is the expectation value for a probability distribution of random variables λ,

$$\langle \mathcal{O} \rangle = \int \mathrm{d}\mu_\lambda\, \lambda\, \mathrm{tr}(\mathrm{pr}_\lambda\, \varrho), \tag{3.9}$$

with

$$I_{\mathbf{H}} = \int \mathrm{d}\mu_\lambda\, \mathrm{pr}_\lambda, \tag{3.10}$$

also known as *completeness relation*.

The next example displays some of the properties discussed above.

Example 2. Let $\mathbf{H}$ be a two-dimensional Hilbert space, with orthonormal basis states $|0\rangle$ and $|1\rangle$, e.g. of horizontal and vertical polarisations of a photon. Suppose there is a pure state $|\psi\rangle\langle\psi|$ in the superposition

$$|\psi\rangle = a\,|0\rangle + b\,|1\rangle \implies |\psi\rangle\langle\psi| = \begin{pmatrix} |a|^2 & a\bar{b} \\ \bar{a}b & |b|^2 \end{pmatrix}. \tag{3.11}$$

The inner product on the definition of $\mathbf{H}$ is a mechanism to interpret a and b as probability amplitudes. The orthogonality of basis elements says that $|0\rangle$ and $|1\rangle$

are different samples expected in measurements, and as so, the physical system can never be in both, but is in either one or the other state, i.e. after an experiment, $|\psi\rangle$ is projected onto one of them. For instance,

$$|\psi\rangle \xmapsto{\text{measurement}} \frac{\mathrm{pr}_1 |\psi\rangle}{\sqrt{\langle\psi|\mathrm{pr}_1|\psi\rangle}} = \frac{|1\rangle\langle 1|\,|\psi\rangle}{b} = |1\rangle\,. \tag{3.12}$$

By normalisation, $\langle\psi|\psi\rangle = |a|^2 + |b|^2 = 1$, we see that the geometric interpretation of the norm is replaced by a notion of how much access one has to these samples; in this example, by definition, we have full access, i.e. every expected outcome is available to happen. In eq. (3.12), the probability of that simulated result is

$$\mathrm{prob}(1) = \langle 0|\mathrm{pr}_1|\psi\rangle\,\langle\psi|0\rangle + \langle 1|\mathrm{pr}_1|\psi\rangle\,\langle\psi|1\rangle\,, \tag{3.13}$$

wherein the first term in the right-hand side vanishes, and the second reduces to $|\langle\psi|1\rangle|^2 = |b|^2$.

A curious consequence of quantum behaviour is that of interference. Consider a new state $|\psi\rangle = a\,|\mathrm{R}\rangle + b\,|\mathrm{L}\rangle$, for right-handed and left-handed circular polarisations, under the same measurement as above. Now $|\psi\rangle\langle\psi|$ constructed with respect to the rectangular basis is different, following

$$|\mathrm{R}\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \quad |\mathrm{L}\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}. \tag{3.14}$$

Then $\mathrm{tr}(\mathrm{pr}_1\,|\psi\rangle\langle\psi|)$ yields $\mathrm{Re}(a\bar{b})$. One notices the contribution from both probability amplitudes.

Finally, the last axiom pertains to the dynamics of observables, encoding the interactions and evolutions of physical systems.

Axiom 4 (of dynamics). Let $\mathcal{O}$ be an observable, and let H be the Hamiltonian operator whose spectrum contains the values of energy the system can take. Given a product $[\_\,,\,\_]$ for the algebra of operators, the time evolution of the observable is a solution to

$$\frac{\partial\mathcal{O}}{\partial t} = -\mathrm{i}[\mathcal{O}, H], \tag{3.15}$$

the Heisenberg equation.

Notice that axiom 4 is the ideal (Heisenberg) picture for treating relativistic systems. There the spatial and temporal coordinates play a symmetric role; for

fields, they will both serve as variables for operators. This is contrast with the Schrödinger picture, for which operators are fixed in time, giving room for states to evolve.

Let us review the non-relativistic quantum harmonic oscillator, in terms adequate for further development. This precedes concepts relevant for the study of fields in curved spacetime in chapter 4.

Example 3. Consider a total of J particles of the same mass m moving in one dimension, each subjected to an independent quadratic potential

$$H = \frac{\boldsymbol{p}^2}{2m} + \frac{\boldsymbol{q}^\dagger K \boldsymbol{q}}{2}, \tag{3.16}$$

for $(\boldsymbol{q}, \boldsymbol{p})$ the position and momentum vectors with the j^{th} particle operator in its j^{th} entry, and a matrix K coupling particles one-to-one, e.g. $q_j K_{jj} q_j$ the diagonal term representing a single particle in a quadratic potential.

Pick the algebra product to be

$$[q_j, p_{j'}] = \mathrm{i}\delta_{jj'} I. \tag{3.17}$$

The equations of motion 3.15 are coupled differential equations.

For K a positive-definite matrix, one can make a linear transformation diagonalising it with a unitary matrix U. The transformed Hamiltonian is, thus,

$$\begin{aligned} H \overset{U}{\mapsto} \widetilde{H} &= \frac{1}{2m} \overbrace{\boldsymbol{p}^\dagger U}^{\tilde{\boldsymbol{p}}^\dagger} U^{-1}\boldsymbol{p} + \frac{1}{2}\boldsymbol{q}^\dagger U \overbrace{U^{-1} K U}^{\widetilde{K}} \underbrace{U^{-1}\boldsymbol{q}}_{\tilde{\boldsymbol{q}}} \\ &= \sum_k \frac{\tilde{p}_k^2}{2m} + \frac{m\omega_k^2}{2}\tilde{q}_k^2. \end{aligned} \tag{3.18}$$

The problem is now indexed by the W normal modes of oscillation, with frequency

$$\omega_k = \sqrt{\frac{\widetilde{K}_{kk}}{m}} \tag{3.19}$$

for mode k. If nondegenerate, K implies there is one mode for each particle, and $W = J$.

Heisenberg's equation lead to harmonic solutions $\tilde{\boldsymbol{q}}_k \propto (a_k \mathrm{e}^{-\mathrm{i}\omega_k t} + a_k^\dagger \mathrm{e}^{\mathrm{i}\omega_k t})$ (and corresponding momenta). This is the Heisenberg picture of quantum mechanics, wherein operators $\tilde{\boldsymbol{q}}_k(t)$ are time-dependent. Together with $\tilde{\boldsymbol{p}}_k$, they also obey the canonical commutation relation $[\tilde{\boldsymbol{q}}_k, \tilde{\boldsymbol{p}}_{k'}] = \mathrm{i}\delta_{kk'} I$.

In this context, the amplitudes a_k take the role of the creation and annihilation operators with commutation rule

$$\left[a_k, a_{k'}^\dagger\right] = \delta_{kk'}. \tag{3.20}$$

They determine the number of mode excitations from the vacuum state $|0\rangle$, e.g.

$$\left(a_k^\dagger\right)^n |0\rangle = |n_k\rangle \qquad \text{: an integer } n \text{ of excitations with frequency } \omega_k. \tag{3.21}$$

$$a_k^\dagger a_{k'}^\dagger |0\rangle = |1_k, 1_{k'}\rangle \quad \text{: one excitation for modes } k \text{ and } k', \text{ and so forth.} \tag{3.22}$$

Finally, the diagonalised Hamiltonian is $\widetilde{H} = \sum_k^M \omega_k a_k^\dagger a_k + \omega_k/2$. With

$$\text{Spectr}(H) = \left\{ E \in \mathbb{R} \mid \text{for } n_k \in \mathbb{N}, E = \sum_k^W \omega_k \left(n_k + \frac{1}{2}\right) \right\} \tag{3.23}$$

as its spectrum.

3.2 Entanglement entropy

The factorization of states into a tensor product is related to important consequences. In this section we present the notion of *entanglement entropy*. The ideas to follow concern the phenomenon of *entanglement*, as a purely quantum correlation between observations, and the entropy function measuring it. This is one of our main topics, and will continue to be detailed as the text progresses, in particular for its role in relativistic and gravitational systems.

Let us start by elaborating on example 2. Recall that we had given a two-dimensional Hilbert space of polarisation degrees of freedom. Add in a second particle. One is then able to construct a standard example of entangled system: a *Bell state*.

Example 4. Let $\mathbf{H}$ be a four-dimensional Hilbert space, constructed from the polarisation states of two particles as a tensor product $\mathbf{H} = \mathbf{H}_{\mathtt{A}} \otimes \mathbf{H}_{\mathtt{B}}$, referring to the system of particle $\mathtt{A}$, that of particle $\mathtt{B}$, and states thereof. Let us work with the superposition of polarisation states of two particles, the pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|0_{\mathtt{A}}\rangle\, |1_{\mathtt{B}}\rangle + |1_{\mathtt{A}}\rangle\, |0_{\mathtt{B}}\rangle \big). \tag{3.24}$$

Under this basis, $|\psi\rangle$ cannot be written as $|\psi_{\mathtt{A}}\rangle\,|\psi_{\mathtt{B}}\rangle$. Let us abbreviate the notation by writing $|ij\rangle$ for $|i_{\mathtt{A}}\rangle\,|j_{\mathtt{B}}\rangle$. A separable state would have the aspect

$$\begin{aligned}|\psi_{\mathtt{A}}\rangle\,|\psi_{\mathtt{B}}\rangle &= \big(a_0\,|0_{\mathtt{A}}\rangle + a_1\,|1_{\mathtt{A}}\rangle\,\big) \otimes \big(b_0\,|0_{\mathtt{B}}\rangle + b_1\,|1_{\mathtt{B}}\rangle\,\big) \\ &= a_0b_0\,|00\rangle + a_0b_1\,|01\rangle + a_1b_0\,|10\rangle + a_1b_1\,|11\rangle\,.\end{aligned} \tag{3.25}$$

The span of such a state is constrained and $|\psi\rangle$ is not in it, for a null contribution of $|00\rangle$ implies a null contribution of either $|01\rangle$ or $|10\rangle$.

This example inspires a explanation of separability of states in quantum mechanics, and what this property (or the lack of it) means for a system. Due to our interests, the discussion to follow encompasses only bipartite systems with pure states, but the subject is vast as one can learn from ref. [41].

Nonseparability of operators ϱ in physics means entanglement, the properties that a state have when it is not enough to know the configuration of its parts, without acknowledging correlations thereof. A pure state $\varrho \in \mathbf{H}$ is *entangled* if it *cannot* be written as a tensor product of two states $\varrho_{\mathtt{A}}$ and $\varrho_{\mathtt{B}}$ in separated subsystems $\mathbf{H}_{\mathtt{A}}$ and $\mathbf{H}_{\mathtt{B}}$, i.e. $\varrho \neq \varrho_{\mathtt{A}} \otimes \varrho_{\mathtt{B}}$. In terms of a vector defining a pure state, this means that

$$|\psi\rangle = \sum_{\alpha,\beta} C_{\alpha\beta}\,|\alpha\rangle\,|\beta\rangle\,, \tag{3.26}$$

in which $C_{\alpha\beta}$ is a matrix with at least two linearly independent rows, i.e. it has rank ≥ 2. In the product state of eq. (3.25), the matrix of coefficients is

$$C_{\alpha\beta} = \begin{pmatrix} a_0b_0 & a_0b_1 \\ a_1b_0 & a_1b_1 \end{pmatrix}, \tag{3.27}$$

Thus

$$|\psi_{\mathtt{A}}\rangle = \sum_{\alpha} a_\alpha\,|\alpha\rangle \tag{3.28}$$

and

$$|\psi_{\mathtt{B}}\rangle = \sum_{\beta} b_\beta\,|\beta\rangle\,, \tag{3.29}$$

implying $|\psi_{\mathtt{A}}\rangle\,|\psi_{\mathtt{B}}\rangle$ has components

$$a_\alpha b_\beta^{\intercal} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \begin{pmatrix} b_0 & b_1 \end{pmatrix} = \begin{pmatrix} a_0b_0 & a_0b_1 \\ a_1b_0 & a_1b_1 \end{pmatrix}. \tag{3.30}$$

whose columns are proportional to each other, hence rendering C a matrix of rank 1 which describes eq. (3.25) but *not* eq. (3.24).

We can rework the matrix $C_{\alpha\beta}$, as it appears in eq. (3.26), to be singular-value decomposed. More generally, this process diagonalises the smallest subspace of a matrix. It is realised by the factorisation

$$C = U\sqrt{P}V^\dagger, \tag{3.31}$$

for U and V unitary matrices[1] acting on the rectangular diagonal matrix $\sqrt{P}$; e.g.

$$C = U \begin{pmatrix} \sqrt{p_1} & 0 & & & 0 \\ 0 & \sqrt{p_2} & \cdots\cdots\cdots & \cdots & 0 \\ & & \ddots & \cdots & \vdots \\ & & & \sqrt{p_n} & 0 \end{pmatrix} V^\dagger, \tag{3.32}$$

for $n = \min\{\dim \mathbf{H}_\mathtt{A}, \dim \mathbf{H}_\mathtt{B}\}$. Let us pick, without loss of generality, $n = \dim \mathbf{H}_\mathtt{A}$, then the singular-value decomposition corresponds to the expansion[2]

$$|\psi\rangle = \sum_{i,j=1} \sqrt{P_{ij}}\, |i_\mathtt{A}\rangle\, |j_\mathtt{B}\rangle = \sum_{i=1}^{n} \sqrt{p_i}\, |i_\mathtt{A}\rangle\, |i_\mathtt{B}\rangle\,, \tag{3.33}$$

in which we recovered the indices of subsystem to make clear to which subspace the vectors belong. The new vectors $|i_\mathtt{A}\rangle$ and $|j_\mathtt{B}\rangle$ are basis for $\mathtt{A}$ and $\mathtt{B}$. The vectors $|i_\mathtt{B}\rangle$ accessed by the sum in the second part of 3.33, however, cannot always be a basis for subsystem $\mathtt{B}$ because there are not enough vectors, after all $n \leq \dim \mathbf{H}_\mathtt{B}$.

The number of nonzero singular values (the ones in the "diagonal") is precisely the *rank* of C. In the singular-value form, entangled states reach a straightforward definition. To better understand this we introduce the notion of reduced density matrix derived from the trace.

Definition 6. Let $\varrho \in \mathrm{Op}(\mathbf{H})$ be a state of the product Hilbert space $\mathbf{H} = \mathbf{H}_\mathtt{A} \otimes \mathbf{H}_\mathtt{B}$. The *partial trace* of ϱ, *over the subspace* $\mathbf{H}_\mathtt{B}$, is the unique linear operator

$$\mathrm{tr}_\mathtt{B} \colon \mathrm{LinOp}\left(\mathbf{H}_\mathtt{A} \otimes \mathbf{H}_\mathtt{B}\right) \to \mathrm{LinOp}(\mathbf{H}_\mathtt{A}) \tag{3.34}$$

such that, for $A \in \mathrm{LinOp}(\mathbf{H}_\mathtt{A})$ and $B \in \mathrm{LinOp}(\mathbf{H}_\mathtt{B})$,

$$\mathrm{tr}_\mathtt{B}(A \otimes B) = A\,\mathrm{tr}(B). \tag{3.35}$$

The image can be expressed as $\mathrm{Op}(\mathbf{H}_\mathtt{A} \otimes \mathbb{R})$, because the effect of a trace is to send any element of $\mathrm{LinOp}(\mathbf{H})$ to $\mathbb{R}$.

[1] The dimensions of these matrices can be distinct, meaning that the subsystems also have different dimensions.

[2] One of the sums collapses because the nonzero contribution is diagonal: $P_{ij} = p_i\delta_{ij}$.

Similarly to the trace, one has a explicit expression in terms of bases. Consider the following general state of $\mathbf{H}_{\mathtt{A}} \otimes \mathbf{H}_{\mathtt{B}}$,

$$\varrho = \sum_{i,j} \sum_{i',j'} C_{iji'j'} \, |ij\rangle\langle i'j'| \, . \tag{3.36}$$

The partial trace over $\mathtt{B}$ is

$$\mathrm{tr}_{\mathtt{B}} \, \varrho = \sum_{i,j} \sum_{i',j'} C_{iji'j'} \, |i\rangle\langle i'| \left(\sum_{\beta} \langle\beta| \, |j\rangle\langle j'| \, |\beta\rangle \right) , \tag{3.37}$$

for orthonormal basis elements $|j\rangle$ and $|\beta\rangle$. The operation reduces the state to

$$\varrho_{\mathtt{A}} \equiv \mathrm{tr}_{\mathtt{B}} \, \varrho = \sum_{i,i'} \underbrace{\sum_{j} C_{iji'j}}_{\tilde{C}_{ii'}} |i\rangle\langle i'| \, , \tag{3.38}$$

depending now only on the pair i and i', belonging to $\mathbf{H}_{\mathtt{A}}$.

The final piece in giving a precise definition of an entangled state is a different type of state a quantum system can find itself in. This comes in opposition to the demonstrated pure states $|\psi\rangle\langle\psi|$ of definition 5.

Definition 7. A state ϱ is *mixed* if

$$\mathrm{tr} \, \varrho^2 < \mathrm{tr} \, \varrho, \tag{3.39}$$

and, hence, ceasing to be a projection operator $\varrho^2 \neq \varrho$. In this case it is a combination[3]

$$\varrho = \sum_{i} p_i \, |\psi_i\rangle\langle\psi_i| \, , \quad \text{such that} \quad \sum_{i} p_i = 1, \tag{3.40}$$

with $p_i \neq 0$ for at least two values of i. Furthermore, $|\psi_i\rangle$ does not need to constitute a basis for $\mathbf{H}$.

The combination $|\psi_i\rangle\langle\psi_i|$ above is not the same as a quantum superposition. It is given by a probability distribution representing classical ignorance of the state of the system, and not the fundamental nescience of quantum nature. Accordingly, the i indexes the statistical ensemble on which the mixture inhabits. A pure state is recognised as the situation where $p_i = 1$ for a single i.

These tools grants us with a working idea of entanglement, as follows.

[3]This is a type of linear combination known as convex combination.

Definition 8. Let a system $\mathbf{H}$ be factorised into $\mathbf{H}_{\mathtt{A}} \otimes \mathbf{H}_{\mathtt{B}}$. An *entangled state* ϱ is such that it has at least two singular values p_i, given a singular-value decomposition. It yields a *mixed reduced state*

$$\mathrm{tr}_{\mathtt{B}}\, \varrho = \sum_i p_i \left|\psi_i\right\rangle\!\left\langle\psi_i\right| , \tag{3.41}$$

in which $\sum_i p_i = 1$.

The singular-value decomposition thus allows for a clear definition of entangled state, as in eq. (3.33). Supplying eq. (3.38) with the coefficients of eq. (3.33) results in

$$\begin{aligned} \varrho_{\mathtt{A}} &= \sum_j \sum_{i,i'} \delta_{ij} \sqrt{p_i} \left|i\right\rangle\!\left\langle i'\right| \delta_{i'j} \sqrt{p_{i'}} \\ &= \sum_j p_j \left|j\right\rangle\!\left\langle j\right| . \end{aligned} \tag{3.42}$$

The sum is convex for states whose trace equals one. Let us verify this for the running example of polarisation states.

Example 5. The density matrix of eq. (3.24), with rows and columns corresponding in order to $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$, is

$$\varrho = |\psi\rangle\!\langle\psi| = \frac{1}{2} \begin{pmatrix} \boxed{\begin{matrix} 0 & 0 \\ 0 & 1 \end{matrix}} & \boxed{\begin{matrix} 0 & 0 \\ 1 & 0 \end{matrix}} \\ \boxed{\begin{matrix} 0 & 1 \\ 0 & 0 \end{matrix}} & \boxed{\begin{matrix} 1 & 0 \\ 0 & 0 \end{matrix}} \end{pmatrix} . \tag{3.43}$$

The elements of the reduced state $\varrho_{\mathtt{A}}$ are found out after tracing out the basis of subsystem $\mathtt{B}$. The partial trace is the sum of diagonal terms of each boxed submatrix above. These are the numbers accompanying basis vectors for which the second indices (referent to $\mathtt{B}$) equal one another; the first indices (of $\mathtt{A}$), on the other hand, determine what component of the reduced density matrix one reads. Take, for instance, the upper-right submatrix. The diagonal refers to the italicised characters in $|\mathbf{0}\mathit{0}\rangle\!\langle\mathbf{1}\mathit{0}|$ and in $|\mathbf{0}\mathit{1}\rangle\!\langle\mathbf{1}\mathit{1}|$, whilst the characters in bold signify entry $|\mathbf{0}\rangle\!\langle\mathbf{1}|$ of $\varrho_{\mathtt{A}}$. The reduced matrix is found to be

$$\varrho_{\mathtt{A}} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} , \tag{3.44}$$

mixed and with singular values $p_j = 1/2$.

Taking the partial trace over a subsystem conveys the inaccessibility of degrees of freedom there located. By tracing out subsystem $\mathtt{B}$, an experimenter also disregards the measurements made on it; to her perspective, measurements on $\mathtt{A}$ concur with the classical mixture of eq. (3.44). She would perceive quantum correlations only after checking experiments made on the traced-out system, and then conclude that she was dealing with the superposition $(|01\rangle + |10\rangle)/\sqrt{2}$ (cf. eq. (3.24)).

An example would be the spin polarisations of two particles. After computing $\mathrm{tr}_{\mathtt{B}}\,\varrho$, the persisting subsystem reproduces an ensemble of particles created half of the time with the spin of qubit $|0\rangle$, and the other half with the spin of qubit $|1\rangle$. The fact that the state $|0\rangle$ ($|1\rangle$) of $\mathtt{A}$ is always accompanied by state $|1\rangle$ ($|0\rangle$) of $\mathtt{B}$ would only be acknowledged when comparing observations made on both subsystems.

Equation (3.44) comes from a maximally entangled state, because the defining eigenvalues of the reduced matrix have the aspect of $1/\dim \mathbf{H}_{\mathtt{A}}$: a mixture of equally probable outcomes (and therefore multiple of the identity). This suggests a way of quantifying the amount of entanglement in states, and that will be the entanglement entropy $\mathcal{S}$.

Two conditions for it to be a good measure of entanglement are

- $\mathcal{S} = 0$ for pure states.
- $\mathcal{S}$ is maximised for maximally mixed states ϱ.

An expression to account for them is the von Neumann entropy.

Definition 9. The *von Neumann entropy* $\mathcal{S}$ is

$$\mathcal{S}(\varrho) \equiv -\operatorname{tr}(\varrho \ln \varrho). \tag{3.45}$$

Mixed states, written as $\sum_i p_i\,|\psi_i\rangle\langle\psi_i|$, are evidently self-adjoint operators. For the cases where we can regard the $|\psi_i\rangle$ as a basis, the p_i are eigenvalues in the diagonal of the operator.It follows that one can compute the trace of eq. (3.45) by knowing the probabilities p_i, as

$$\begin{aligned}\mathcal{S}(\varrho) &= -\operatorname{tr}\left(\varrho \ln \varrho\right) \\ &= \sum_{\{i\in\mathbb{N}|p_i\neq 0\}} -p_i \ln p_i.\end{aligned} \tag{3.46}$$

This is the *Shannon entropy* of information theory.

$\mathcal{S}(\varrho) = 0$ for a pure state, and $\mathcal{S}(\varrho_{\mathtt{A}})$ for the maximally entangled states. Example 6 concludes the discussion of entanglement of Bell states.

Example 6. Consider the full and the reduced states, respectively

$$\varrho = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \varrho_{\mathtt{A}} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}, \tag{3.47}$$

as before. The entropies are then computed to be

$$\begin{aligned} \mathcal{S}(\varrho) &= -\left(1 \ln 1 + 1 \ln 1\right) \\ &= 0, \end{aligned} \tag{3.48}$$

and

$$\begin{aligned} \mathcal{S}(\varrho_{\mathtt{A}}) &= -\ln\left(\frac{1}{2}\right) \\ &= \ln 2. \end{aligned} \tag{3.49}$$

Hence their status as a pure and maximally mixed state.

Notice that the reduced matrix is already in diagonal form, but ϱ can be brought into this shape with a single nonvanishing eigenvalue; the eigenvector for it is precisely $|\psi\rangle$. That is

$$\varrho = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{3.50}$$

and one has $\mathcal{S}(\varrho) = 0$ again.

A second signature of maximally entangled states is the fact that $\mathcal{S} = \ln \dim \mathbf{H}$; assume we have such a state, and $n = \dim \mathbf{H}$. Because it is maximally entangled, then $\forall i$, $p_i = 1/n$, and

$$\begin{aligned} \mathcal{S} &= \sum_{i=1}^{n} -\frac{1}{n} \ln\left(\frac{1}{n}\right) \\ &= \ln n. \end{aligned} \tag{3.51}$$

$\mathcal{S}$ also possesses properties useful for its general study. Given three disjoint subsystems $\mathtt{A}, \mathtt{B}, \mathtt{C}$, and $\mathcal{S}(\varrho_{\mathtt{A}}) \equiv \mathcal{S}_{\mathtt{A}}$, then strong subadditivity holds (see ref. [40] and references therein):

$$\mathcal{S}_{\mathtt{A}\cup\mathtt{B}\cup\mathtt{C}} + \mathcal{S}_{\mathtt{B}} \leq \mathcal{S}_{\mathtt{A}\cup\mathtt{B}} + \mathcal{S}_{\mathtt{B}\cup\mathtt{C}} \tag{3.52}$$

$$\mathcal{S}_{\mathtt{A}} + \mathcal{S}_{\mathtt{C}} \leq \mathcal{S}_{\mathtt{A}\cup\mathtt{B}} + \mathcal{S}_{\mathtt{B}\cup\mathtt{C}}. \tag{3.53}$$

These relations imply the following, clearer, properties:

Subadditivity: the entropy of parts sum to at least the entropy of the whole system $\mathtt{A} \cup \mathtt{B}$.

Triangle inequality: the entropy of the full system is at least the difference of the entropies of its parts.

We can conjoin these features in the expression

$$|\mathcal{S}_{\mathtt{A}} - \mathcal{S}_{\mathtt{B}}| \leq \mathcal{S}_{\mathtt{A}\cup\mathtt{B}} \leq \mathcal{S}_{\mathtt{A}} + \mathcal{S}_{\mathtt{B}}. \tag{3.54}$$

The last feature deserves a status of theorem, and next will follow a proof It plays an important role in the subject matter, and we name it accordingly.

Theorem 1. Let ϱ be a pure state of a Hilbert space split into $\mathbf{H}_{\mathtt{A}} \otimes \mathbf{H}_{\mathtt{A}^{\complement}}$. The entanglement entropy of the parts are equal,

$$\mathcal{S}_{\mathtt{A}^{\complement}} = \mathcal{S}_{\mathtt{A}}, \tag{3.55}$$

given that $\mathtt{A}^{\complement}$ is the complement of the set defining the subsystem $\mathbf{H}_{\mathtt{A}}$.

Proof. Let the vector associated to the state be

$$|\psi\rangle = \sum_{\alpha=1}^{d_{\mathtt{A}}} \sum_{\beta=1}^{d_{\mathtt{A}}^{\complement}} C_{\alpha\beta} \, |\alpha\rangle \, |\beta\rangle \, , \tag{3.56}$$

and write the vector space dimensions of $\mathbf{H}_{\mathtt{A}}$ and $\mathbf{H}_{\mathtt{A}^{\complement}}$ as $d_{\mathtt{A}}$ and $d_{\mathtt{A}}^{\complement}$, respectively.

Now, under a singular value decomposition $C = U\sqrt{P}V^{\dagger}$, $|\psi\rangle$ is written as

$$|\psi\rangle = \sum_{\alpha,\beta} \sum_{i=1}^{d_{\mathtt{A}}} \sum_{j=1}^{d_{\mathtt{A}}^{\complement}} \sqrt{p_i} U_{\alpha i} \, |\alpha\rangle \, \delta_{ij} {V^{\dagger}}_{j\beta} \, |\beta\rangle \, . \tag{3.57}$$

We can define the transformed vectors $|i\rangle = \sum_{\alpha} U_{\alpha i} \, |\alpha\rangle$ and $|j\rangle = \sum_{\beta} {V^{\dagger}}_{j\beta} \, |\beta\rangle$, and thus write the state as

$$\varrho = \sum_{i,j} \sum_{i',j'} \sqrt{p_i}\sqrt{p_{i'}} \delta_{ij}\delta_{i'j'} \, |ij\rangle\langle i'j'| \, . \tag{3.58}$$

The last step is to compare $\mathrm{tr}_{\mathtt{A}} \, \varrho$ with $\mathrm{tr}_{\mathtt{A}^{\complement}} \, \varrho$. These are

$$\begin{aligned} \mathrm{tr}_{\mathtt{A}} \, \varrho &= \sum_{\substack{i,j \\ i',j'}} \sqrt{p_i p_{i'}} \delta_{ij}\delta_{i'j'} \Bigg(\sum_{\alpha} \underbrace{\langle\alpha| \, |i\rangle\langle i'| \, |\alpha\rangle}_{\delta_{\alpha i}\delta_{\alpha i'}} \Bigg) \otimes |j\rangle\langle j'| \\ &= \sum_{ii'} \sqrt{p_i p_{i'}} \delta_{ii'} \, |i\rangle\langle i'| \\ &= \sum_{i} p_i \, |i\rangle\langle i| \, ; \end{aligned} \tag{3.59}$$

and similarly

$$\begin{aligned}\mathrm{tr}_{\mathtt{AC}}\,\varrho &= \sum_{\substack{i,j\\ i',j'}} \sqrt{p_i p_{i'}}\delta_{ij}\delta_{i'j'}\,|i\rangle\langle i'|\otimes\left(\sum_{\beta}\langle\beta|\,|j\rangle\langle j'|\,|\beta\rangle\right)\\ &= \sum_{jj'}\sqrt{p_j p_{j'}}\delta_{jj'}\,|j\rangle\langle j'|\\ &= \sum_{j} p_j\,|j\rangle\langle j|\,.\end{aligned} \tag{3.60}$$

Up to the dummy indices, the reduced states are equal, hence rendering the entropies equal as well. □

When treating quantum fields more details will be introduced, in particular because of the presence of infinitely many degrees of freedom. These details include states of the thermal variety appearing in the study of spatial degrees of freedom, made relevant when gravity is added to the quantum system.

Chapter 4

Field theory

In this section we will treat quantised theories of fields on curved spacetimes. We are interested in a system of matter or radiation fields and spacetime, and many of the concepts of the previous sections will have a part in the following constructions.

In the studies here carried, the metric tensor field will not be itself quantised nor it will interact dynamically with the other fields, i.e. there will be no consideration of back-reactions on the metric by the dynamics of other fields. With this we mean the metric constitutes a mere background where the physics of the universe occurs. This is in contradiction to the spirit of general relativity, but approaches of semiclassical gravity such as this one must content with being incomplete whilst investigative in nature, hoping to give the next step for a complete quantum description of gravitation. Mathematically, we are essentially studying quantum fields on Lorentzian differentiable manifolds.

This chapter is dedicated to introducing tools for the study of quantum field theories. The first section brings the concepts behind classical mechanics of fields; on the next subsection, the idea of *quantisation* will be elaborated upon. More detailed analyses will follow when treating specific problems, they will come alongside definitions built on top of the ones supplied here. The topics of quantum field theory in general, and in curved spacetime are based on refs. [42, 43, 44, 45, 46]. Discussions of symplectic geometry, quantisation was based on refs. [47, 37].

4.1 Classical field dynamics

A theory is defined once an *action functional* $\mathcal{I}$ is given. This surmounts to give $\mathcal{I}$ with the following form:

$$\mathcal{I}[g_{\mu\nu}, \Phi_{\mathrm{s}}] = \int_{\mathbb{M}} \mathrm{d}x^0\, \mathrm{d}x^1\, \mathrm{d}x^2\, \mathrm{d}x^3\, \mathcal{L}(g_{\mu\nu}, \Phi_{\mathrm{s}}, \nabla\Phi_{\mathrm{s}}). \tag{4.1}$$

The Lagrangian density $\mathcal{L}$ is the component of a volume-form on the four-dimensional spacetime manifold $\mathbb{M}$, and is expressed in terms of the set of dynamical field species[1] Φ_{s}, their derivatives, and the metric tensor field $g_{\mu\nu}$. One could be more general by including higher order derivatives, and product of fields at different events e of spacetime, such as $\Phi(\mathsf{e})\Phi(\mathsf{e}')$, but we are mainly interested in actions as the one here presented; this is a way of establishing that the dynamics are local, depending on the fields at single event, i.e. the dynamics at e will not be affected by phenomena happening at e', unless it is in a neighbourhood of e.

In the Lagrangian formalism the action is sufficient to determine the evolution of a system through the equations of motion. By taking the functional variation $\delta\mathcal{I}$ we are lead to the Euler–Lagrange equations, and by solving them we understand the classical dynamics of the theory. That is to say, given a particular field of interest,

$$\Phi\colon \mathbb{M} \to \mathbb{V} \tag{4.2}$$

defines it as a map from the spacetime manifold to a target space $\mathbb{V}$ describing its values. A concrete example is to take Φ to be a real scalar field,

$$\begin{aligned} \Phi\colon \mathbb{M} &\to \mathbb{R} \\ \mathsf{e} &\mapsto \Phi(\mathsf{e}). \end{aligned} \tag{4.3}$$

We assume $\mathbb{M}$ to be globally hyperbolic and foliated into spacelike submanifolds $\mathbb{D}$, under conditions elaborated in section 2.2. The field at fixed x^0 forms the infinite-dimensional configuration space $\mathbf{C}$ of the theory. For example, $\mathbf{C} \cong \mathbf{C}^\infty(\mathbb{D};\mathbb{R})$: the space of real-valued smooth functions on the spatial section $\mathbb{D}$. We will denote these points with the fixed time as subscripts, e.g. $\Phi_t(x^i) \equiv \Phi(x^\mu)\big|_{x^0=t}$.

In addition to this, trajectories in $\mathbf{C}$ denote the dynamical evolution of the field between two arbitrary configurations. We call these curves *field histories*, and they are the proper functions Φ, as depicted in fig. 4.1 by paths. This means that the action is a real-valued functional with domain in the space of field histories, for instance $\mathbf{C}^\infty(\mathbb{M};\mathbb{R})$ such that $\mathcal{I}\colon \mathbf{C}^\infty(\mathbb{M}) \to \mathbb{R}$. The space of field histories does not contain only configuration obeying the equations of motion. The contribution of configurations which do not obey the Euler–Lagrange equations makes an important appearance when one tries to quantise a theory using the path integral.

The behaviour of the system is encoded in the explicit form of the Lagrangian, and one bases quantum field theory on its construction. To guide this task the symmetries of the universe are taken into account; they may pertain to spacetime, whose conserved current densities assigned through Noether's theorem can be energy, linear or angular momenta, or pertain to internal redundancies, with associated

[1] E.g. $\Phi_{(1)} \equiv$ scalar field, $\Phi_{(2)} \equiv A_\mu$, etc. We shall omit this index unless the expression allows for sufficient generality.

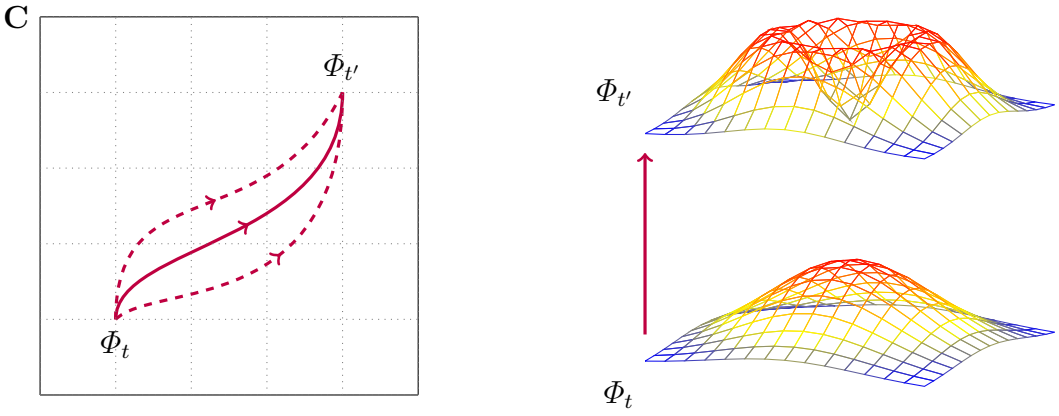

Figure 4.1: Examples of field histories, of which the central trajectory is a solution to the equations of motion. Φ and Φ' denote different field configurations at times $t' > t$, as illustrated to the right.

electric, colour and other charges. The Lagrangian must be built such as to be invariant under the action of operators in the symmetry groups.

The Euler-Lagrange equations originating from $\delta\mathcal{I} = 0$ are

$$\frac{\partial\mathcal{L}}{\partial\Phi_{\mathrm{s}}} - \partial_\mu \frac{\partial\mathcal{L}}{\partial(\partial_\mu\Phi_{\mathrm{s}})} = 0, \tag{4.4}$$

valid for any type of field, whether it is a scalar, a spinor or vector with internal degrees of freedom. The solutions determine classically allowed physical histories.

Example 7. Let the universe be a flat spacetime, with metric

$$\mathrm{d}s^2 = \mathrm{d}t^2 - \mathrm{d}\mathbf{x}^2, \tag{4.5}$$

populated by a free, massless scalar field Φ. Its Poincaré-invariant Lagrangian is

$$\mathcal{L} = \frac{1}{2}\partial_\mu\Phi\partial^\mu\Phi, \tag{4.6}$$

leading to the wave equation

$$\partial_\mu\partial^\mu\Phi = 0 \tag{4.7}$$

as its equation of motion.

The space of solutions of the Euler–Lagrange equations, **Sol**, is a vector space in the cases that will be studied in this text. This property will follow from the

linearity of eq. (4.4), allowing linear combinations of solutions to be elements of **Sol** as well. To work with quantum mechanics it will be useful to allow for complex functions, a property that does not present difficulties when working with $\mathbb{R}$-valued fields as long as we impose $\overline{\Phi}_{\mathrm{s}} = \Phi_{\mathrm{s}}$, setting constraints on the possible spectrum of particles arising from field excitations.

By introducing the space of solutions as a vector space, it is natural and it will be helpful to find a convenient orthonormal basis of functions satisfying eq. (4.4); to attain this goal one needs to provide an inner product. Complexification will play a role in interpreting the formalism, and we take this opportunity to split **Sol** into the direct sum $\mathbf{S}^+ \oplus \mathbf{S}^-$, with the quantum theory in mind, as follows:

Definition 10. Let $\langle \_, \_ \rangle \colon \mathbf{Sol} \times \mathbf{Sol} \to \mathbb{R}$ be a nondegenerate Hermitian form and $\{f_\lambda\}$ be an orthonormal basis with respect to it. The space of solutions is split into $\mathbf{Sol} = \mathbf{S}^+ \oplus \mathbf{S}^-$ according to the following: suppose f_λ and $f_{\lambda'}$ belong to $\mathbf{S}^+$, then

$$\langle f_\lambda, f_{\lambda'} \rangle = \delta(\lambda, \lambda') \tag{4.8a}$$

$$\implies \langle \overline{f_\lambda}, \overline{f_{\lambda'}} \rangle = -\delta(\lambda', \lambda) \qquad \implies \overline{f_\lambda}, \overline{f_{\lambda'}} \in \mathbf{S}^-. \tag{4.8b}$$

That is, complex conjugation maps $\mathbf{S}^+ \to \mathbf{S}^- \colon f_\lambda \mapsto \overline{f_\lambda}$. This Hermitian form is a positive-definite inner product on $\mathbf{S}^+$ and negative-definite on $\mathbf{S}^-$.

In summary, the Lagrangian programme amounts to finding in $\mathbf{C}$ the trajectories minimising eq. (4.1) given initial data, e.g. $\Phi(x^\mu)\big|_{x^0=0}$ and $\partial_0 \Phi(x^\mu)\big|_{x^0=0}$. These constructions are in parallel with the Hamiltonian formalism, necessary to the canonical approach to quantisation. Define the Hamiltonian as the Legendre transform of the Lagrangian density,

$$H \equiv \int_{\mathbb{D}} \mathrm{d}\mathbf{vol} \sum_{\text{species}} \partial^0 \Phi_{\mathrm{s}} \Pi_{\mathrm{s}} - \mathcal{L}(g_{\mu\nu}, \Phi_{\mathrm{s}}, \nabla \Phi_{\mathrm{s}}), \tag{4.9}$$

in which Π_{s} is the canonical momentum conjugate to Φ_{s}, equal to[2]

$$\Pi_{\mathrm{s}} = \frac{\partial \mathcal{L}}{\partial(\partial^0 \Phi_{\mathrm{s}})}. \tag{4.10}$$

For instance, in example 7, the Lagrangian for a free, massless scalar field yields $\Pi = \partial_0 \Phi$. Recall that $g_{\mu\nu}$ is not considered here a dynamical variable, so there is

[2]Due to the definition as a Legendre transform of $\mathcal{L}$ with respect to $\partial^0 \Phi$.

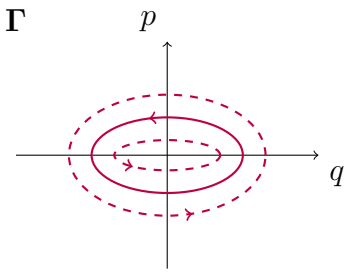

Figure 4.2: Phase space for one Newtonian particle moving in one-dimensional euclidean space under a harmonic potential, $H = p^2/2m + m\omega^2 q^2/2$. Ellipses are level sets of the Hamiltonian in $\mathbf{\Gamma}$, and dynamical evolution thus defines flows in it given by the arrows. The fact that $\mathbf{\Gamma}$ is two-dimensional implies one-dimensional level sets, hence their equivalence with the one-dimensional flows.

no reason in assigning a conjugate momentum to it. We shall not take into account the configuration space of the metric.

Phase space is the cotangent bundle to $\mathbf{C}$, with (canonical) coordinates (Φ_t, Π_t) and, as such, it is a vector space with symplectic structure. Evolution of the physical system are curves in this space (constrained to the level sets of H due to conservation of energy). A notable interest in the Hamiltonian arises with quantum mechanics in mind. In this context it is useful to introduce the concept of observables: functions with domain in $\mathbf{\Gamma}$.

This framework for mechanics can be cast for fields of any species, given their own intricacies. From this point onwards, in this essay, we shall restrict attention to the case of a *real scalar field*, that we denote as Φ, and its conjugate field momentum Π.

The quantisation procedure requires one to equip the space of functions of $\mathbf{\Gamma}$ with a product, realising the classical algebra of observables. In order to do so, we introduce the symplectic structure of $\mathbf{\Gamma}$ and the inherited symplectic structure of its dual space, $\mathbf{\Gamma}^*$.

Definition 11. The *symplectic structure* on a vector space $\mathbf{\Gamma}$ is a bilinear map[3]

$$\begin{array}{rccc} \Omega\colon & \mathbf{\Gamma}\times\mathbf{\Gamma} & \to & \mathbb{R} \\ & \left(\Xi, \widetilde{\Xi}\right) & \mapsto & \Omega_{\mathsf{ab}}\Xi^{\mathsf{a}}\widetilde{\Xi}^{\mathsf{b}}, \end{array} \tag{4.11}$$

which is also

1. Nondegenerate: $\forall\Xi$, $\exists\widetilde{\Xi}\colon \Omega_{\mathsf{ab}}\Xi^{\mathsf{a}}\widetilde{\Xi}^{\mathsf{b}} \neq 0$.

[3]Symplectic indices will be sans-serif Latin letters.

2. Antisymmetric: $\Omega_{\mathsf{ab}}\Xi^{\mathsf{a}}\widetilde{\Xi}^{\mathsf{b}} = -\Omega_{\mathsf{ab}}\widetilde{\Xi}^{\mathsf{a}}\Xi^{\mathsf{b}}$.

3. Closed (as a two-form): $\partial_{\mathsf{a}}\Omega_{\mathsf{bc}} + \partial_{\mathsf{b}}\Omega_{\mathsf{ca}} + \partial_{\mathsf{c}}\Omega_{\mathsf{ab}} = 0$.[4]

The second condition implies that Ω_{ab} is a two-form. The first condition implies that Ω_{ab} is invertible. Take its inverse to be Ω^{ab}, such that $\Omega^{\mathsf{ab}}\Omega_{\mathsf{ab}} = \delta^{\mathsf{a}}_{\mathsf{b}}$; this is the symplectic structure acting on $\mathbf{\Gamma}^*$.

The Hamiltonian provides the time-evolution in phase space $\mathbf{\Gamma}$, whose curves are restricted to the level sets of H and are parametrised by the time coordinate of $\mathbb{M}$.

We will denote the space of observables as $\mathbf{C}^\infty(\mathbf{\Gamma})$. An example of an element of this space is the field itself: given the coordinates (Φ, Π), then there is a function $\mathcal{O}$ such that $\mathcal{O}(\Phi, \Pi) = \Phi$; we refer to it just as Φ. The algebra of observables, however, needs the extra structure defined below.

Definition 12. The *Poisson bracket* is a bilinear map[5]

$$\{\_, \_\}\colon \mathbf{C}^\infty(\mathbf{\Gamma}) \times \mathbf{C}^\infty(\mathbf{\Gamma}) \to \mathbf{C}^\infty(\mathbf{\Gamma}), \tag{4.12}$$

whose action on $\mathcal{O} \in \mathbf{C}^\infty(\mathbf{\Gamma})$ is

$$\{\mathcal{O}_1, \mathcal{O}_2\} \equiv \Omega^{\mathsf{ab}}\frac{\partial\mathcal{O}_1}{\partial\Xi^{\mathsf{a}}}\frac{\partial\mathcal{O}_2}{\partial\Xi^{\mathsf{b}}}. \tag{4.13}$$

This bilinear product is the designated product of a Lie algebra on $\mathbf{C}^\infty(\mathbf{\Gamma})$; it also obeys the Jacobi identity, and the product rule in addition to it (configuring a Poisson algebra).

Example 8. In this example we have, in one-dimensional euclidean space, N non-relativistic particles. Then $\mathbf{\Gamma} = (\mathbb{R}^{2N}, \Omega)$ and the position column vector therein is

$$\begin{aligned}\Xi &= \begin{pmatrix}\Xi^1 & \dots & \Xi^n & \dots & \Xi^N & \Xi^{N+1} & \dots & \Xi^{N+n} & \dots & \Xi^{2N}\end{pmatrix}^{\mathsf{T}} \\ &= \begin{pmatrix}q_1 & \dots & q_N & p_1 & \dots & \dots & \dots & p_N\end{pmatrix}^{\mathsf{T}};\end{aligned} \tag{4.14}$$

notice how the index a runs from 1 to $2N$ by double-counting the particle number n. Let us choose a symplectic structure of the form

$$\Omega = \begin{pmatrix}0 & I_N \\ -I_N & 0\end{pmatrix}, \tag{4.15}$$

[4] For the reader familiar with differential forms, $\mathrm{d}\Omega = 0$.

[5] $\partial_{\mathsf{a}}\mathcal{O}$ are components of the one-form $\mathrm{d}\mathcal{O} = \partial\mathcal{O}/\partial\Phi\ \mathrm{d}\Phi + \partial\mathcal{O}/\partial\Pi\ \mathrm{d}\Pi$.

for I_N the $N \times N$ identity matrix.

Equation (4.13) is, by making explicit the sum over the particle number n, the familiar Poisson brackets of classical mechanics

$$\{\mathcal{O}_1, \mathcal{O}_2\} = \sum_{n=1}^{N} \frac{\partial \mathcal{O}_1}{\partial q_n}\frac{\partial \mathcal{O}_2}{\partial p_n} - \frac{\partial \mathcal{O}_1}{\partial p_n}\frac{\partial \mathcal{O}_2}{\partial q_n}. \tag{4.16}$$

It satisfies the product rule due to the presence of derivatives.

From nondegeneracy of the symplectic form, an analogue of the Riesz theorem (see, for example, refs. [37, 48]) dictates that $\Omega_{\mathsf{ab}}\Xi^{\mathsf{b}} = \xi_{\mathsf{a}} \in \mathbf{\Gamma}^*$ holds for every ξ and Ξ. As a consistency check with definition 12, notice that $\partial_{\mathsf{a}}\mathcal{O}$ is component of a covector ξ.

Example 9. The couple $(\Phi_t(x^i), \Pi_t(x^i))$ is an analogue for an infinite number of components, each pertinent to the field value at a point in space (i.e. spatial coordinates of events serve as an indexing set for the field observables). They are analogous to the $(d+1)$-tuple (x^μ) in spacetime: each entry is a coordinate, and therefore a function of $\mathbf{\Gamma}$ (similarly to $\mathcal{O}$). A continuous version of eq. (4.16) is

$$\{\mathcal{O}_1, \mathcal{O}_2\} = \int_{\mathbb{D}} \mathrm{d}\mathbf{vol}_x \int_{\mathbb{D}} \mathrm{d}\mathbf{vol}_y \, \Omega^{\mathsf{ab}}(x^i, y^i) \frac{\partial \mathcal{O}_1}{\partial \Xi^{\mathsf{a}}(x^i)} \frac{\partial \mathcal{O}_2}{\partial \Xi^{\mathsf{b}}(y^i)}. \tag{4.17}$$

We leave the symplectic form unspecified.

Notice that the role the indices a and b play in this equation is different from what we had in example 8. In symplectic geometry one has two types of coordinates, differing by a minus sign; here, a and b pick one of these types and, therefore, only admits the values 1 and 2.

The Hamiltonian approach is a rich environment for the study of dynamics. One can see this from the freedom there exists on defining the canonical coordinates: in the instances studied above, both the particle number and space points played the role of indexing sets of phase space coordinates.

Poisson brackets supplies a substitute to the Euler–Lagrange equations. The time evolution of observables can be cast as

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \{\mathcal{O}, H\}. \tag{4.18}$$

It reduces to the familiar Hamilton's equations when applied to Φ and Π.

Supplying the framework with *canonical brackets* thus reduce all information about the system to three relations. These are the same-time ($x^0 = y^0 = t$) canonical brackets

$$\{\Phi_t(x^i), \Pi_t(y^i)\} = \delta(x^i - y^i), \tag{4.19}$$
$$\{\Phi_t(x^i), \Phi_t(y^i)\} = 0, \tag{4.20}$$
$$\{\Pi_t(x^i), \Pi_t(y^i)\} = 0. \tag{4.21}$$

If fields of any two different species are present, the bracket operation yields zero. This reflects the fact that observables are functions of (Φ_t, Π_t) at any given time and, being such, the dynamics are determined by knowing how these evolve and interrelate.

The canonical brackets stated above is a choice of symplectic form. Spelling out in phase space coordinates, it is

$$\begin{aligned}\{\Xi^{\mathsf{a}}(x^i), \Xi^{\mathsf{b}}(y^i)\} &= \int_{\mathbb{D}} \mathrm{d}\mathbf{vol}_{\tilde{x}} \int_{\mathbb{D}} \mathrm{d}\mathbf{vol}_{\tilde{y}}\, \Omega^{\mathsf{ab}}(\tilde{x}^i, \tilde{y}^i) \frac{\partial \Xi^{\mathsf{a}}(x^i)}{\partial \Xi^c(\tilde{x}^i)} \frac{\partial \Xi^{\mathsf{b}}(y^i)}{\partial \Xi^d(\tilde{y}^i)} \\ &= \int_{\mathbb{D}} \mathrm{d}\mathbf{vol}_{\tilde{x}} \int_{\mathbb{D}} \mathrm{d}\mathbf{vol}_{\tilde{y}}\, \Omega^{\mathsf{ab}}(\tilde{x}^i, \tilde{y}^i) \delta^{\mathsf{a}}_{\mathsf{c}} \delta(x^i - \tilde{x}^i) \delta^{\mathsf{b}}_{\mathsf{c}} \delta(y^i - \tilde{y}^i) \\ &= \Omega^{\mathsf{ab}}(x^i, y^i),\end{aligned} \tag{4.22}$$

from which it follows that $\Omega^{12}(x^i, y^i) = \delta(x^i - y^i)$ for eq. (4.19). The diagonal components are $\Omega^{11} = \Omega^{22} = 0$, and the remaining off-diagonal gives

$$\begin{aligned}\{\Pi_t(y^i), \Phi_t(x^i)\} &= \Omega^{21}(y^i, x^i) \\ &= -\delta(x^i - y^i).\end{aligned} \tag{4.23}$$

Mathematically, these observables span the vector space underlying the Poisson algebra, in the sense that we consider other observables $\mathcal{O}$ arising from linear combinations of Φ and Π. Each monomial in the field and its conjugate momentum is an element of the basis, but it is enough to know the behaviour of the linear one. Upon necessity bracket operations with higher-order polynomials can be found by using the product rule. Nonetheless, eqs. (4.19) to (4.21) close a infinite-dimensional analogue to the Heisenberg algebra $\mathfrak{h}$ if one includes the brackets of field and conjugate momentum with the function which is identically 1 on $\mathbf{\Gamma}$: $\{\Phi, 1\} = 0$ and $\{\Pi, 1\} = 0$. The most general element of $\mathfrak{h}$ is $\mathcal{O}(\Xi) = c + c_{\mathsf{a}}\Xi^{\mathsf{a}}$, for some constants c and c_{a}.

The mathematical approach of quantum mechanics is an extension of this abstract reasoning of physics, with the energy in the form of the Hamiltonian playing a central role. Despite this necessity, one remains interested in Lagrangian mechanics because it is a treatment better suited for relativistic systems, after all

the Lagrangian $\mathcal{L}$ is invariant under symmetry transformations, something that the energy fails to be, by virtue of the fact that it is merely a component of a tensor, whilst $\mathcal{L}$ is a true scalar.

The interplay of quantum and relativistic phenomena seems to demand a connection between both treatments. By coming across this necessity, we find ourselves selecting Cauchy data as the set of boundary conditions, for it will allow us to go back and forth between the formalisms reducing one's work to solving the Euler–Lagrange equations. This paves the way for quantisation, as it will be presented in the following section.

As guaranteed by the uniqueness (and existence) of solutions to Hamilton's equations, the pair of initial-value functions $\Phi\big|_{x^0}$ and $(\partial^0\Phi)\big|_{x^0}$ provided as Cauchy conditions is in one-to-one correspondence with a full solution in **Sol**. Notice as well how $\partial_0\Phi$ is what defines, in eq. (4.10), the canonical momentum conjugate to $\Phi_t(x^i)$ (cf. example 7); by taking the time derivative of a solution, and later fixing its time coordinate, one has the coordinate $\Pi_t(x^i)$ of $\mathbf{\Gamma}$. We shall choose smooth functions with compact support as initial conditions, $\mathbf{\Gamma} \cong \mathbf{C}^\infty_c(\mathbb{D})$, and **Sol** follows as the solutions to Euler–Lagrange generated from these functions by time-evolution.

It turns out that Cauchy data is a choice of point in phase space, as

$$\mathbf{Sol} \ni \Phi(x^\mu) \iff \begin{pmatrix} \Phi_t(x^i) \\ \Pi_t(x^i) \end{pmatrix} \in \mathbf{\Gamma}. \tag{4.24}$$

Finally, because **Sol** was taken to be a space of complex solutions, the phase space shall also be complexified: $\mathbf{\Gamma}_\mathbb{C} \equiv \mathbf{\Gamma} \otimes \mathbb{C}$. We will elaborate on this in section 6.1.

This statement relies on the fact that our spacetime is globally hyperbolic, as studied in section 2.2. The Cauchy surfaces slicing $\mathbb{M}$ provides the stage on which to define the initial conditions, and the global hyperbolicity dictates that the solutions found are valid throughout spacetime. The time coordinate that has been central to the present discussion is that defined with respect to the slicing, where ∂_0 is the vector field on $\mathbb{M}$, perpendicular to the $\mathbb{D}$ hypersurfaces, parametrised by t.

At hands with the methods of quantisation, one is able to treat the quantum theory of fields; amidst developments in next section, we will outline steps to this end. As a start, we can prescribe a relation of the inner product on **Sol** with the symplectic form Ω_{ab} on $\mathbf{\Gamma}_\mathbb{C}$, as follows.

Definition 13. Let f_1^{a} and f_2^{b} be the coordinates in phase space associated to solutions $f_1, f_2 \in \mathbf{Sol}$. We choose the Hermitian form to be

$$\langle f_1, f_2 \rangle \equiv \mathrm{i} \int_\mathbb{D} \mathrm{d}\mathbf{vol}_x \int_\mathbb{D} \mathrm{d}\mathbf{vol}_y \, \Omega_{\mathsf{ab}}(x^i, y^i) \overline{f_1}^{\mathsf{a}}(x^i) f_2^{\mathsf{b}}(y^i), \tag{4.25}$$

for Ω antisymmetric under exchange of composite indices ${}_{\mathsf{a}}(x^i) \longleftrightarrow {}_{\mathsf{b}}(y^i)$.

The components f_1^{a} of a solution are $f_1^1 = f_1\big|_{x^0=t} = \Phi_t$ and, based on the discussion above we know that $\Pi = \partial^0\Phi$, thus having $f_1^2 = (\partial_0 f_1)\big|_{x^0=t} = \Pi_t$. Let $\Omega_{\mathsf{ab}}(x^i, y^i) = \delta_{\mathsf{ab}}\delta(x^i - y^i) = -\Omega_{\mathsf{ba}}(y^i, x^i)$ be fixed as a component of the symplectic form, we use this to implement eq. (4.25) as

$$\langle f_1, f_2\rangle = \mathrm{i}\int_{\mathbb{D}} \mathrm{d}\mathbf{vol}\, \overline{f_1}\,(\partial_0 f_2) - \left(\overline{\partial_0 f_1}\right) f_2. \tag{4.26}$$

The splitting of **Sol** into $\mathbf{S}^+ \oplus \mathbf{S}^-$ in definition 10 is only possible because we recognise the isomorphism $\mathbf{Sol} \cong \mathbf{\Gamma}_{\mathbb{C}}$ and then exploit the symplectic structure of phase space.

4.2 Canonical quantisation

The defining inputs of a quantum theory are Hilbert spaces and an operator algebra, the Hamiltonian operator within being a special element. The observables introduced in the previous sections are no longer functions with definite values at points in the phase space but operators acting on Hilbert spaces, a change of perspective capturing the nature of quantum physics. We first study the notion of observables, and then proceed to make sense of physical states and systems.

Quantisation is an *attempt*[6] at constructing a representation of the algebra of functions on phase space. For a Hilbert space $\mathbf{H}$, chosen so as to comply with axiom 1, the representatives of the algebra are operators mapping $\mathbf{H} \to \mathbf{H}$. Thus, we have

$$\begin{array}{ccc} \text{Algebra on } \mathbf{C}^\infty(\mathbf{\Gamma}) & & \text{Algebra on } \mathrm{LinOp}(\mathbf{H}) \\ & \xmapsto{\text{quantisation}} & \\ \text{with } \{\_,\_\} & & \text{with } \mathrm{i}[\_,\_]. \end{array} \tag{4.27}$$

As an algebra representation, they should preserve the product relations, i.e. functions satisfying $\{\mathcal{O}_1, \mathcal{O}_2\} = \mathcal{O}_3$ are represented as operators satisfying $[\mathcal{O}_1, \mathcal{O}_2] = \mathcal{O}_3$ uniquely, and that $-\mathrm{i}I$ acting on $\mathbf{H}$ represents the unit constant function on $\mathbf{\Gamma}$.[7]

[6] An attempt because it is not fully realised. Later on we will mention problems with the formalism.

[7] We will omit I from the end of this section onwards.

In particular, the coordinates of phase space (or functions thereof) are represented by operators on $\mathbf{H}$, rendering the fields themselves as operator-valued distributions

$$\Phi\colon \mathbf{X}(\mathbb{M}) \to \mathrm{LinOp}(\mathbf{H}), \tag{4.28}$$

from the suitable space of functions on spacetime, $\mathbf{X}(\mathbb{M})$.

Any relationship the functions in $\mathbf{C}^\infty(\mathbf{\Gamma})$ had, prior to the representation, must be preserved by corresponding relations in $\mathrm{LinOp}(\mathbf{H})$. Quantisation is then required to imply

$$\big[\Phi_t\big(x^i\big), \Pi_t\big(y^i\big)\big] = \mathrm{i}\delta\big(x^i - y^i\big)I, \tag{4.29a}$$
$$\big[\Phi_t\big(x^i\big), \Phi_t\big(y^i\big)\big] = 0, \tag{4.29b}$$
$$\big[\Pi_t\big(x^i\big), \Pi_t\big(y^i\big)\big] = 0, \tag{4.29c}$$

given that eqs. (4.19) to (4.21) are satisfied. This is realised by representing the field and conjugate momentum functions as operators $-\mathrm{i}\Phi$ and $-\mathrm{i}\Pi$. One can interpret the above condition as a statement of causality: two measurement operations taking place at points spacelike separated cannot influence each other.

The algebra of operators, $\mathfrak{A}$, is a subset of $\mathrm{LinOp}(\mathbf{H})$ whose elements obey the canonical commutation relations, and whose self-adjoint elements are the observables as laid out in chapter 3. Algebraic quantum field theory is an example of engaging physics with the algebra of observables as the main subject of study. In its treatment of subalgebras associated to localisation of operators in spacetime, one can deduce and prove important implications of the formalism; one of them is the Reeh–Schlieder theorem, demonstrated in section 5.1.1, stating consequences of the entanglement of quantum field vacua. Modern comprehensive reviews of the algebraic formulation of quantum field can be found in refs. [49, 50, 51].

The next step in quantising the field is to make the association between the symplectic structure and the splitting of the solution space. We will make use of a basis of functions spanning $\mathbf{Sol}$, and the direct sum $\mathbf{S}^+ \oplus \mathbf{S}^-$, as laid out in definition 10. Generically, a full solution is a linear combination of the mode basis with mode amplitudes z_λ, as in

$$\Phi(x^\mu) = \int \mathrm{d}\mu_\lambda \left(z_\lambda f_\lambda(x^\mu) + \overline{z_\lambda}\,\overline{f_\lambda}(x^\mu)\right), \tag{4.30}$$

for the same measure $\mathrm{d}\mu_\lambda$ appearing in definition 10.[8] One sees the contribution from $\mathbf{S}^+$ and $\mathbf{S}^-$, whose bases are indexed by the spectrum λ of the differential operator. With the aid of the Hermitian form one could write the mode amplitudes as $z_\lambda = \langle f_\lambda, \Phi\rangle$ and $\overline{z_\lambda} = -\langle \overline{f_\lambda}, \Phi\rangle$.

[8] These details will become more clear when we explicitly solve the equations of motion.

From the discussion in the previous section, we have a vector in phase space associated to this solution, and the mode basis vectors in $\mathbf{\Gamma}_{\mathbb{C}}$, providing new coordinates z and $\overline{z}$ for that same vector. In a finite-dimensional analogy, that would mean

$$\underbrace{\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} u & \overline{u} \\ v & \overline{v} \end{pmatrix} \begin{pmatrix} z \\ \overline{z} \end{pmatrix}}_{\Xi^{\mathsf{a}} = M^{\mathsf{a}}{}_{\mathsf{b}} \Upsilon^{\mathsf{b}}} \tag{4.31}$$

is a change of coordinates, given the change of basis. In this way, u and v (and their conjugates) are the coordinates of the new basis vectors *in the old basis*.

Example 10. Let us return to the example of N particles in a one-dimensional harmonic potential with characteristic frequency ω, and whose complexified phase space is $\mathbf{\Gamma}_{\mathbb{C}} = \mathbb{C}^{2N}$. An explicit, inverse transformation to that of eq. (4.31) is

$$\begin{pmatrix} \vdots \\ z_i \\ \vdots \\ \overline{z}_j \\ \vdots \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} (m\omega)^{1/2} I_N & \mathrm{i}(m\omega)^{-1/2} I_N \\ (m\omega)^{1/2} I_N & -\mathrm{i}(m\omega)^{-1/2} I_N \end{pmatrix} \begin{pmatrix} \vdots \\ q_i \\ \vdots \\ p_j \\ \vdots \end{pmatrix}. \tag{4.32}$$

The Poisson brackets of the mode amplitudes are

$$\begin{aligned} \{z_i, \overline{z}_j\} &= \frac{1}{2} \left((m\omega)\{q_i, q_j\} + (m\omega)^{-1}\{p_i, p_j\} + \mathrm{i}\{p_i, q_j\} - \mathrm{i}\{q_i, p_j\} \right) \\ &= -\frac{\mathrm{i}}{2}(\{p_i, q_j\} + \{p_j, q_i\}) \\ &= -\frac{\mathrm{i}}{2}(\delta_{ij} + \delta_{ji}) \\ &= -\mathrm{i}\delta_{ij}. \end{aligned} \tag{4.33}$$

and $\{z_i, z_j\} = 0 = \{\overline{z}_i, \overline{z}_j\}$.

Upon quantisation, the amplitudes are the parts of eq. (4.30) that turn out to be represented by operators acting on $\mathbf{H}$. To make this step, one recognises coordinates as linear functions on phase space and, hence, observables belonging to $\mathbf{\Gamma}^*_{\mathbb{C}}$; both pairs q and p, z and $\overline{z}$ in the preceding expression. Moreover, these coordinates become bases themselves, dual to the original basis of $\mathbf{\Gamma}_{\mathbb{C}}$, which makes it possible to write elements of the dual space in their own coordinates, i.e.

$$\mathbf{\Gamma}^*_{\mathbb{C}} \ni \underbrace{c_1 q + c_2 p}_{= c_{\mathsf{a}} \Xi^{\mathsf{a}}} = \underbrace{\tilde{c}_1 z + \tilde{c}_2 \overline{z}}_{= \tilde{c}_{\mathsf{a}} \Upsilon^{\mathsf{a}}}. \tag{4.34}$$

This is an element of the Heisenberg algebra mentioned earlier. In fact, the algebra can be written as $\mathfrak{h} = \mathbb{C} \oplus \mathbf{\Gamma}^*_{\mathbb{C}}$, with $\mathbb{C}$ providing the constant function.

We realise the canonical commutation relations by representing z and $\overline{z}$ as operators a and $a^\dagger$ (with adjoint conjugation), and taking advantage of the normalisation of vectors in **Sol** in the continuum case. Whence, through the mode expansion, we set

$$\left[a_\lambda, a^\dagger_{\lambda'}\right] \equiv \langle f_\lambda, f_{\lambda'}\rangle I. \tag{4.35}$$

Which, under normalisation, becomes

$$\left[a_\lambda, a^\dagger_{\lambda'}\right] = \delta(\lambda, \lambda')I, \tag{4.36a}$$

supplemented with

$$[a_\lambda, a_{\lambda'}] = 0, \tag{4.36b}$$

$$\left[a^\dagger_\lambda, a^\dagger_{\lambda'}\right] = 0. \tag{4.36c}$$

One can promptly verify that eqs. (4.36a) to (4.36c) imply eqs. (4.29a) to (4.29c). Finally, the canonical operators are

$$\Phi_t\big(x^i\big) = \int \mathrm{d}\mu_\lambda \left(a_\lambda u_\lambda + a^\dagger_\lambda \overline{u_\lambda}\right) \tag{4.37}$$

$$\Pi_t\big(x^i\big) = \int \mathrm{d}\mu_\lambda \left(a_\lambda v_\lambda + a^\dagger_\lambda \overline{v_\lambda}\right), \tag{4.38}$$

setting $u_\lambda \equiv f_\lambda\big|_{x^0=t}$ and $v_\lambda \equiv (\partial_0 f_\lambda)\big|_{x^0=t}$, as in the finite-dimensional analogue.

The argument taken to arrive at eq. (4.35) covers many necessities of creating a model for quantum fields. The procedure of canonical quantisation is used due to the ease in creating classical and invariant field Lagrangians. One then works with Poisson brackets and Hamiltonians, in order for the algebra quantisation indicated in this section to be achieved. The way out of the conflict between using energy as the main subject for dynamics and preserving relativistic covariance lies on the relation between the symplectic form and the inner product of solutions. Relating the symplectic structure of phase space to the space of solutions of the Euler–Lagrange equations (innately relativistic) there is the inner product in eq. (4.35).

On top of the algebra with commutation relations, and the Hilbert space on which the algebra's operators act, quantum theory requires the distinguished Hamiltonian operator. By starting with the invariant Lagrangian, and therefore constructing both the space of solutions to $\delta\mathcal{I} = 0$ with its inner product, and the Hamiltonian by way of a Legendre transform, axiom 4 guarantees that the

represented quantum observables will obey the same equations as the classical ones. The canonical operators, as they stand in eqs. (4.37) and (4.38), are in the Schrödinger picture and thus time-independent. In order to make connection with the Heisenberg equation, we consider the equivalent version in the Heisenberg picture:

$$\begin{aligned} \Phi(x^\mu) &= U^\dagger(x^0)\Phi_t(x^i)U(x^0) \\ &= \int \mathrm{d}\mu_\lambda \left(a_\lambda f_\lambda(x^\mu) + a_\lambda^\dagger \overline{f_\lambda}(x^\mu)\right) \end{aligned} \tag{4.39}$$

and

$$\begin{aligned} \Pi(x^\mu) &= U^\dagger(x^0)\Pi_t(x^i)U(x^0) \\ &= \int \mathrm{d}\mu_\lambda \left(a_\lambda \partial_0 f_\lambda(x^\mu) + a_\lambda^\dagger \overline{\partial_0 f_\lambda}(x^\mu)\right), \end{aligned} \tag{4.40}$$

wherein $U(x^0) = \mathrm{e}^{-\mathrm{i}Hx^0}$ is the operator of time translations. The covariance thus persists to the quantum model in such a way that eq. (4.18) is replaced by eq. (3.15),

$$\text{Hamilton's} \quad \frac{\partial \mathcal{O}}{\partial t} = \{\mathcal{O}, H\} \longmapsto \text{Heisenberg's} \quad \frac{\partial \mathcal{O}}{\partial t} = -\mathrm{i}[\mathcal{O}, H]. \tag{4.41}$$

See refs. [34, 42] for more details on the initial-value formulation and its relation to quantisation.

Example 11. Consider again the universe of example 7: a flat spacetime populated by a free, massless scalar field; its Hamiltonian is $H = (\Pi^2 + \partial^i\Phi\partial_i\Phi)/2$. The Heisenberg equations for the operator are

$$\frac{\partial \Phi}{\partial t} = -\mathrm{i}[\Phi, H] \tag{4.42}$$

and

$$\frac{\partial \Pi}{\partial t} = -\mathrm{i}[\Pi, H]. \tag{4.43}$$

They can be cast as an Euler–Lagrange equation for operators after we solve the commutators. One finds

$$\frac{\partial \Phi}{\partial t} = \Pi \quad \text{(as expected)}, \tag{4.44}$$

$$\frac{\partial \Pi}{\partial t} = \partial^i\partial_i\Phi. \tag{4.45}$$

Inserting one equation into the other, one concludes

$$\frac{\partial^2 \Phi}{\partial t^2} - \frac{\partial}{\partial x_i}\frac{\partial \Phi}{\partial x^i} = 0, \tag{4.46}$$

the field equation for operators.

The fact that the normal mode expansion explicated here contains amplitudes z related by complex conjugation stems from our choice of working with a real scalar field. The meaning behind this is that there is a single degree of freedom at each point in space, as opposed to the more detailed cases of spinor fields or vector field, bearing internal degrees of freedom such as spin.

4.3 Fock space

We will now construct pure quantum states. These are uniquely determined by rays in a Hilbert space, so in order to do so we need to find that Hilbert space. Restricting our analysis to scalar fields, quantisation reduces to considerations of a symmetry Fock space, whereby bosonic particles of zero spin arise. See ref. [37] for more details.

Recall that the Hermitian form is positive-definite on $\mathbf{S}^+$, hence it defines an inner product on that space. We will take the one-particle Hilbert space of the quantum theory to be the completion of $\mathbf{S}^+$ with respect to the norm induced by $\langle \_ , \_ \rangle$.

Consider the closure of the space of positive frequency solutions, $\underline{\mathbf{S}^+}$ (i.e. insert in the space the limit of every sequence of elements in $\mathbf{S}^+$); completion surmounts in identifying Cauchy sequences $\{v_n\}_{n\in\mathbb{N}}$ in equivalence classes whenever their limits (now inside $\underline{\mathbf{S}^+}$) are equal. The span of these classes and their limits forms the Hilbert space $\mathbf{H}$ of one-particle quantum state.

To complete the step into the quantum theory, we write $|\lambda\rangle$ for the Hilbert space version of the basis elements $f_\lambda \in \mathbf{S}^+$. The quantum mechanical $\langle \_ | \_ \rangle$ inner product is, therefore, the Hermitian form of solutions restricted to positive frequency ones $\langle \_ , \_ \rangle \big|_{\mathbf{S}^+}$ (see ref. [39] for more details).

The full Hilbert space of the quantum theory is bigger. Starting with the just defined Hilbert space, the bosonic *Fock space* over $\mathbf{H}$ is

$$\mathbf{F}_{\mathrm{S}}(\mathbf{H}) \equiv \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathrm{sym}\big(\mathbf{H}^{\otimes n}\big) \tag{4.47}$$

in which $\mathrm{sym}(\mathbf{H}^{\otimes n})$ symmetrises the n^{th} tensor power of $\mathbf{H}$. The vacuum space, $\mathbb{C}$ as a Hilbert space, turns out to define single state because any two vectors related by multiplication by a constant belong to the same ray (cf. chapter 3).

To recover a proper Hilbert space in this construction, one must only consider vectors whose components (vectors in each of the elements of the direct sum) form convergent sequences themselves. It is also important to consider a vector with finitely many nonzero components under the sum, in order to not arrive at problems when treating the tensor product of an infinite number of vectors, at $n \to \infty$.

A general element of $\mathbf{F}_{\mathrm{S}}(\mathbf{H})$ is a linear combination of vectors of the form

$$|\phi\rangle = c_0 \,|0\rangle \oplus c_1 \,|\lambda\rangle \oplus c_2 \,\mathrm{sym}(|\lambda'_{\mathit{1}}\rangle \,|\lambda''_{\mathit{2}}\rangle) \oplus \dots \tag{4.48}$$

for

1. the vacuum state $|0\rangle$ defined as

$$\forall\lambda\colon a_\lambda \,|0\rangle = 0; \tag{4.49}$$

2. the state $|\lambda\rangle$ of a single particle with mode λ;

3. the state of two identical bosonic particles $\mathrm{sym}(|\lambda'_{\mathit{1}}\rangle \,|\lambda''_{\mathit{2}}\rangle) \in \mathrm{sym}(\mathbf{H}^{\otimes 2})$ such that

$$\mathrm{sym}(|\lambda'_{\mathit{1}}\rangle \,|\lambda''_{\mathit{2}}\rangle) \equiv \frac{1}{2}\left(|\lambda'_{\mathit{1}}\rangle \,|\lambda''_{\mathit{2}}\rangle + |\lambda''_{\mathit{1}}\rangle \,|\lambda'_{\mathit{2}}\rangle\right), \tag{4.50}$$

   is symmetric under exchange of modes $\lambda' \leftrightarrow \lambda''$, with *1* and *2* labelling particles and order of entries in the tensor product;

4. the state of n particles, symmetrised as

$$\mathrm{sym}(|\lambda_{\mathit{1}}\rangle \dots |\lambda'_n\rangle) = \frac{1}{n!}\sum_{\varpi} \left|\lambda_{\varpi(\mathit{1})}\right\rangle \dots \left|\lambda'_{\varpi(n)}\right\rangle, \tag{4.51}$$

   wherein ϖ are elements of the permutation group of n elements.

In terms of occupation number, a state with a definite number of total particles, otherwise written as $\mathrm{sym}(|\lambda\rangle \dots |\lambda\rangle \,|\lambda'\rangle \dots |\lambda'\rangle \,|\lambda''\rangle \dots)$, is more succinctly written as $|\, n_\lambda \dots n_{\lambda'} \dots\rangle$, for n_λ particles with mode λ, $n_{\lambda'}$ particles with mode λ', etc., and assuming symmetrisation. One may assume an ordering of the modes, whereby the relative positioning of numbers n indicate the mode. The two particle state exemplified above is $|1_{\lambda'}1_{\lambda''}\rangle$, with 0 particles in every other mode being implied. For $\sum_\lambda n_\lambda < \infty$, $|\, n_\lambda \dots n_{\lambda'} \dots\rangle$ span $\mathbf{F}_{\mathrm{S}}(\mathbf{H})$.

The occupation number states are eigenstates of the number operator for each mode, $\hat{n}_\lambda \equiv a^\dagger_\lambda a_\lambda$. For example,

$$\hat{n}_{\lambda'} \,|1_{\lambda'}1_{\lambda''}\rangle = 1 \,|1_{\lambda'}1_{\lambda''}\rangle, \tag{4.52}$$

but

$$\hat{n}_k \,|1_{\lambda'}1_{\lambda''}\rangle = 0. \tag{4.53}$$

The action of the creation and annihilation operators is to insert states (by taking a tensor product) and to remove states (by taking a inner product), respectively:

$$\begin{aligned} \left(a^\dagger_\lambda\right)^n |n_\lambda \dots n_{\lambda'} \dots\rangle &= \sqrt{\frac{(n_\lambda + n)!}{n_\lambda!}}\,\mathrm{sym}(|\lambda\rangle^{n_\lambda+n} \dots |\lambda'\rangle^{n_{\lambda'}} \dots) \\ (a_\lambda)^n \,|n_\lambda \dots n_{\lambda'} \dots\rangle &= \sqrt{\frac{n_\lambda!}{n!}}\,\langle\lambda|\lambda\rangle^n\,\mathrm{sym}(|\lambda\rangle^{n_\lambda-n} \dots |\lambda'\rangle^{n_{\lambda'}} \dots) \end{aligned} \tag{4.54}$$

This agrees with the annihilation of the vacuum by a_λ, since we are taking an inner product of $|\lambda\rangle$ with the zero vector that populates every order of the direct sum greater than 1.

To achieve normalised states, the action of the ladder operator are accompanied by constants. A general state with nonzero particles is created from the vacuum as

$$|n_\lambda \dots n_{\lambda'}\rangle = \prod_\lambda \frac{\left(a_\lambda^\dagger\right)^{n_\lambda}}{\sqrt{n_\lambda!}} |0\rangle \,. \tag{4.55}$$

And individually, one has

$$\begin{aligned} a_\lambda^\dagger |n_\lambda \dots n_{\lambda'} \dots\rangle &= \sqrt{n_\lambda + 1}\, |(n_\lambda + 1) \dots n_{\lambda'} \dots\rangle \\ a_\lambda |n_\lambda \dots n_{\lambda'} \dots\rangle &= \sqrt{n_\lambda}\, |(n_\lambda - 1) \dots n_{\lambda'} \dots\rangle \,. \end{aligned} \tag{4.56}$$

The global (Fock) vacuum, which will be an important subject in this text, is the product of all mode vacua: $|0\rangle = |000\dots\rangle$.

Remarks on limitations of canonical quantisation

We laid out in these introductory sections a framework for treating quantum fields in the continuum, with their infinite number of degrees of freedom, in a way inspired by an extension of existing methods in the case of finite-dimensional phase space, as in standard quantum mechanics. We now briefly discuss theorems in the theory of quantisation to draw attention to obstructions that already appear in the finite-dimensional case, and that will be avoided throughout the text given the choices of systems that we study.

For physical systems with a finite number (N) of degrees of freedom, i.e. whose phase space is $\mathbf{\Gamma} \cong \mathbb{R}^{2N}$, modelling quantum theories under quantisation is facilitated by the following theorem, which we only enunciate.

Theorem 2 (Stone–von Neumann). Let $\mathbf{\Gamma} = (\mathbb{R}^{2N}, \Omega)$ be the phase space of a classical system. Let $(\mathbf{H}, \mathfrak{A})$ and $(\mathbf{H}', \mathfrak{A}')$ be two irreducible,[9] unitary representations of the classical algebra of observables. Then, as quantisations, they are related by a unitary transformation. That is, there exists a unitary operator mapping vectors in $\mathbf{H}$ to $\mathbf{H}'$ and operators in $\mathfrak{A}$ to $\mathfrak{A}'$, all yielding the same expectation values.

This theorem guarantees that, given such a representation of the classical observables, any different way of constructing quantum observables are equivalent,

[9] An irreducible representation is such that there is no subspace of the chosen representing space, say $\mathbf{H}$, that is invariant under the action of any one representing operator.

given the assumptions are satisfied. For a quantum field in the continuum, on the other hand, one faces the conundrum of interpreting unitarily *inequivalent* representations of the classical algebra of observables, since in this case the Stone–von Neumann theorem does not hold.

The construction above, of the space of quantum pure states, relied on the choice of splitting of the space of solutions into $\mathbf{S}^+$ and $\mathbf{S}^-$, and thus relied on a choice of a basis of solutions. In spacetimes with symmetries, such as the case of stationary spaces (of which flat space is a very particular case) one may pick a set of preferred solutions, enabling a preferred representation as well. Curved spacetimes in general, however, do not provide such a choice, and quantisation is therefore made non-unique in this context.

In the next section we explicit an example of this non-uniqueness in the form of the Unruh effect, and the implications this property of quantum fields have in the interpretation of particles, quantum states and the relation of these to observers.

In addition to this set-back in the procedure of canonical quantisation, a *no-go theorem*, as we now enunciate, impedes a second feature to be realised.

Theorem 3 (Groenewold–van Hove). Let $\mathbf{\Gamma} = (\mathbb{R}^2, \Omega)$ be the phase space of a classical system. There is *no* representation of polynomials $\mathcal{O}$ on $\mathbf{\Gamma}$ as operators acting on $\mathbf{H}$ such that polynomials of degree less than or equal to two is a proper subalgebra.

The choice of a two-dimensional phase space is because, from the structure of the Poisson algebra of functions, there is no obstruction in constructing a representation of polynomials such as $q_1q_2p_3$ (given the phase space $\mathbb{R}^{2\times 3}$ of three particles, for instance), since canonical coordinates of different particles commute, implying that both as functions and as operators $q_1q_2p_3 = q_2p_3q_1$ (see ref. [37] for more details).

4.4 Unruh effect and the notion of particle

In this section we will discussion an important conceptual issue regarding the interplay between the canonical approach to quantum field theory and the arbitrary manifolds of spacetime, following the review [52] and refs. [25, 33, 53].

The problem at hands is that of defining what a *particle* means in physics. In the study of particle physics, this notion is taken for granted and justifiably so: the experiment and phenomenology are studied in a regime wherein the notion of particle is close to being well-defined. The reason for this is that detectors are working in an approximately flat spacetime.

Whilst set in a spacetime which is in general curved, it is always possible to define coordinates in the neighbourhood of a point for which the metric admits flat components, $\mathrm{d}t^2 - \mathrm{d}\boldsymbol{x}^2$, up to second order in the coordinates: the *local inertial frames*.[10]

The laboratories of particle physics rely on this idea. For the scale of the experiment, it is enough to consider $\mathbb{M} = \mathbb{R}^4$ with all its ten symmetries coming along. These symmetries are then crucial for what we mean by particle. The question arises more prominently in the general case of gravity and cosmology, but we will only make explicit the case for flat spacetime, for it already presents the issue that must be made clear in the rest of this text.

Starting from the choice of basis of **Sol**, a choice must be made that is not a priori natural. The basis elements are what constitute the particle states in the construction of the Fock space, the vacuum thereby and the operator annihilating it. All of this is connected to the choice of foliation of spacetime: the creation and annihilation operators were a representation of the field amplitudes with respect to the chosen basis, for a hypersurface of initial conditions.

This suggests that different notions of particle apply to different choices of foliation $\mathbb{D}$ and basis of solutions. The particle content as viewed by an observer is as arbitrary as the choice of coordinates she chooses to describe spacetime. Detecting particles is analogous to experiencing the effect of a fictitious force in a non-inertial frame.

This is illustrated in the Unruh effect. Consider a massless scalar field in flat spacetime. We may expand the classical solutions to the Klein–Gordon equation in plane wave basis. The time coordinate can be taken as the parameter generating the integral curves of the timelike Killing vector ∂_0. The positive and negative frequency solutions are also defined with respect to it,

$$\partial_0 f_k = \frac{\partial}{\partial t} \exp(-\mathrm{i}k_\mu x^\mu) = -\mathrm{i}k_0 \exp(-\mathrm{i}k_\mu x^\mu), \tag{4.57}$$

for the positive frequency solutions $f_k \in \mathbf{S}^+$, and

$$\frac{\partial}{\partial t} \exp(\mathrm{i}k_\mu x^\mu) = \mathrm{i}k_0 \exp(\mathrm{i}k_\mu x^\mu) \tag{4.58}$$

for the negative ones.

We can pick as non-inertial frame one which is under constant proper acceleration. These coordinates are defined such that, at each instant of their proper time τ they correspond to one inertial frame reached from one boost operation with rapidity η.

[10]The non-vanishing nature of second-order contributions to the metric stem from the non-vanishing curvature at the point (the Riemann tensor depends on second derivatives of the metric).

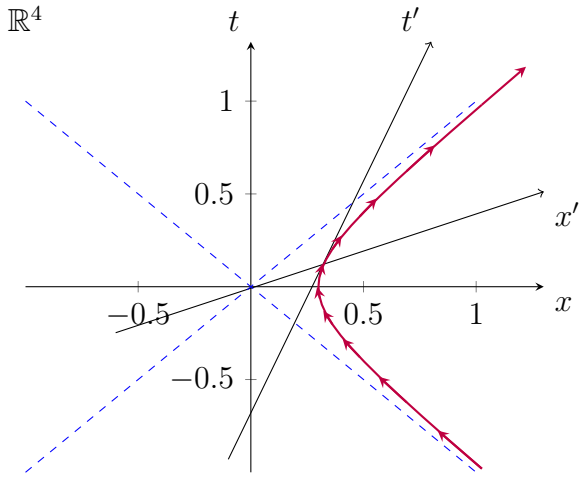

Figure 4.3: The dashed lines represent the light cones of frame (t, x), and the hyperbola to the right is the worldline of the accelerated frame. The primed coordinates are those for the boosted, t- and x-translated frame when its instantaneously moving in the direction of increasing x, asymptotically approximating the speed of light.

Recall example 1. There, η parametrised integral curves of a Killing vector; tangent to the integral curve at a point is a timelike vector of the instantaneous inertial frame. In fig. 4.3 we plot the frame of a hypothetical detector moving along one of these integral curves.

The Killing vector field of boosts to the right of the light cone in fig. 4.3 is everywhere timelike and future directed. Rapidity η then defines the time coordinate of the accelerated frame, for which the boost vector has the form $\partial/\partial\eta$, with a role similar to $\partial/\partial t$.

Because we are using boosts along one of the spatial coordinates, the other two remain unchanged and even decouple in the field equations. Because of this, we will ignore them and work in the two-dimensional problem. With the aid of a new spatial coordinate, the full coordinate transformation to the accelerated frame is $(t, x) \mapsto (\eta, \chi)$ satisfying

$$t = \chi \sinh \eta \tag{4.59}$$

$$x = \chi \cosh \eta, \quad \chi > 0, -\infty < \eta < \infty. \tag{4.60}$$

These coordinates are so chosen in order as to reproduce the worldline of each possible constant accelerated frame, at each possible proper distance χ to the original inertial frame.

Notice, however, that these coordinate only cover the part of spacetime such that $z > |t|$. We can treat that region as a globally hyperbolic spacetime in its own

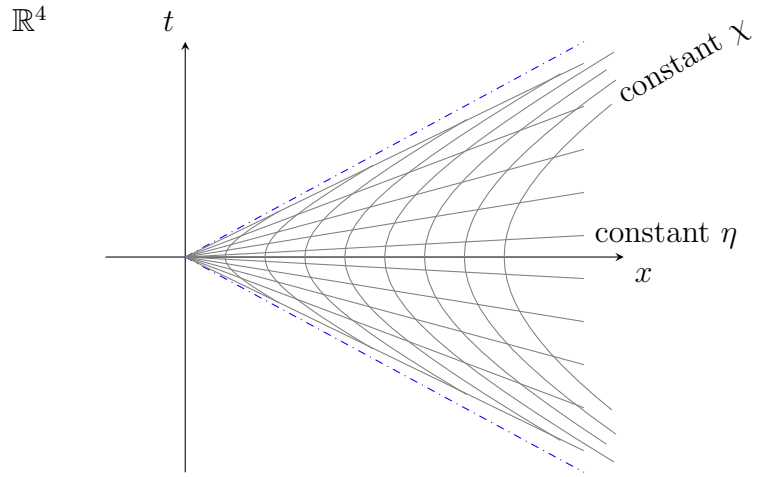

Figure 4.4: To the right one sees the accelerated frame grid, with hyperbolae indicating constant χ surfaces and straight lines indicating constant η surfaces; in fact, the straight lines can be viewed as the positive half of the boosted spatial coordinates whose origin is shared with the inertial frame. To the right one sees the accelerated frame grid, and how much it covers the full flat spacetime.

right, but to relate with the full Minkowski spacetime, we need the other parts. A similar discussion leads to the coordinates for the left-half $z < |t|$,

$$t = -\chi \sinh \eta \tag{4.61}$$
$$x = -\chi \cosh \eta. \tag{4.62}$$

with the subtlety that in the left-half, η runs backwards: as t increases, η decreases (the same intervals of validity for χ and η are taken).

We can slightly rework these coordinates by defining $\chi = \mathrm{e}^{\alpha\zeta}/\alpha$ and $\eta = \alpha\tau$, for α constant. In these terms, α is the acceleration as seen by the inertial observer, and τ works as a proper time for an accelerated observer (which is at rest in the (χ, η) system). The transformation from (t, x) then is

$$t = \frac{\mathrm{e}^{\alpha\zeta}}{\alpha} \sinh(\alpha\tau) \tag{4.63}$$
$$x = \frac{\mathrm{e}^{\alpha\zeta}}{\alpha} \cosh(\alpha\tau), \tag{4.64}$$

for the right-half, constituting the *Rindler coordinates*. The physical interpretation of these coordinates can be seen using the definition of acceleration in relativity: in the inertial system, the accelerated particle has wordline parametrised as above

for a given ζ, e.g. $\zeta = 0$ ($\chi = 1/\alpha$). Its acceleration has components

$$\left(\frac{\mathrm{d}^2 x^\mu}{\mathrm{d}\tau^2}\right) = (\alpha \sinh(\alpha\tau), \alpha\cosh(\alpha\tau), 0, 0), \tag{4.65}$$

of magnitude

$$\sqrt{\frac{\mathrm{d}^2 x^\mu}{\mathrm{d}\tau^2}\frac{\mathrm{d}^2 x_\mu}{\mathrm{d}\tau^2}} = \alpha. \tag{4.66}$$

These two parts are called the *right*, and *left Rindler wedges*. They are causally disconnected, as can be seen from the the fact that the light cone of the inertial system works as a horizon: no lightlike curve that leaves any event in one of the wedges can reach the opposite one (for instance, a photon carrying information).

The metric in Rindler coordinates assumes the form[11]

$$\mathrm{e}^{2\alpha\zeta}(\mathrm{d}\tau^2 - \mathrm{d}\zeta^2), \tag{4.67}$$

and the field equation becomes

$$\left(\frac{\partial^2}{\partial\tau^2} - \frac{\partial^2}{\partial\zeta^2}\right)\Phi = 0, \tag{4.68}$$

exactly the same as the it is in Cartesian coordinates. Using separation of variables, the functional form of the solutions are similar to what we had before,

$$\frac{\partial}{\partial\tau} f_{\mathrm{R}\lambda} = \frac{\partial}{\partial\tau}\mathrm{e}^{\mp\mathrm{i}(\lambda_0\tau - \lambda_1\zeta)} = \mp\mathrm{i}\lambda_0 \mathrm{e}^{\mp\mathrm{i}(\lambda_0\tau-\lambda_1\zeta)}, \tag{4.69}$$

for the positive- and negative-frequency solutions. The same can be found for the left Rindler wedge, although one needs to invert the sign of τ, because $\partial/\partial\eta$ is past-directed there (with respect to the inertial frame). This consideration leads to

$$\frac{\partial}{\partial\tau} f_{\mathrm{L}\lambda} = \frac{\partial}{\partial\tau}\mathrm{e}^{\mp\mathrm{i}(-\lambda_0\tau - \lambda_1\zeta)} = \pm\mathrm{i}\lambda_0 \mathrm{e}^{\mp\mathrm{i}(-\lambda_0\tau-\lambda_1\zeta)} \tag{4.70}$$

as positive- and negative solutions. Let us rename the mode conjugate to time-translation as $\lambda_0 \equiv w_\lambda$, to better distinguish from the others and due to its recurrence in what follows.

From the definition of the coordinates, these solutions only have support in their respective wedge. It follows that we need to consider them both to form a complete basis of **Sol**. The quantised scalar field can then be written either as

$$\begin{aligned}\Phi &= \int \mathrm{d}\mu_k\, a_k f_k + a_k^\dagger \overline{f_k} \quad \text{or as} \\ &= \int \mathrm{d}\mu_\lambda\, b_{\mathrm{R}\lambda} f_{\mathrm{R}\lambda} + b_{\mathrm{R}\lambda}^\dagger \overline{f_{\mathrm{R}\lambda}} + b_{\mathrm{L}\lambda} f_{\mathrm{L}\lambda} + b_{\mathrm{L}\lambda}^\dagger \overline{f_{\mathrm{L}\lambda}},\end{aligned} \tag{4.71}$$

[11] Recall that we are working in the two dimensional case.

such that $a_k \left|0\right\rangle = 0$, $b_{\mathrm{R}\lambda} \left|0_{\mathrm{R}}\right\rangle = 0$, etc.

The quantisation procedure follows for both expansion, each with a their own vacuum state, subject to the discussion in section 4.3. The fact that the Rindler vacuum $\left|0_{\mathrm{R}}\right\rangle$ is intrinsically different from the Minkowski vacuum $\left|0\right\rangle$ is at the heart of the Unruh effect. The disagreement between the particle content seen by observer in different comes from the distinction between b_{R} and b_{L} and a.

The bases can be written as a combination of one another and thus so can the creation and annihilation operators. First, let us choose an inner product with respect to which both bases are orthonormal, referring to the "boost time" Killing vector (i.e. the time derivative in its definition is with respect to τ).

From the mode expansion, we can extract $b_{\mathrm{R}k}$ by taking the inner product of Φ (in either basis) with $f_{\mathrm{R}\lambda}$, $\langle f_{\mathrm{R}\lambda}, \Phi\rangle$. This leads to

$$b_{\mathrm{R}\lambda} = \int \mathrm{d}\mu_k \, \langle f_{\mathrm{R}\lambda}, f_k\rangle a_k + \langle f_{\mathrm{R}\lambda}, \overline{f_k}\rangle a_k^\dagger, \tag{4.72}$$

and similarly for $b_{\mathrm{L}k}$. This is a *Bogoliubov transformation*, a symplectic transformation relating the mode amplitudes in mode basis of phase space.

The generic non-vanishing nature of $\langle f_k, f_{\mathrm{R}\lambda}\rangle$ and $\langle f_k, f_{\mathrm{L}\lambda}\rangle$ already suggests that expressions such as $\langle 0|b_{\mathrm{R}\lambda}^\dagger b_{\mathrm{R}\lambda}|0\rangle$ are also non-vanishing. A second complete basis of functions, due to Unruh, can be defined as

$$h_{\mathrm{I}\lambda} = \frac{1}{\sqrt{2\sinh \pi w_\lambda/\alpha}}(\mathrm{e}^{\pi w_\lambda/2\alpha} f_{\mathrm{R}\lambda} + \mathrm{e}^{-\pi w_\lambda/2\alpha}\overline{f_{\mathrm{L}\lambda}}) \tag{4.73}$$

$$h_{\mathrm{II}\lambda} = \frac{1}{\sqrt{2\sinh \pi w_\lambda/\alpha}}(\mathrm{e}^{\pi w_\lambda/2\alpha} f_{\mathrm{L}\lambda} + \mathrm{e}^{-\pi w_\lambda/2\alpha}\overline{f_{\mathrm{R}\lambda}}), \tag{4.74}$$

and their complex conjugate. It can be shown (see [33]) that they are an analytic continuation of (each) Rindler mode to all of spacetime. We can verify the orthonormality of these modes with respect to the previously used Hermitian form,

$$\begin{aligned}
\langle h_{\mathrm{I}\lambda}, h_{\mathrm{I}\lambda'}\rangle &= \frac{\left(\mathrm{e}^{\pi(w_\lambda+w_{\lambda'})/2\alpha}\langle f_{\mathrm{R}\lambda}, f_{\mathrm{L}\lambda'}\rangle + \mathrm{e}^{-\pi(w_\lambda+w_{\lambda'})/2\alpha}\langle\overline{f_{\mathrm{R}\lambda}}, \overline{f_{\mathrm{L}\lambda'}}\rangle\right)}{2\sqrt{\sinh\left(\frac{\pi w_\lambda}{\alpha}\right)\sinh\left(\frac{\pi w_{\lambda'}}{\alpha}\right)}} \\
&= \frac{\left(\mathrm{e}^{\pi(w_\lambda+w_{\lambda'})/2\alpha}\delta(\lambda,\lambda') - \mathrm{e}^{-\pi(w_\lambda+w_{\lambda'})/2\alpha}\right)}{2\sqrt{\sinh\left(\frac{\pi w_\lambda}{\alpha}\right)\sinh\left(\frac{\pi w_{\lambda'}}{\alpha}\right)}\delta(\lambda,\lambda')} \\
&= \frac{1}{\sinh(\pi w_\lambda/\alpha)}\frac{\left(\mathrm{e}^{\pi w_\lambda/\alpha} - \mathrm{e}^{-\pi w_\lambda/\alpha}\right)}{2}\delta(\lambda,\lambda') \\
&= \delta(\lambda,\lambda').
\end{aligned} \tag{4.75}$$

The orthonormal conditions for the other solutions follow from the same arguments. Given their associated creation and annihilation operators c_{I}, c_{II}, etc., the Rindler annihilation operators can be written as $\langle f_{\mathrm{R}}, \Phi\rangle$ and $\langle f_{\mathrm{L}}, \Phi\rangle$; that is,

$$b_{\mathrm{R}\lambda} = \frac{1}{\sqrt{2\sinh \pi w_\lambda/\alpha}}(\mathrm{e}^{\pi w_\lambda/2\alpha} c_{\mathrm{I}\lambda} + \mathrm{e}^{-\pi w_\lambda/2\alpha} c^\dagger_{\mathrm{II}\lambda}) \tag{4.76}$$

$$b_{\mathrm{L}\lambda} = \frac{1}{\sqrt{2\sinh \pi w_\lambda/\alpha}}(\mathrm{e}^{\pi w_\lambda/2\alpha} c_{\mathrm{II}\lambda} + \mathrm{e}^{-\pi w_\lambda/2\alpha} c^\dagger_{\mathrm{I}\lambda}). \tag{4.77}$$

The advantage of using these modes relies on how they do not mix Minkowski operators, and in fact they also annihilate the Minkowski vacuum: $c_{\mathrm{I}}\,|0\rangle = c_{\mathrm{II}}\,|0\rangle = 0$. The answer to the question of what is the particle content of the Minkowski vacuum seen by an accelerated observer in the right Rindler wedge is $\langle 0|b^\dagger_{\mathrm{R}\lambda} b_{\mathrm{R}\lambda}|0\rangle$, which follows as

$$\begin{aligned}
\langle 0|b^\dagger_{\mathrm{R}\lambda} b_{\mathrm{R}\lambda}|0\rangle &= \frac{\langle 0|\left(\mathrm{e}^{\pi w_\lambda/2\alpha} c^\dagger_{\mathrm{I}\lambda} + \mathrm{e}^{-\pi w_\lambda/2\alpha} c_{\mathrm{II}\lambda}\right)\left(\mathrm{e}^{\pi w_\lambda/2\alpha} c_{\mathrm{I}\lambda} + \mathrm{e}^{-\pi w_\lambda/2\alpha} c^\dagger_{\mathrm{II}\lambda}\right)|0\rangle}{2\sinh \pi w_\lambda/\alpha} \\
&= \frac{1}{2\sinh \pi w_\lambda/\alpha}\,\langle 0|\mathrm{e}^{-\pi w_\lambda/\alpha} c_{\mathrm{II}\lambda} c^\dagger_{\mathrm{II}\lambda}|0\rangle \\
&= \frac{1}{\mathrm{e}^{2\pi w_\lambda/\alpha} - 1},
\end{aligned} \tag{4.78}$$

wherein we have used that $\langle 0|c_{\mathrm{II}\lambda} c^\dagger_{\mathrm{II}\lambda}|0\rangle$ is normalised. The same can found for the left Rindler wedge.

The particle interpretation is thus not trivial even in flat spacetime, when considering non-inertial observers. In curved spacetime that leads to a plethora of possible notions of particles, each one related to the coordinate systems with which we endow the manifold and, moreover, related by inequivalent unitary representations of the algebra of observables, since the Stone–von Neumann fails for infinite degrees of freedom.

At the beginning of this section it is stated that the discussed phenomenon does not severely affect the study of particle physics. That this is true can be seen from the fact that, in the regime of special relativity, the existence of Poincaré symmetry of flat spacetime justifies a choice of *preferred* representation. The special status of inertial frames picks as favourite the particles which have been defined with respect to the associated flow of time, with its causal structure and quantisation. None of this necessarily exist for an arbitrary spacetime. Based on the symmetry argument, one could at least save the particle interpretation of asymptotically stationary spacetimes, for which case although it does not always exist, it can be agreed upon in the asymptotic regions.

The expectation for the occupation number found in eq. (4.78) is that for a thermal distributions of bosons. In what follows we make explicit the relation between thermal states and the Bose–Einstein distribution.

Thermal states

The most general state of a thermal system can be written as

$$\varrho_T = \frac{\mathrm{e}^{-H/T}}{\mathcal{Z}}, \tag{4.79}$$

in which the partition function for the grand canonical ensemble is

$$\mathcal{Z} \equiv \mathrm{tr}\big(\mathrm{e}^{-H/T}\big), \tag{4.80}$$

normalising the state:

$$\mathrm{tr}(\varrho_T) = \frac{\mathrm{tr}\big(\mathrm{e}^{-H/T}\big)}{\mathcal{Z}} = 1. \tag{4.81}$$

This works as an ansatz for the state in one of the Rindler wedges, as it refers to a restriction to the degrees of freedom in that region (due to its causal structure, an accelerated observer only has access to detectors measuring modes in her wedge, modelled after $b_{\mathrm{R}\lambda}^\dagger b_{\mathrm{R}\lambda}$).

The expectation value for a single mode number operator in thermal states is the thermal distribution, Bose–Einstein for our case, or Fermi–Dirac otherwise. That is,

$$\mathrm{tr}(\varrho_T \hat{n}_k) = \frac{1}{\mathcal{Z}} \sum_{n_k} \langle n_k | \mathrm{e}^{-H/T} \hat{n}_k | n_k \rangle \,. \tag{4.82}$$

Because H is diagonalised in the basis of the number operator, we can compute the expected occupation number per mode k, $\mathrm{tr}(\varrho_T n_k) = \langle \hat{n}_k \rangle$, to be

$$\langle \hat{n}_k \rangle = \frac{1}{\mathcal{Z}} \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} \langle n_1 n_2 \ldots n_M | \exp\left(- \sum_{l=0}^{M} \omega_l \hat{n}_l / T \right) \hat{n}_k | n_1 n_2 \ldots n_M \rangle \,, \tag{4.83}$$

wherein the sum is over all the possible occupation number configurations, with $n_{k'}$ ranging from 0 to ∞.

Writing $\{n'_k\}$ for the collection of numbers of particle at each one of the M total modes,

$$\begin{aligned} \langle \hat{n}_k \rangle &= \frac{1}{\mathcal{Z}} \sum_{\{n_{k'}\}}^{\infty} \langle \{n_{k'}\} | \exp\left(- \sum_{l} \omega_l \hat{n}_l / T \right) \hat{n}_k | \{n_{k'}\} \rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{\{n_{k'}\}}^{\infty} \prod_{l} \mathrm{e}^{-\omega_l \hat{n}_l / T} n_k, \end{aligned} \tag{4.84}$$

wherein each number operator finds its eigenvalue in the collection $\{n_{k'}\}$. We can then group the exponentials in the sum over its argument, and find

$$\begin{aligned}
\langle \hat{n}_k \rangle &= \frac{1}{\mathcal{Z}} \left[\prod_{l \neq k} \left(\sum_{n_l} \mathrm{e}^{-\omega_l n_l / T} \right) \right] \sum_k \mathrm{e}^{-\omega_k n_k / T} n_k \\
&= \frac{1}{\mathcal{Z}} \left(\prod_{l \neq k} \frac{1}{1 - \mathrm{e}^{-\omega_l / T}} \right) \frac{\partial}{\partial \frac{\omega_k}{T}} \sum_k \mathrm{e}^{-\omega_k n_k / T} \\
&= \frac{1}{\mathcal{Z}} \left(\prod_{l \neq k} \frac{1}{1 - \mathrm{e}^{-\omega_l / T}} \right) \frac{\partial}{\partial \frac{\omega_k}{T}} \frac{1}{1 - \mathrm{e}^{-\omega_k / T}} \\
&= \frac{1}{\mathcal{Z}} \left(\prod_{l \neq k} \frac{1}{1 - \mathrm{e}^{-\omega_l / T}} \right) \frac{1}{\left(1 - \mathrm{e}^{-\omega_k / T}\right)^2} \mathrm{e}^{-\omega_k / T},
\end{aligned} \tag{4.85}$$

with steps in which the geometric series has been used. To simplify further, we compute the partition function for this system explicit. That is,

$$\begin{aligned}
\mathcal{Z} &= \sum_{\{n_l\}} \mathrm{e}^{-\sum_l \omega_l n_l / T} \\
&= \prod_l \left(\sum_{n_l} \mathrm{e}^{-\omega_l n_l / T} \right) \\
&= \prod_l \frac{1}{1 - \mathrm{e}^{-\omega_l / T}},
\end{aligned} \tag{4.86}$$

which is very similar to one of the previous steps, except that the product runs over all of the modes. Inserting back into the equation for $\langle \hat{n}_k \rangle$ leads to

$$\begin{aligned}
\langle \hat{n}_k \rangle &= \left(\prod_{l'} \frac{1}{1 - \mathrm{e}^{-\omega_{l'} / T}} \right)^{-1} \left(\prod_{l \neq k} \frac{1}{1 - \mathrm{e}^{-\omega_l / T}} \right) \frac{\mathrm{e}^{-\omega_k / T}}{\left(1 - \mathrm{e}^{-\omega_k / T}\right)^2} \\
&= \left(1 - \mathrm{e}^{-\omega_k / T}\right) \frac{\mathrm{e}^{-\omega_k / T}}{\left(1 - \mathrm{e}^{-\omega_k / T}\right)^2} \\
&= \frac{1}{\mathrm{e}^{\omega_k / T} - 1}.
\end{aligned} \tag{4.87}$$

Relating back to w as the energy/frequency associated to the λ modes in one of the Rindler wedges,

$$\langle 0 | b_{\mathrm{R}\lambda}^\dagger b_{\mathrm{R}\lambda} | 0 \rangle \equiv \langle n_{\mathrm{R}\lambda} \rangle = \frac{1}{\mathrm{e}^{2\pi w_\lambda / \alpha} - 1}, \tag{4.88}$$

we find that

$$T = \frac{\alpha}{2\pi}. \tag{4.89}$$

This is the *Unruh effect*. The particle content, found in eq. (4.78), is that for a thermal distribution with the temperature of eq. (4.88). When the inertial observer lies in the global vacuum state of Minkowski spacetime, a detector whose worldline follows the trajectory in fig. 4.3 perceives a thermal bath with temperature proportional to its acceleration.

This is closely related to the Hawking radiation. In contrast with the vacuum seen by a freely falling detector, an observer lying at asymptotic null infinity in a black hole spacetime perceives a thermal bath. To her perspective, the event horizon is a black body with temperature proportional to the surface gravity of the black hole.

What has been shown does not suffices, however, to prove that the state is a thermal state; instead, it was shown that the Bose-Einstein distribution is a necessary condition. That the Minkowski vacuum is indeed a thermal state in the Rindler modes can be shown, and we refer the reader to [52, 33] for the full argument. It can be written as

$$|0\rangle\langle 0| = \frac{1}{\mathrm{e}^{-w_\lambda/T} - 1} \sum_{n_{\mathrm{R}\lambda}} \mathrm{e}^{-n_{\mathrm{R}\lambda} w_\lambda/T} \, |n_{\mathrm{R}\lambda}\rangle\langle n_{\mathrm{R}\lambda}| \,, \tag{4.90}$$

in which $|n_{\mathrm{R}\lambda}\rangle$ are the particle number eigenstates of $b_{\mathrm{R}\lambda}^\dagger b_{\mathrm{R}\lambda}$ (or its left counterpart).

Chapter 5

Vacuum correlations and entanglement entropy in flat spacetime

5.1 Correlations

Quantum correlations in arbitrary spacetimes are given by n-point functions of operators acting on the Hilbert space. Particularly for Gaussian states, the two-point function carries all the information available on the theory, it is then of interest to study such distributions. For a general operator $\mathcal{O}$, covariances are expressed as

$$\langle 0|\mathcal{O}_1\mathcal{O}_2|0\rangle - \langle 0|\mathcal{O}_1|0\rangle \langle 0|\mathcal{O}_2|0\rangle . \tag{5.1}$$

Without loss of generality, one can set the first moments $\langle\mathcal{O}\rangle$ to zero by displacement operations on phase space.

Scalar field two-point correlations can be expressed by the expectation value of Φ on the Fock vacuum of the theory. For arbitrary pure states, the correlator, once chosen a vacuum state, reduces to

$$Q(x^\mu, y^\mu) = \langle 0|\Phi(x^\mu)\Phi(y^\mu)|0\rangle , \tag{5.2}$$

in which the first statistical moment vanishes ($\langle\Phi\rangle = 0$) as can be verified through the normal mode expansion.

By expressing the field in its normal modes expansion, through the creation and annihilation operators, we know how to act on $|0\rangle$ explicitly. Generically, this means

$$\langle 0| \int \mathrm{d}\mu_\lambda \, \mathrm{d}\mu_{\lambda'} \left(a_\lambda f_\lambda(y) + a^\dagger_\lambda \overline{f_\lambda}(y)\right) \left(a_{\lambda'} f_{\lambda'}(x) + a^\dagger_{\lambda'} \overline{f_{\lambda'}}(x)\right) |0\rangle . \tag{5.3}$$

Applying a to the ground state yields 0, meaning that the only non-vanishing coefficient in this expression is proportional to $\int f\overline{f}aa^\dagger\,|0\rangle$. Using the commutation relations to rearrange this term, we get

$$\begin{aligned}\int \mathrm{d}\mu_\lambda\,\mathrm{d}\mu_{\lambda'}\,f_\lambda(y)\overline{f_{\lambda'}}(x)\,\langle 0|a_\lambda a^\dagger_{\lambda'}|0\rangle &= \int \mathrm{d}\mu_\lambda\,\mathrm{d}\mu_{\lambda'}\,f_\lambda(y)\overline{f_{\lambda'}}(x)\left\langle a^\dagger_{\lambda'}a_\lambda + \delta_\mu(\lambda,\lambda')\right\rangle \\ &= \int \mathrm{d}\mu_\lambda\,\mathrm{d}\mu_{\lambda'}\,f_\lambda(y)\overline{f_{\lambda'}}(x)\delta_\mu(\lambda,\lambda').\end{aligned} \tag{5.4}$$

Recall that the definition of the measure signifies

$$\int \mathrm{d}\mu_\lambda\,\delta_\mu(\lambda,\lambda')f(\lambda') = f(\lambda), \tag{5.5}$$

allowing for the integration on λ', which leads to

$$Q(x,y) = \int \mathrm{d}\mu_\lambda\,f_\lambda(y)\overline{f_\lambda}(x). \tag{5.6}$$

As mentioned above, Gaussian states are completely determined by their two-point correlations because of the following theorem.

Theorem 4 (Wick). Let $\mathcal{O}_n$ be either configuration or momentum operators. Then

$$\langle 0|\mathcal{O}_1\mathcal{O}_2\ldots\mathcal{O}_n|0\rangle = \sum_{\varpi}\left\langle\mathcal{O}_{\varpi(1)}\mathcal{O}_{\varpi(2)}\right\rangle\ldots\left\langle\mathcal{O}_{\varpi(n-1)}\mathcal{O}_{\varpi(n)}\right\rangle, \tag{5.7}$$

where ϖ denotes *all* possible permutations of the n numbers.[1]

This theorem guarantees that any higher-order statistical moment of the quantum distribution can be decomposed as a combination of the covariance.

In our approach, Gaussian states are *defined* as the ones obeying eq. (5.7). From now on, attention will be focused on such cases. In the following section we prove a second theorem that demonstrates (non-quantitatively) the amount of entanglement of the Gaussian state of the vacuum.

5.1.1 Reeh–Schlieder theorem

In this section we will follow closely the proof of a theorem, given in ref. [54], that demonstrates qualitatively the amount of entanglement residing in the vacuum

[1] E.g. $\varpi(1) = 2$, $\varpi(2) = 3$ and $\varpi(3) = 1$ give the cyclic permutation $(123) \mapsto (231)$.

state of a field between degrees of freedom localised in space. We will restrict our attention in this context to the case of flat space $\mathbb{M} = \mathbb{R}^4$.

Before enunciating the theorem, we shall explicit two formal ideas that will aid in its understanding. One of them concerns operators, and the other is a recapitulation of a property of pure states.

Definition 14. Let $\mathcal{O}$ be an operator in the algebra of observables. Then it is

$$\mathcal{O}_f \equiv \int_{\mathbb{M}} \mathrm{dvol}\, \mathcal{O}(x^\mu) f(x^\mu) : \tag{5.8}$$

an operator-valued distribution.

This comes as rigorous way to define the observables that were introduced in section , guaranteeing that the resulting vectors of the Hilbert space are of finite norm. In section we will make explicit the necessity of this *smearing*: the property that the operator is only defined after an integration. Notice also that we are bypassing the dependence of $\mathcal{O}$ on Ξ^{a} as its definition would require, and writing it directly in terms of points in spacetime.

Definition 15. A dense subspace of a Hilbert space $\mathbf{H}$ is a set[2]

$$\mathbf{D} \equiv \left\{ |\upsilon\rangle \in \mathbf{H} \mid \sqrt{\langle \upsilon - \eta | \upsilon - \eta \rangle} < \epsilon \text{ for some } |\eta\rangle \in \mathbf{H}, \epsilon > 0 \right\}, \tag{5.9}$$

of vectors arbitrarily close to at least one other vector.

The definition of a dense subspace is akin to the requirement of completeness, i.e. that any vector can be approximated by a linear combination of elements of the Schauder basis. We are now ready to read the topic of this section.

Theorem 5 (Reeh–Schlieder). Let $\mathfrak{A}(\mathbb{X})$ be the subalgebra of operators whose collective support lies in a compact region of space $\mathbb{X}$. Let $|0\rangle \in \mathbf{H}$ be the vacuum state of the quantum field residing in the spatial slice $\mathbb{R}^3$ that contains $\mathbb{X}$. Then the subspace

$$\mathfrak{A}(\mathbb{X})\,|0\rangle = \{ |\upsilon\rangle \in \mathbf{H} \mid \mathcal{O}_f\,|0\rangle = |\upsilon\rangle \} \tag{5.10}$$

is dense in $\mathbf{H}$, i.e. any state $|\psi\rangle \in \mathfrak{A}(\mathbb{X})\,|0\rangle$ is arbitrarily close to other appropriate state in $\mathbf{H}$.

[2] In which we define for now $|\upsilon - \eta\rangle \equiv |\upsilon\rangle - |\eta\rangle$.

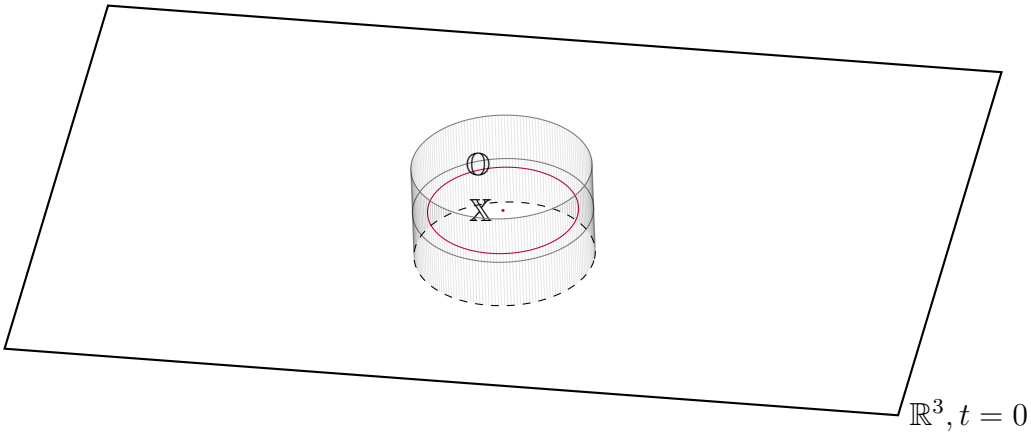

Figure 5.1: Compact subregion $\mathbb{X}$ contained in a spatial slice, within a cylindrical open neighbourhood $\mathbb{O}$.

More explicitly, the collective support to which we refer is a collection of smearing functions $f_i(x)$ whose support are contained in $\mathbb{X}$. Despite these details, in the proof that follows we will work with the non-smeared operators.

Proof. Consider n operators $\mathcal{O}(x_i)$, such that $x_i \in \mathbb{X}$. Let $\mathbb{X}$ be a spacelike region entirely inside a spatial slice $\mathbb{R}^3$, and let $\mathbb{O}$ be an open neighbourhood of $\mathbb{X}$ that also contains points timelike separated from those in $\mathbb{X}$ (cf. fig. 5.1). Choose a vector $|\eta\rangle$ such that

$$\langle\eta|\mathcal{O}(x_1)\mathcal{O}(x_2)\dots\mathcal{O}(x_n)|0\rangle = 0 \quad \forall x_1,\dots,x_n \in \mathbb{X}, \tag{5.11}$$

and define the function $g(t)$ to be a version of the above after time translation of the last operator by t:

$$g(t) \equiv \langle\eta|\mathcal{O}(x_1)\mathcal{O}(x_2)\dots\mathcal{O}(x_n^0+t,\boldsymbol{x}_n)|0\rangle\,. \tag{5.12}$$

By making explicit the action of the time translation operators we can simplify the expression to

$$\begin{aligned} g(t) &= \langle\eta|\mathcal{O}(x_1)\mathcal{O}(x_2)\dots \mathrm{e}^{\mathrm{i}Ht}\mathcal{O}(x_n)\mathrm{e}^{-\mathrm{i}Ht}|0\rangle \\ &= \langle\eta|\mathcal{O}(x_1)\mathcal{O}(x_2)\dots \mathrm{e}^{\mathrm{i}Ht}\mathcal{O}(x_n)|0\rangle\,. \end{aligned} \tag{5.13}$$

To study the behaviour of $g(t)$ more closely, we consider it as a function of a complex variable $t = \tau + \mathrm{i}\beta$. The spectrum of H is positive for a quantum field, as one can check by decomposing the field into normal modes. For this reason $g(t)$

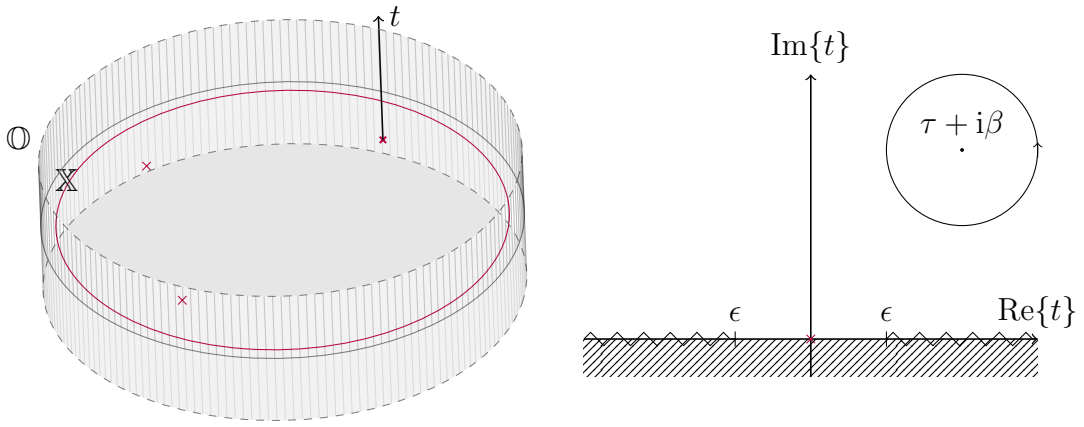

Figure 5.2: Time evolution by t of one of the points in the definition of the n-point function $g(t)$, and its analytical structure in the complex plane (hashed region and sawtooth line is where $g(t)$ is not guaranteed analytical) with a possible contour.

is analytic on the upper-half complex plane: $\beta > 0$, with $\mathrm{e}^{\mathrm{i}Ht} = \mathrm{e}^{\mathrm{i}H\tau}\mathrm{e}^{-H\beta}$ therein, and continuous on the real axis.

Exploiting the residue formula for analytic functions, one may write $g(t)$ as

$$g(t) = \frac{1}{2\pi\mathrm{i}} \oint \frac{g(t')}{t' - t}\,\mathrm{d}t'\,, \tag{5.14}$$

for any closed contour in the upper-half complex plane encircling the simple pole at $t' = t$. Recall that $g(\tau) = 0$ for $\beta = 0$, $-\epsilon < \tau = t < \epsilon$, given that ϵ defines the neighbourhood $\mathbb{O}$ (see fig. 5.2).

In this definition, we can always pick a contour lying on the edge on which $g(t) = 0$; this choice renders part of the integration in eq. (5.14) null, allowing one to remove the pole from within the contour, and still maintain $g(t)$. From Morera's theorem, $g(t)$ is also analytic on $-\epsilon < t < \epsilon$.

In addition, from the Schwarz reflection principle, an analytic function such as $g(t)$ has an analytical continuation to the complex conjugate of its domain (the lower-half complex plane in our case) equal to $\overline{g}(\overline{t})$. But $\overline{g}(\overline{t}) = g(t)$, from which follows that $g(t)$ is analytic (and continuous) in the whole complex plane.

Finally, from the expansion of an analytic function as a power series, if two functions are equal in a region of their domain, then they are equal on the whole domain (their coefficients of expansion are equal). $g(t)$ is equal to 0 on a portion of the real axis and, thence, $g(t) = 0$ on the whole complex plane. In summary, if $g(t)$ vanishes in $\mathbb{X}$, then by time translating and applying Lorentz transformations, it will continue to vanish for any x_n in all of spacetime.

It remains to do the same for the other points of the n-point function. Notice that time translating by the same amount t two points in $\mathbb{X}$, we have

$$g(t) = \langle\eta|\mathcal{O}(x_1)\dots \mathrm{e}^{\mathrm{i}Ht}\mathcal{O}(x_{n-1})\mathcal{O}(x_n)|0\rangle\,, \tag{5.15}$$

from which the rest of the argument follows unchanged. On top of this, we can again time translate x_n again by a different amount t', and rerun the argument once again. Applying this same procedure for every point up to x_1 allows us to assert that, if the n-point function vanishes for points in $\mathbb{X}$, then it must vanish for all $x_1, \dots, x_n \in \mathbb{M}$.

The full algebra of operators acting on the vacuum, $\mathfrak{A}\,|0\rangle$, is clearly dense in the Hilbert space. Considering this, the only vector which is orthogonal to any other vector (or to any vector that arbitrarily approximates a second one) is the 0 vector. That is, if

$$\langle\eta|\mathcal{O}(x_1)\mathcal{O}(x_2)\dots\mathcal{O}(x_n)|0\rangle = 0 \tag{5.16}$$

for any collection of points in spacetime, then $|\eta\rangle$ must be the zero vector.

The fact that the vanishing of $\langle\eta|\mathcal{O}(x_1)\mathcal{O}(x_2)\dots\mathcal{O}(x_n)|0\rangle$ for points in $\mathbb{X}$ leads to its nullity for all of $\mathbb{M}$, ultimately implying that $|\eta\rangle = 0$, allows us to conclude that $\mathfrak{A}(\mathbb{X})\,|0\rangle$ is also dense in $\mathbf{H}$. □

5.2 Vacuum correlations

Let the background be Minkowski $(1+3)$-dimensional spacetime, $\mathbb{M} = \mathbb{R}^{1+3}$, i.e. $\mathbb{R}^4$ manifold with metric of Lorentzian signature $\big(+\ \ -\ \ -\ \ -\big)$; its line element is

$$\mathrm{d}s^2 = \mathrm{d}t^2 - \mathrm{d}\boldsymbol{x}^2, \tag{5.17}$$

where $\mathrm{d}\boldsymbol{x}^2 = \delta_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j$ is the three-dimensional distance in flat space given by the metric $g_{ij} = -\delta_{ij}$ restricted to each spacelike foliation (corresponding to a single value of t). From hereafter we will maintain the use of the spatial vector notation $\boldsymbol{x} = x^i$ and $t = x^0$.

A massive Klein–Gordon field $\Phi(t, \boldsymbol{x})$ is described by the Lagrangian

$$\mathcal{L} = \frac{\sqrt{-g}}{2}\left[g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi - (m^2 + \xi R)\Phi^2\right], \tag{5.18}$$

wherein $\sqrt{-g} = 1$; in this background, the curvature scalar is $R = 0$. We use ∇ interchangeably with the spatial part ∂_i, and also omit the variables dependence of the field to declutter notation.

Varying the action with respect to the scalar field results in the usual Euler–Lagrange equation. In its most general form, applied to this context, we have the Klein–Gordon equation

$$(g^{\mu\nu}\partial_\mu\partial_\nu + m^2)\Phi = 0. \tag{5.19}$$

We will denote the first term succinctly by $\Box$.

Solutions and the mass shell

The solution to eq. (5.19) is straightforward in flat spacetime, it is an equation for four harmonic oscillators. We can use the Fourier components, $\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} = \mathrm{e}^{-\mathrm{i}kx}$, as a basis for the general form of Φ. That is

$$\Phi(x^\mu) = \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega_{\boldsymbol{k}}}} (a_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}kx} + \overline{a}_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}kx}). \tag{5.20}$$

The spectral variables $\boldsymbol{k}$ naturally index the decoupled normal modes of field oscillations in $\mathbb{M}$. The frequency is then $\boldsymbol{k}$-dependent; explicitly

$$\omega_{\boldsymbol{k}}^2 = \boldsymbol{k}^2 + m^2. \tag{5.21}$$

We set out to calculate two-point functions of a real scalar field in Minkowski spacetime vacuum, that is, $\left\langle \tilde{\Phi}(\boldsymbol{x};\boldsymbol{h})\tilde{\Phi}(\boldsymbol{y};\boldsymbol{r}) \right\rangle \equiv \langle 0|\tilde{\Phi}(\boldsymbol{x};\boldsymbol{h})\tilde{\Phi}(\boldsymbol{y};\boldsymbol{r})|0\rangle$, for the smeared field $\tilde{\Phi}(\boldsymbol{x})$ defined as

$$\tilde{\Phi}\big(x^0, \boldsymbol{h}\big) \equiv \int_{\mathbb{R}^3} \mathrm{d}\boldsymbol{x}\, \Phi(x^\mu) f(\boldsymbol{x} - \boldsymbol{h}, \sigma), \tag{5.22}$$

where σ is a smearing parameter, given by the function $f \in \mathsf{S}_{\mathbb{M}}$. At all moments we are picking a particular time-slice, for a vanishing time interval $x^0 - y^0 = 0$ between measurements that can always be satisfied for spacelike intervals, given an appropriate reference frame.

In order to act on the Fock vacuum, we express the quantized field Φ in its normal modes expansion

$$\Phi(x^\mu) = \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega_{\boldsymbol{k}}}} \big(a_{\boldsymbol{p}} \mathrm{e}^{-\mathrm{i}kx} + a_{\boldsymbol{p}}^\dagger \mathrm{e}^{\mathrm{i}kx}\big), \tag{5.23}$$

where $u_{\boldsymbol{k}} = \mathrm{e}^{-\mathrm{i}kx}$ constitutes the basis of solutions to the Klein–Gordon equation, and a_k together with its Hermitian conjugate annihilates and creates particles with 4-momentum k^μ respectively, obeying the canonical commutation relation $\left[a_{\boldsymbol{k}}, a_{\boldsymbol{k}'}^\dagger\right] = \delta(\boldsymbol{k} - \boldsymbol{k}')$.

Let us first pick the smearing function to be a Gaussian function, where the σ parameter is its standard deviation. The correlation function smeared at a coincident point ($\boldsymbol{h} = \boldsymbol{r} = 0$) is

$$\left\langle \tilde{\Phi}(\boldsymbol{x};0)\tilde{\Phi}(\boldsymbol{y};0) \right\rangle = \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} \frac{1}{2\omega_{\boldsymbol{k}}} \mathrm{e}^{-\boldsymbol{k}^2\sigma^2}. \tag{5.24}$$

We perform this simple integration in the cases of a massless ($\omega_{\boldsymbol{k}} = |\boldsymbol{k}|$) and massive theory.

As for correlations with smearing centred at distinct points in space, $\boldsymbol{r} = 0$ and some non-vanishing $\boldsymbol{h}$, the calculation takes a few more steps and results in

$$\left\langle \tilde{\Phi}(\boldsymbol{x};\boldsymbol{h})\tilde{\Phi}(\boldsymbol{y};0)\right\rangle = \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\frac{1}{2\omega_{\boldsymbol{k}}}\mathrm{e}^{-\boldsymbol{k}^2\sigma^2}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{h}}, \tag{5.25}$$

which leads, for a massless field, after a choice of frame where $\boldsymbol{h} = \begin{pmatrix}0 & 0 & h\end{pmatrix}^{\intercal}$ and integration in spherical coordinates, to

$$\left\langle \tilde{\Phi}(\boldsymbol{x};\boldsymbol{h})\tilde{\Phi}(\boldsymbol{y};0)\right\rangle = \frac{1}{4\pi^2\sigma h}\,\mathrm{D}\left(\frac{h}{2\sigma}\right), \tag{5.26}$$

where $\mathrm{D}(x)$ is the Dawson function. We plot this result in section 5.2 alongside the massive counterpart, with correlations noticeably weaker and more damped.

5.3 Entanglement entropy in flat space

Entanglement entropy, as introduced in chapter 3, is divergent when applied to the continuum. The regularisation provided by the more rigorous definition of quantum fields in terms of operator-valued distributions, as discussed in chapter 4, can be difficult to calculate even for simple free theories. It is common to resort to regularisation by discretisation in this case.

In ref. [2], Srednicki treats quantum fields on a lattice, simulating countable degrees of freedom, in order to achieve a finite value for the entanglement-area relation. In this setting, the ever-shorter excitations of the quantum fields contributing to correlations near the boundary are suppressed because one cannot get arbitrarily close to the entangling surface. The divergent aspect of these correlations are not accounted in $\mathcal{S}$, thus rendering it finite.

5.3.1 Discretisation and normal mode decomposition

Our choice of discretisation is defined as follows, to motivate the calculation of the finite entanglement entropy in systems with a finite number of degrees of freedom.

Definition 16. The *discretisation* of a manifold $\mathbb{D}$ is a graph, constituted by two sets and a bijection, $\mathtt{D} = (\mathrm{Vt}(\mathbb{D}), \mathrm{Ed}(\mathbb{D}), \iota)$, such that

- $\mathrm{Vt}(\mathbb{D})$ is the set of points in a spatial hypersurface $\mathbb{D}$ at a particular time slice, given a coordinate system.

- $\mathrm{Ed}(\mathbb{D})$ is the set of edges, whose elements are unordered pairs of vertices at a constant geodesic distance ε (*ultraviolet cutoff*).

- ι is the incidence map:

$$\begin{aligned} \iota\colon \mathrm{Ed}(\mathbb{D}) &\to \binom{\mathrm{Vt}(\mathbb{D})}{2} \\ \mathrm{edge} &\mapsto \{\mathrm{v}_1, \mathrm{v}_2\}, \end{aligned} \tag{5.27}$$

  a map that associates to each edge an unordered pair of vertices.

The set $\mathrm{Vt}(\mathbb{D})$ is a countable choice of points in the spatial manifold; its elements are referred to as nodes, sites or vertices. The set of edges (or links) $\mathrm{Ed}(\mathbb{D})$ is then fixed through the bound function, with edges being unordered pairs of points that are at the neighbourhood of each other.

`D` encodes events in space and their connectivity. $\mathrm{Vt}(\mathbb{D})$ is a discrete subset of $\mathbb{D}$; $\mathrm{Ed}(\mathbb{D})$, on the other hand, represents the end-points of an edge. The connectivity that the edge set and the adjacency encodes should reproduce a notion of proximity that resembles continuum space and preserve an intuitive notion of topology and continuity (in the sense that two events are linked only if they are nearby). Moreover, derivatives are substituted by finite differences. The full spacetime is $\mathtt{D} \times \mathbb{R}$.

Example 12. This discretisation is dependent on the choice of local coordinates for the manifold. Figure 5.3 is an example of discretisation of flat space in terms of global rectangular coordinates. The edges connect the four nearest neighbours to each vertex, all equally spaced. In the scheme presented in the picture, the set $\mathrm{Vt}(\mathbb{D})$ has sites parametrised by two indices (x, y), each referring to one of the coordinate functions. If the graph is finite, with size L, we can introduce a single ordering for the vertices; for instance,

$$\begin{aligned} &n = 1 \mapsto (x = 0, y = 0) \\ &n = 2 \mapsto (0, 1) \\ &\quad\vdots \\ &n = L \mapsto (0, L) \\ &n = L + 1 \mapsto (1, 0), \end{aligned} \tag{5.28}$$

and so on, up to the total number of sites L^2, for which $n = N$.

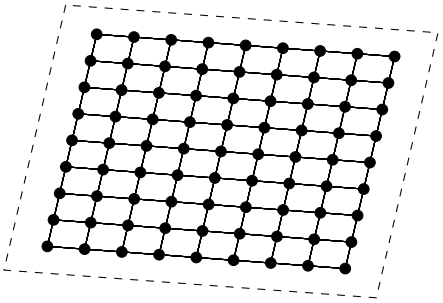

Figure 5.3: Regular square lattice with euclidean plane as base manifold. The discretisation picks values of rectangular coordinates at fixed intervals. The vertices in coordinates are $(x\varepsilon, y\varepsilon) \in \varepsilon\mathbb{Z}^2$, in which ε is the constant lattice spacing, multiplied by the integers x and y, whose value at the origin of the global chart is $x = 0 = y$. The edges connect nearest neighbours e' and e, for which either $x' = x \pm 1$ with $y' = y$, *or* $y' = y \pm 1$ with $x' = x$.

This procedure has the important effect of translating the problem of a quantum field in the continuum to a collection of harmonic oscillators. Functions previously defined on the manifold, when restricted to the graph $(f\big|_{\mathsf{D}})$, change their range from $f(\mathbb{D})$ to $f(\mathrm{Vt}(\mathbb{D}))$. When quantum fields were introduced, we picked smooth functions for our relevant configurations and, hence, phase space had two smooth functions as coordinates: the field $\Phi_t(x^i)$ and its conjugate canonical momentum $\Pi_t(x^i)$. After restricting the range of functions on the spacetime manifold through discretisation, only the values of the field and its momentum at points in $\mathrm{Vt}(\mathbb{D})$ count as degrees of freedom.

We will be mainly interested in cases for which $\mathrm{Vt}(\mathbb{D})$ has a finite number of elements. This amounts to introducing an upper limit to the possible distances between two points in the manifold (an *infrared cutoff*). Only in this manner the original phase space is reduced from an infinite-dimensional vector space to a finite-dimensional one. If we had $\mathrm{Vt}(\mathbb{D})$ still infinite, despite being countable, $\mathbf{\Gamma}$ would still be infinite-dimensional (one degree of freedom at each point in space).

We thus realise the dictionary translating systems with an infinite number of degrees of freedom to systems with a finite number of degrees of freedom. The classical states $(\Phi_t(x^i), \Pi_t(x^i))$ are now substituted by (Φ_n, Π_n) , that can be put into vector form

$$\begin{pmatrix}\Phi_1 & \dots & \Phi_n & \dots & \Pi_n & \dots & \Pi_N\end{pmatrix}^{\intercal} \in \mathbf{\Gamma} \cong \mathbb{R}^{2N}, \tag{5.29}$$

given that N is the total number of sites in the lattice. Also notice that the triplet of structures in our definition of a graph will not be constructed, but merely implied in what follows.

Notwithstanding the use of discretisation in regularising the theory, it has physical motivation. Considerations of quantum effects in gravity possibly lead to the concept of a fundamental minimal length, as suggested by the following argument.

Suppose we can saturate the uncertainty principle whilst localising a particle of mass m in a region of the order of the Planck length, $\ell_{\mathrm{P}} \approx \sqrt{G}$. This implies a relativistic energy of at least

$$E = \sqrt{\frac{1}{4G} + m^2}, \tag{5.30}$$

for the particle at the instant of measurement. In order to do this, we may probe such particle using a photon whose wavelength is also ℓ_{P} and whose energy is $E_{\mathrm{photon}} = 2\pi/\sqrt{G}$. The total energy at that region, of size ℓ_{P}, is the sum $E + E_{\mathrm{photon}}$. Consider, on the other hand, a black hole whose Schwarszchild radius is the Planck length. Its mass (or rest energy) is approximately $E_{\mathrm{BH}} = 1/2\sqrt{G}$. Therefore, this thought experiment packs in a region of size ℓ_{P} an energy higher than that which is enough to form a black hole:

$$\sqrt{\frac{1}{4G} + m^2} + \frac{2\pi}{\sqrt{G}} > \frac{1}{2\sqrt{G}}. \tag{5.31}$$

The many quantum corrections needed to validate this argument will alter its results, so it should not be taken at face value. Other, more elaborate arguments supporting the minimal length hypothesis can be found in ref. [55].

Let us now go back to the entanglement entropy of the vacuum state for a massless, real, scalar field. This vacuum is a Gaussian state, as we will see in the following. This will be done in two steps: first, the fields are decoupled in normal modes conjugate to the two variables parametrising a choice of entangling surface; second, the remaining variable, transverse to the entangling surface, is discretised.

The Hamiltonian for a massless scalar field in the continuum, rectangular coordinates of flat space is

$$H = \frac{1}{2} \int \mathrm{d}\boldsymbol{x} \left(\Pi^2 + \partial_i \Phi \partial^i \Phi \right). \tag{5.32}$$

To rewrite H in the graph and in terms of angular modes, we need to know what form the integral takes and how the gradient of Φ is expressed as a finite difference.

Spherical harmonics form a complete basis of functions; we thus write the canonical fields in flat space as

$$\Phi(r, \theta, \alpha) = \sum_{l=0}^{\infty} \sum_{k=-l}^{l} \frac{\Phi_{lk}(r)}{r} \mathrm{Y}_{lk}(\theta, \alpha), \tag{5.33}$$

and

$$\mathit{\Pi}(r,\theta,\alpha)=\sum_{l=0}^{\infty}\sum_{k=-l}^{l}\frac{\mathit{\Pi}_{lk}(r)}{r}\mathrm{Y}_{lk}(\theta,\alpha), \tag{5.34}$$

for the *multipole components* $\mathit{\Phi}_{lk}$ and $\mathit{\Pi}_{lk}$. In this expansion we have used the *real* spherical harmonics, instead of the complex variety, in order to avoid adding conditions on the multipoles. Refer to appendix for their relations; for now it is enough to know that they all share the same properties (e.g. normalisation).

In spherical coordinates the volume form is $\mathrm{d}\boldsymbol{x}\mapsto r^2\sin\theta\mathrm{d}r\mathrm{d}\theta\mathrm{d}\alpha$. The gradient, conversely, is

$$\partial_i\mathit{\Phi}\partial^i\mathit{\Phi}=\left(\frac{\partial\mathit{\Phi}}{\partial r}\right)^2+\frac{1}{r^2}\left(\frac{\partial\mathit{\Phi}}{\partial\theta}\right)^2+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial\mathit{\Phi}}{\partial\alpha}\right)^2. \tag{5.35}$$

Writing in terms of the normal modes, the derivatives on θ and α operate solely on the spherical harmonics,[3] i.e.

$$\partial_i\mathit{\Phi}\partial^i\mathit{\Phi}=\sum_{\substack{l,k\\l',k'}}\left[\left(\frac{\partial}{\partial r}\frac{\mathit{\Phi}_{lk}}{r}\right)^2(\mathrm{Y}_{lk})^2+\frac{(\mathit{\Phi}_{lk})^2}{r^4}\left[\underbrace{\left(\frac{\partial\mathrm{Y}_{lk}}{\partial\theta}\right)^2+\frac{1}{\sin^2\theta}\left(\frac{\partial\mathrm{Y}_{lk}}{\partial\alpha}\right)^2}_{=\partial_c\mathrm{Y}_{lk}\partial^c\mathrm{Y}_{l'k'}}\right]\right], \tag{5.36}$$

in which $c=2$ or 3, are spatial indices restricted to angular variables.

Let us simplify the angular dependence, by working in the geometry of $\mathbb{S}^2$. In terms of the spherical harmonics, H is

$$H=\sum_{\substack{l,k\\l',k'}}\int\frac{\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\alpha\,r^2\sin\theta}{2}\left[\frac{(\mathit{\Pi}_{lk})^2}{r^2}(\mathrm{Y}_{lk})^2+\left(\frac{\partial}{\partial r}\frac{\mathit{\Phi}_{lk}}{r}\right)^2(\mathrm{Y}_{lk})^2\right.$$
$$\left.+\frac{(\mathit{\Phi}_{lk})^2}{r^4}\partial_c\mathrm{Y}_{lk}\partial^c\mathrm{Y}_{l'k'}\right]. \tag{5.37}$$

As mentioned above, the Y_{lk} are an orthonormal basis for functions on $\mathbb{S}^2$, by applying this property, we can simplify the first term as

$$H=\sum_{\substack{l,k\\l',k'}}\int\frac{\mathrm{d}r\,r^2}{2}\left[\left(\frac{(\mathit{\Pi}_{lk})^2}{r^2}+\left(\frac{\partial}{\partial r}\frac{\mathit{\Phi}_{lk}}{r}\right)^2\right)\delta_{ll'}\delta_{kk'}\right.$$
$$\left.+\frac{(\mathit{\Phi}_{lk})^2}{r^4}\int\mathrm{d}\theta\,\mathrm{d}\alpha\sin\theta\partial_c\mathrm{Y}_{lk}\partial^c\mathrm{Y}_{l'k'}\right]. \tag{5.38}$$

[3]The components being squared should be understood as having both primed and unprimed indices l and k.

The second term is integrated by parts as functions on the sphere. That is,

$$\int_{\mathbb{S}^2} \partial_c \mathrm{Y}_{lk} \partial^c \mathrm{Y}_{l'k'} = \underbrace{\int_{\mathbb{S}^2} \nabla_c (\mathrm{Y}_{lk} \partial^c \mathrm{Y}_{l'k'})}_{=0} - \int_{\mathbb{S}^2} \mathrm{Y}_{lk} \nabla_c \partial^c \mathrm{Y}_{l'k'}, \tag{5.39}$$

in which the boundary contribution, that arises from the use of the divergence theorem (cf. chapter 2), vanishes identically because $\partial\mathbb{S}^2 = \varnothing$: the sphere does not have a boundary. This leads to

$$H = \sum_{\substack{l,k \\ l',k'}} \int \frac{\mathrm{d}r\, r^2}{2} \Bigg[\left(\frac{(\Pi_{lk})^2}{r^2} + \left(\frac{\partial}{\partial r} \frac{\Phi_{lk}}{r} \right)^2 \right) \delta_{ll'} \delta_{kk'} + \frac{(\Phi_{lk})^2}{r^4} \left(- \int \mathrm{d}\theta\, \mathrm{d}\alpha \sin\theta \mathrm{Y}_{lk} \nabla_c \partial^c \mathrm{Y}_{l'k'} \right) \Bigg]. \tag{5.40}$$

The second part is again simplified by recognising that the Laplacian and the spherical harmonics satisfy the eigenvalue equation $\nabla_c \partial^c \mathrm{Y}_{lk} = -l(l+1)\mathrm{Y}_{lk}$. Inserting this into the second integral above, and applying orthonormality on it, yields

$$\begin{aligned} H &= \sum_{\substack{l,k \\ l',k'}} \int \frac{\mathrm{d}r\, r^2}{2} \left(\frac{(\Pi_{lk})^2}{r^2} + \left(\frac{\partial}{\partial r} \frac{\Phi_{lk}}{r} \right)^2 + \frac{(\Phi_{lk})^2}{r^4} l'(l'+1) \right) \delta_{kk'} \delta_{ll'} \\ &= \sum_{l,k} \int \frac{\mathrm{d}r\, r^2}{2} \left(\frac{\Pi_{lk}^2}{r^2} + \left(\frac{\partial}{\partial r} \frac{\Phi_{lk}}{r} \right)^2 + \frac{\Phi_{lk}^2}{r^4} l(l+1) \right), \end{aligned} \tag{5.41}$$

with the squares now referring to the single, unprimed, pair l, k.

We now finally apply the discretisation of the radial coordinate. Instead of picking a cubic lattice, similar to that of fig. 5.3, we are associating a graph to flat space in spherical coordinates (r, θ, α) (with $0 < r$ and $0 < \theta < \pi$ and $0 < \alpha < 2\pi$). With the choice of spherical entangling surface $\mathbb{S}^2$, the angular functions are decomposed into normal modes, as shown above, and the radius is what remains to be discretised.

The r coordinate is replaced by vertices at constant spacing ε, as shown in fig. 5.4, after discretisation. This is irrespective of the angles and, in this way, the graph sets up a collection of concentric spheres whose radius reach the position of the vertices. Under the prescription $r \mapsto (j + 1/2)\varepsilon$ the phase space coordinates of interest are rendered as Φ_{lkj} and Π_{lkj}/ε: the multipole components at site j.

Under this prescription, the integral in eq. (5.41) becomes a sum, its volume element, $r^2\, \mathrm{d}r$, becomes $(j + 1/2)^2 \varepsilon^3$, and the derivative is replaced by a finite

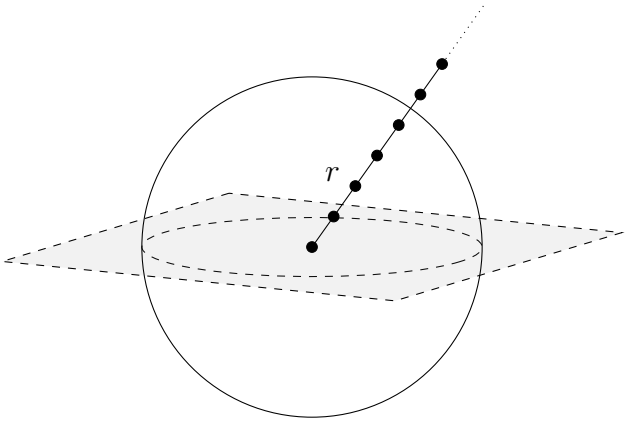

Figure 5.4: Shown above is the sphere associated to the fourth vertex, $n = 4$, at a distance $r = (n + 1/2)\varepsilon$ from the origin.

difference,

$$\frac{\partial}{\partial r}\frac{\Phi_{lk}}{r} \mapsto \frac{1}{\varepsilon^2}\left(\frac{\Phi_{lkj+1}}{j+3/2} - \frac{\Phi_{lkj}}{j+1/2}\right). \tag{5.42}$$

This is the important implication of discretisation, namely to introduce regularisation containing the infinities of the theory, follow from this procedure as it was discussed in the beginning of this section. $N\varepsilon$ prevents infinities stemming from a continuum of low-energy modes, as a natural infra-red cut-off, whilst ε does so for high-energy modes, introducing a finite resolution in space.

Finally, we can rewrite H as

$$H = \sum_{lk}\sum_{j=0}^{N}\left[\frac{\Pi_{lkj}^2}{2\varepsilon} + \frac{(j+1/2)^2}{2\varepsilon}\left(\frac{\Phi_{lk,j+1}}{j+3/2} - \frac{\Phi_{lkj}}{j+1/2}\right)^2 + \frac{l(l+1)}{2\varepsilon}\frac{\Phi_{lkj}^2}{(j+1/2)^2}\right], \tag{5.43}$$

from which we define the coupling matrix,

$$K_{xy} = \left[\frac{(x-1/2)^2}{(x+1/2)^2} + \frac{l(l+1)}{(x+1/2)^2} + 1\right]\delta_{xy} - \left[\frac{(x-1/2)}{(x+1/2)}\right]\delta_{x-1,y} - \left[\frac{(y-1/2)}{(y+1/2)}\right]\delta_{x,y-1}. \tag{5.44}$$

This is the Hamiltonian of N coupled harmonic oscillators, as we were set out to demonstrate. In more familiar shape, and changing the indexing of sites, we can express the per-mode contributions, H_{lk} (of $H = \sum_{lk} H_{lk}$), as

$$H_{lk} = \frac{1}{2\varepsilon}\left(\sum_{x=0}^{N}\Pi_{lkx}^2 + \sum_{x,y=0}^{N}\Phi_{lkx}K_{xy}\Phi_{lky}\right), \tag{5.45}$$

where we can identify the diagonal contribution K_{xy} as that of a simple harmonic oscillator, whilst the off-diagonal contribution, $x = y \pm 1$, is responsible for coupling the neighbouring oscillators. Also, from the full expression of matrix K in eq. (5.43), we see that longer-distance couplings are assumed non-existent.

In summary we have a field defined on a one-dimensional graph, whose configurations at neighbouring sites x and y are coupled through matrix K_{xy} in eq. (5.44).

$$H = \frac{1}{2}\Xi^{\intercal}\begin{pmatrix} K & 0 \\ 0 & I \end{pmatrix}\Xi. \tag{5.46}$$

This new matrix couples the first N coordinates of phase space, the ones that refer to configuration: Φ_x. The rest results in the standard kinetic term $\Pi^2/2$.

It is important to understand what is the effect of decoupling the angular variables into normal modes: the phase space of that problem is actually larger than $\mathbb{R}^{2(N+1)}$, for N the number of vertices in the one-dimensional graph. For every l and k, one has lattice phase spaces $\mathbf{\Gamma}_{lk} = \mathbb{R}^{2(N+1)}$, that sum up to

$$\mathbf{\Gamma} = \bigoplus_{l=1}^{\infty}\bigoplus_{k=-l}^{l}\mathbb{R}^{2N}, \tag{5.47}$$

and a bigger coupling matrix X such that

$$\begin{aligned} X &= \bigoplus_{l=1}^{\infty}\bigoplus_{k=-l}^{l} X_{lk} \\ &= \begin{pmatrix} \ddots & & & & & & \\ & K_{lk} & 0 & & & & \\ & 0 & I & & & & \\ & & & \ddots & & & \\ & & & & K_{l'k'} & 0 & \\ & & & & 0 & I & \\ & & & & & & \ddots \end{pmatrix}, \end{aligned} \tag{5.48}$$

wherein each X_{lk} leading to a mode Hamiltonian H_{lk}, as in eq. (5.45).

A full decomposition into normal modes and introduction of creation and annihilation operators would diagonalise H completely. Had we used the full diagonalisation of H, with respect to the full decomposition into normal modes, we could write the state ϱ as a product state of Gaussian functions, one for each mode. Instead, we express it using the non-diagonal form, to exploit the coupling between spatial degrees of freedom that leads to entanglement.

5.3.2 Entropy of spherical regions

In the following we will make a partial trace over degrees of freedom residing in specific regions of space and, to this end, the form of H that makes explicit these regions come in hand. The interest lies in the vacuum state for the scalar field, for which the energy expectation value is minimised; this still corresponds to a Gaussian, ground state, since we are treating harmonic oscillators. This property also facilitates the partial trace, for it reduces the problem to a Gaussian integral. The state for each lk mode, in configuration basis $\langle\phi|\varrho|\phi\rangle$ is, therefore,

$$\varrho_{lk}(\Phi,\Phi') = \frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}} \exp\left(-\frac{\Phi^{\intercal} K^{1/2}\Phi}{2}\right) \exp\left(-\frac{\Phi'^{\intercal} K^{1/2}\Phi'}{2}\right), \tag{5.49}$$

wherein the coefficients in front of the exponentials guarantee that $\operatorname{tr}\varrho = 1$, and $K^{1/2}$ is the non-diagonal matrix of square roots of eigenvalues of K.[4] From this point onwards we will omit reference to the modes lk, working in a per-mode premise, where the upright Φ is used as the column matrix of field eigenvalues (i.e. $\hat{\Phi}\,|\varphi\rangle = \Phi\,|\varphi\rangle$).

The choice of entangling surface determines the factorisation of the Hilbert space on which ϱ acts. This in turns determines how to trace out one of the regions. Let us choose a submanifold $\mathbb{X}^{\complement}$ in $\mathbb{D}$, the *inner part*, comprised of the points whose coordinates are all r such that $r < r_0$. $\mathbb{X}^{\complement}$ is then a ball with $\partial\mathbb{X}^{\complement}$ as bounding surface. Its complement (the *outer region*), $\mathbb{X}$, is such that $\mathbb{D} = \mathbb{X}\cup\mathbb{X}^{\complement}$, with shared *entangling surface* $\partial\mathbb{X}^{\complement} = \partial\mathbb{X}$. The corresponding graphs follow from the coordinate representation: every $\mathtt{e}_x \in \mathrm{Vt}(\mathbb{D})$ giving $r < r_0$ is a part of $\mathtt{X}^{\complement}$, and analogously for $\mathtt{X}$. The depiction would be a three-dimensional version of fig. 5.5, given the choice of spherical coordinates in flat space. If we pick, for example, $n = 4$ for the last vertex inside $\mathbb{X}$, fig. 5.4 is the appropriate picture to have in mind, with the sphere of radius $r_0 = 9\varepsilon/2$ taking the role of $\partial\mathbb{X}$.

Inspired by the study of black holes, we choose the graph $\mathtt{X}$ to be outside the event horizon, whereas $\mathtt{X}^{\complement}$ is inside it. It is intuitive to trace out the degrees of freedom at sites $i \leq n$, for the vertex[5] n whose coordinate is at the Schwarzschild radius; describing physics exclusively outside the event horizon, the resulting reduced state is $\operatorname{tr}_{\mathtt{X}^{\complement}}\varrho = \varrho_{\mathtt{X}}(\Phi_{n+1},\ldots,\Phi_N,\Phi'_{n+1},\ldots,\Phi'_N)$. To declutter notation, we refer to this reduced state simply as $\varrho_{\mathtt{X}}$.

Next, it is shown how the factorised out-states in terms of angular modes, following from eq. (5.43), are diagonalised, form of which the associated entropy, $\mathcal{S}_\kappa$, is computed exactly. The total entropy $\mathcal{S}_{\text{out}}$ turns out to be a sum over $\mathcal{S}_\kappa$, and then over normal modes.

[4] Suppose that U is the unitary matrix diagonalising K as $U^\dagger K_{\text{diag}} U$. Then $K^{1/2} \equiv U^\dagger K_{\text{diag}}^{1/2} U$, for $K_{\text{diag}}^{1/2}$.

[5] Attention that we are using n as a distinguished site now, whilst i and j are generic points.

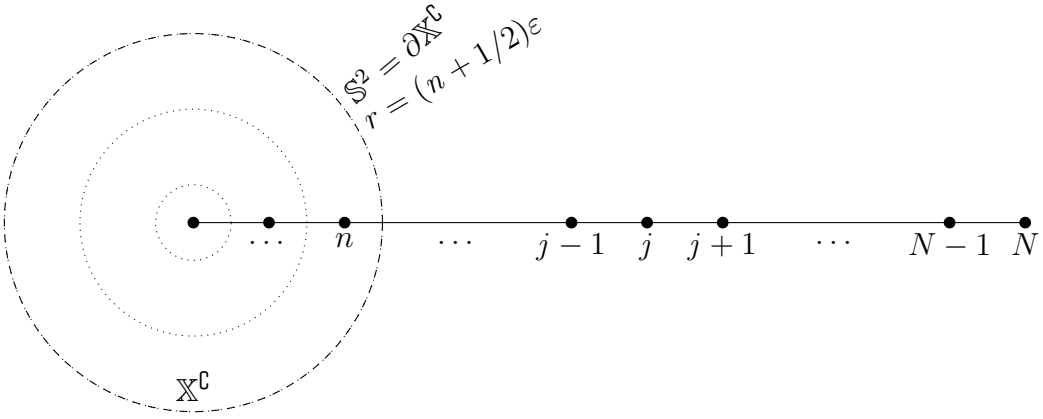

Figure 5.5: One-dimensional lattice in spherical coordinate discretisation of flat space, with lattice size N and entangling surface with radius $r = (n + 1/2)\varepsilon$ enclosing $\mathbb{X}^{\complement}$.

Writing the $K^{1/2}$ matrix through its block components, the vector algebra in eq. (5.49) is

$$\Phi^{\intercal} K^{1/2} \Phi \equiv \begin{pmatrix} \Phi^{\intercal}_{\mathtt{X}^{\complement}} & \Phi^{\intercal}_{\mathtt{X}} \end{pmatrix} \begin{pmatrix} A & B \\ B^{\intercal} & C \end{pmatrix} \begin{pmatrix} \Phi_{\mathtt{X}^{\complement}} \\ \Phi_{\mathtt{X}} \end{pmatrix}, \tag{5.50}$$

where A is the submatrix coupling degrees of freedom entirely inside the entangling surface, B couples them to oscillators in $\mathtt{X}$, which are coupled amongst themselves by C. To compute the trace, we then integrate on the Gaussian functions pertaining to these two couplings, after setting $\Phi^{\intercal}_{\mathtt{X}} = \Phi'^{\intercal}_{\mathtt{X}}$,

$$\varrho_{\mathtt{X}} = \sqrt{\frac{\det K^{1/2}}{\pi^N}} \int \prod_{x=1}^{n} \mathrm{d}\Phi_i \exp \Bigg[- \Phi^{\intercal}_{\mathtt{X}^{\complement}} A \Phi_{\mathtt{X}^{\complement}} - \frac{1}{2} \Phi^{\intercal}_{\mathtt{X}} C \Phi_{\mathtt{X}} - \frac{1}{2} \Phi'^{\intercal}_{\mathtt{X}} C \Phi'_{\mathtt{X}} \\ - \Phi^{\intercal}_{\mathtt{X}^{\complement}} B \left(\Phi'_{\mathtt{X}} + \Phi_{\mathtt{X}} \right) - \left(\Phi'^{\intercal}_{\mathtt{X}} + \Phi^{\intercal}_{\mathtt{X}} \right) B^{\intercal} \Phi_{\mathtt{X}^{\complement}} \Bigg], \tag{5.51}$$

The $\Phi^{\intercal}_{\mathtt{X}^{\complement}} B (\Phi'_{\mathtt{X}} + \Phi_{\mathtt{X}})$ term is the transpose of $(\Phi'^{\intercal}_{\mathtt{X}} + \Phi^{\intercal}_{\mathtt{X}}) B^{\intercal} \Phi_{\mathtt{X}^{\complement}}$, but they are a sum of commuting field operators and, hence, equal. We can thus write them as $(\Phi'^{\intercal}_{\mathtt{X}} + \Phi^{\intercal}_{\mathtt{X}}) B^{\intercal} \Phi_{\mathtt{X}^{\complement}}$.

The operation of interest is thus a collection of Gaussian integrals with linear

and constant contributions, whose result is well-known to be[6]

$$\begin{aligned}\varrho_{\mathtt{X}} &= \sqrt{\frac{(2\pi)^n \det(K^{1/2})}{\pi^N \det(2A)}} \exp\left[\frac{1}{2}\left(\Phi_{\mathtt{X}}'^{\intercal} + \Phi_{\mathtt{X}}^{\intercal}\right) B^{\intercal} A^{-1} B \left(\Phi_{\mathtt{X}}' + \Phi_{\mathtt{X}}\right)\right. \\ &\qquad \left. - \frac{1}{2}\Phi_{\mathtt{X}}^{\intercal} C \Phi_{\mathtt{X}} - \frac{1}{2}\Phi_{\mathtt{X}}'^{\intercal} C \Phi_{\mathtt{X}}'\right] \\ &= \sqrt{\frac{\det K^{1/2}}{\pi^{N-n} \det A}} \exp\left[-\frac{\Phi_{\mathtt{X}}'^{\intercal}\left(C - B^{\intercal}A^{-1}B\right)\Phi_{\mathtt{X}}'}{2} - \frac{\Phi_{\mathtt{X}}^{\intercal}\left(C - B^{\intercal}A^{-1}B\right)\Phi_{\mathtt{X}}}{2}\right. \\ &\qquad \left. + \Phi_{\mathtt{X}}^{\intercal} B^{\intercal} A^{-1} B \Phi_{\mathtt{X}}'\right]. \end{aligned} \tag{5.52}$$

We want to compute $\mathcal{S}_{lk} \equiv -\operatorname{tr}(\varrho_{\mathtt{X}} \ln \varrho_{\mathtt{X}})$, which is most easily done in a basis where $\varrho_{\mathtt{X}}$ is diagonal, for which the trace is a sum of eigenvalues. This is achieved by diagonalising the expression inside the exponential of eq. (5.52), and recognising the result as a tensor product of states of the new degrees of freedom; the steps leading are outlined below.

1. Introduce the diagonal matrix D and the orthogonal matrix V, for which $C - B^{\intercal}A^{-1}B \equiv V^{\intercal}DV$; redefine the fields as $\widetilde{\Phi} \equiv D^{1/2}V\Phi_{\mathtt{X}}$. It follows that

$$\exp\left[-\frac{1}{2}\left(\widetilde{\Phi}'^{\intercal}\widetilde{\Phi}' + \widetilde{\Phi}^{\intercal}\widetilde{\Phi}\right) + \widetilde{\Phi}^{\intercal} D^{-1/2} V B^{\intercal} A^{-1} B V^{\intercal} D^{-1/2} \widetilde{\Phi}'\right], \tag{5.53}$$

   replaces the exponential in eq. (5.52).

2. Introduce the second diagonal matrix Λ and orthogonal matrix W, for which $D^{-1/2}VB^{\intercal}A^{-1}BV^{\intercal}D^{-1/2} \equiv W^{\intercal}\Lambda W$; redefine the fields as $X \equiv W\widetilde{\Phi}$. One has that

$$\exp\left[-\frac{1}{2}\left(X'^{\intercal}X' + X^{\intercal}X\right) + X^{\intercal}\Lambda X'\right], \tag{5.54}$$

   replaces the exponential in item 1.

In component form, the transformed $\varrho_{\mathtt{X}}$ is

$$\varrho_{\mathtt{X}}(X, X') = \sqrt{\frac{\det K^{1/2}}{\pi^{N-n} \det A}} \bigotimes_{\kappa=1}^{n-1} \underbrace{\exp\left[-\frac{1}{2}\left(X_\kappa'^{\,2} + X_\kappa^2\right) + \lambda_\kappa X_\kappa X_\kappa'\right]}_{\equiv\, \varrho_\kappa}, \tag{5.55}$$

[6] See appendix for details.

where λ_κ are the κ eigenvalues of Λ. In this expression, each exponential is a factorised state of the new $n-1$ degrees of freedom, κ, no longer referring to vertices of the graph, but still restricted to the region outside the boundary.

Each one of the tensor product states in eq. (5.55), ϱ_κ, can be diagonalised by finding eigenfunctions f_d such that

$$\int \mathrm{d}X'_\kappa \, \varrho_\kappa(X_\kappa, X'_\kappa) f_d(X'_\kappa) = p_d f_d(X_\kappa). \tag{5.56}$$

This is a solved problem, for which one finds $f_n(X_\kappa) = \mathrm{Herm}_d(X_\kappa)$, the Hermite polynomial of degree $d \in \mathbb{N}$, and

$$p_d = \left(1 - \frac{\lambda_\kappa}{1 + (1-\lambda_\kappa^2)^{1/2}}\right) \Bigg(\underbrace{\frac{\lambda_\kappa}{1 + (1-\lambda_\kappa^2)^{1/2}}}_{\equiv \zeta_\kappa} \Bigg)^d, \tag{5.57}$$

for the eigenvalues.

We are ready to compute $\mathcal{S}_{lk}$, by first computing $\mathcal{S}_\kappa$ and summing over κ. Recall the various simplifications in the preceding steps:

1. The Hamiltonian H was decoupled into angular normal modes, H_{lk}. This provides a factorised states, ϱ_{lk}, implying that the entropy for the reduced density matrix is also assigned to particular modes; we named it $\mathcal{S}_{lk}$. The sum $\mathcal{S}_{\mathrm{out}} = \sum_{lk} \mathcal{S}_{lk}$ defines the *total* entropy outside the entangling surface, $\mathcal{S}_{\mathrm{out}}$.

2. Each $\varrho_{\mathtt{X}}$ was decomposed into a product state $\prod_\kappa \varrho_\kappa$. The meaning of this is that, for each κ, one can compute $\mathcal{S}_\kappa$. Then, $\mathcal{S}_{lk} = \sum_{\kappa=1}^{n-1} \mathcal{S}_\kappa$.

3. To calculate the entropy $\mathcal{S}_\kappa$, we sum over the infinite eigenvalues of each factorised state ϱ_κ: $\mathcal{S}_\kappa = \sum_d \mathcal{S}_d$.

In short, the entanglement entropy is

$$\mathcal{S}_{\mathrm{out}} = \underbrace{\sum_{lk} \sum_{\kappa} \underbrace{\sum_{d} \mathcal{S}_d}_{\mathcal{S}_\kappa}}_{\mathcal{S}_{lk}} . \tag{5.58}$$

Finally, let us compute $\mathcal{S}_\kappa$. Its expression explicitly in terms of ζ_κ is

$$\mathcal{S}_\kappa = -\sum_{d=0}^{\infty} (1-\zeta_\kappa)(\zeta_\kappa)^d \ln\big((1-\zeta_\kappa)(\zeta_\kappa)^d\big). \tag{5.59}$$

In order to compute this sum, we need to establish that $0 < \zeta_\kappa < 1$. Relying on the eigenvalue statement and the normalisation of ϱ_κ, one sees that $0 < p_d < 1$. In turn, by checking eq. (5.57), the condition that p_d is a probability distribution implies that $0 < \zeta_\kappa < 1$. The entropy can then be simplified as follows.

$$\begin{aligned}\mathcal{S}_\kappa &= -(1-\zeta_\kappa)\ln(1-\zeta_\kappa)\sum_d(\zeta_\kappa)^d - (1-\zeta_\kappa)\ln(\zeta_\kappa)\sum_d d(\zeta_\kappa)^d \\ &= -\ln(1-\zeta_\kappa) - (1-\zeta_\kappa)\ln(\zeta_\kappa)\sum_d \frac{\mathrm{d}}{\mathrm{d}\zeta_\kappa}(\zeta_\kappa)^{d+1} - (\zeta_\kappa)^d \\ &= -\ln(1-\zeta_\kappa) - (1-\zeta_\kappa)\left(\frac{\mathrm{d}}{\mathrm{d}\zeta_\kappa}\frac{1}{1-\zeta_\kappa} - \frac{1}{1-\zeta_\kappa}\right)\ln\zeta_\kappa,\end{aligned} \tag{5.60}$$

where we used the geometric series. The last step leads to

$$\mathcal{S}_\kappa = -\ln(1-\zeta_\kappa) - \frac{\zeta_\kappa}{1-\zeta_\kappa}\ln\zeta_\kappa. \tag{5.61}$$

The sum over angular modes can be partially dealt by recognising that H_{lk} does not depend on k; the sum over k is thus trivial, with the effect of making present an additional coefficient, totalling the expression as $\mathcal{S}_{\text{out}} = \sum_{lk}\mathcal{S}_{lk} = \sum_l(2l+1)\mathcal{S}_l$. As aforementioned, $\mathcal{S}_l$ has an expression in terms of $\mathcal{S}_\kappa$. All of these steps culminate in the relation

$$\mathcal{S}_{\text{out}} = \sum_{l=1}^{\infty}(2l+1)\sum_{\kappa=1}^{n-1}\mathcal{S}_\kappa. \tag{5.62}$$

In summary, we were able to factorise the out-states in terms of angular modes, following from the same factorisation of the full states eq. (5.49). These were further factorised in terms of κ, as in eq. (5.55), for which the entropy $\mathcal{S}_\kappa$ is computed exactly and analytically to be eq. (5.61). The total entropy $\mathcal{S}_{\text{out}}$ turned out to be a sum over κ, followed by a sum of angular modes.

The l dependence of $\mathcal{S}_\kappa$ is hidden inside the eigenvalues λ_κ, which were constructed from transformations of the block matrices of the coupling K. In general, this sum is difficult and is done numerically, as did Srednicki [2]. Apart from the use of a Gaussian state, this method is general in quantum mechanics; but it can be made easier. In the next section, we will outline an alternative method which completely relies on the gaussianity of ϱ, being better suited for numerical computations.

The seminal results found in ref. [2] are reproduced and summarised in fig. 5.6, for a lattice of N sites and normalised spacing $\varepsilon = 1$. We compare our results with the most precise version of the coefficient of proportionality found in a lattice due to Lohmayer et al. [56]. Notice that in fig. 5.6 there is included a logarithmic term. This is a *regularisation-independent* contribution that will be discussed in

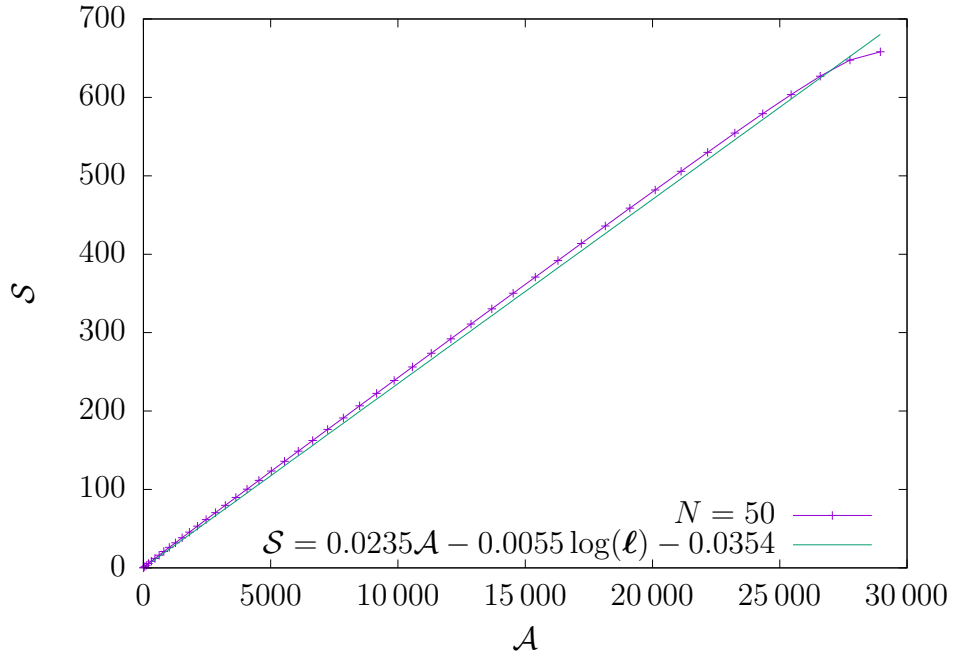

Figure 5.6: Area law of entanglement entropy for massless fields in lattice of size $N = 50$ and best fit found in ref. [56]. The coefficient of proportionality is $\sigma_2 \approx 0.0235$, with more than 99% of agreement with the results in that reference. The slight decay at entropy value for $x \approx 50$ is a numerical artefact appearing at the border of the lattice.

more detail in section 7.2.1. The method we used to reproduce it is the one to be outlined in the next chapter.

Chapter 6

Gaussian states in phase space

6.1 Kähler technology

In section chapter 4 we have introduced the phase space formalism that underlies canonical quantisation of field theory, and we have applied some of it in last section, namely on the use of the covariance of the canonical operators. In that case, we have chosen a particular Gaussian state: the vacuum $|0\rangle$.

As mentioned in preceding sections, the choice of vacuum in a general field theory on curved space might be subject of ambiguity. It is then desirable to expand the formalism of the quantum phase space to allow for this. The formalism that will be introduced in this section, based on refs. [57], clarifies this scenario by parametrising the choice of vacuum (and squeezed state in general) in terms of other structures that are defined on the phase space. We then endow $\mathbf{\Gamma}$ with additional structures that will be used to this end; to start, however, let us discuss in more detail its symplectic structure. The more mathematical underpinnings are based on refs. [58, 48].

Definition 17. The *linear symplectic group* Sp is a collection of transformations $M^{\mathsf{a}}{}_{\mathsf{b}}$ such that

$$\Omega_{\mathsf{cd}} M^{\mathsf{c}}{}_{\mathsf{a}} M^{\mathsf{d}}{}_{\mathsf{b}} = \Omega_{\mathsf{ab}}, \tag{6.1}$$

i.e. it *preserves* the symplectic form. Equivalently, it also preserves the inverse symplectic form

$$\Omega^{\mathsf{cd}} M_{\mathsf{c}}{}^{\mathsf{a}} M_{\mathsf{d}}{}^{\mathsf{b}} = \Omega^{\mathsf{ab}}. \tag{6.2}$$

In summary, the representation of the group elements in terms of matrices is

$$\mathrm{Sp}(\mathbf{V}) = \{M \in \mathrm{GL}(\mathbf{V}) \mid M^{\intercal}\Omega M = \Omega\}, \tag{6.3}$$

in which $\mathrm{GL}(\mathbf{V})$ is the linear group of matrices acting on the vector space $\mathbf{V}$.

This group is responsible for making possible to transform canonical coordinates without modifying the dynamics of the system being described; since the evolution is given, classicaly, by the Poisson brackets, and by the commutation relations in quantum mechanics, both of which are defined in terms of the symplectic form, it follows that action with symplectic transformations on the coordinates do not change the equations of motion. These are the linear canonical transformations (or linear symplectomorphisms in mathematical literature).

This can be extended to the non-linear case, by considering general transformations, and not just the ones given by matrices. We will limit our study to the linear group since our phase space is a vector space, and because we are interested in fields on discretised, compact spaces, for which $\mathbf{\Gamma}$ is finite-dimensional.

We now introduce two other structures: the first one connects symplectic spaces with complex ones.

Definition 18. A *linear complex structure* J on any symplectic vector space $\mathbf{V}$ is such that

$$\begin{aligned} J &\colon \mathbf{V} \to \mathbf{V} \\ J^{\mathsf{a}}{}_{\mathsf{c}} J^{\mathsf{c}}{}_{\mathsf{b}} &= -\delta^{\mathsf{a}}{}_{\mathsf{b}}; \end{aligned} \tag{6.4}$$

it is said compatible when

$$\Omega_{\mathsf{cd}} J^{\mathsf{c}}{}_{\mathsf{a}} J^{\mathsf{d}}{}_{\mathsf{b}} = \Omega_{\mathsf{ab}}, \tag{6.5}$$

i.e. $J \in \mathrm{Sp}(\mathbf{V})$.

Endowing the complexified phase space with a complex structure allows for an explicit separation of it into two complex conjugate subspaces, as we conjectured for **Sol**. A real vector space together with a complex structure can be made into a complex space by defining complex scalar multiplication $(a + \mathrm{i}b)v$ through real scalar multiplication as $av + bJv$ for $v \in \mathbf{V}$. This is *different* from complexification, starting from the fact that the complex dimension of $(\mathbf{V}, J)$ is half the real dimension of $\mathbf{V}$: $\dim_{\mathbb{C}}(\mathbf{V}, J) = \dim(\mathbf{V})/2$, whilst through complexification it follows that $\dim_{\mathbb{C}}(\mathbf{V}_{\mathbb{C}}) = \dim(\mathbf{V})$.

Recall from section chapter 4 that we complexified the phase space as $\mathbf{\Gamma}_{\mathbb{C}}$. This was in response to the splitting of the complex space of solutions **Sol** into $\mathbf{S}^+ \oplus \mathbf{S}^-$ given by introducing a hermitian form (positive-definite only on $\mathbf{S}^+$).

In a complex vector space the complex structure is diagonalisable.[1] Consider a complex structure of the following form. Its eigenvalues are $\pm\mathrm{i}$ (with degeneracy).

[1] After extending it by complex linearity: $J(v \otimes z) \equiv Jv \otimes z$, for $v \in \mathbf{V}$ and $z \in \mathbb{C}$, and recognising that $\mathrm{i}J$ is Hermitian.

That is, starting from a basis of $\mathbf{\Gamma}_{\mathbb{C}}$ with respect to which we write

$$J_0 = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}_{\text{canon}}, \tag{6.6}$$

in a new basis the same complex structure is

$$J_0 = \begin{pmatrix} \mathrm{i}I & 0 \\ 0 & -\mathrm{i}I \end{pmatrix}_{\text{mode}}. \tag{6.7}$$

The two eigenspaces, of eigenvalues $\pm\mathrm{i}$, represent the splitting of the space of solutions. The modes f belonging to $\mathbf{S}^+$ are the eigenvectors of J_0 whose eigenvalues are i, and respectively for $\overline{f}$ and $-\mathrm{i}$, under the isomorphism. In summary, given a complexified phase space $\mathbb{C} \otimes \mathbf{\Gamma} = \mathbf{\Gamma}_{\mathbb{C}} = (\mathbb{C}^{2N}, \Omega)$, a complex structure J splits it into

$$\begin{aligned} (\mathbf{\Gamma}_{\mathbb{C}}, J) &= (\mathbf{\Gamma}, J) \oplus \overline{(\mathbf{\Gamma}, J)} \\ \Xi_{\mathbb{C}} &= \frac{(\Xi - \mathrm{i}J\Xi)}{2} \oplus \frac{(\Xi + \mathrm{i}J\Xi)}{2}, \end{aligned} \tag{6.8}$$

in which $\Xi_{\mathbb{C}}$ denotes a vector with complex entries, and Ξ its real counterpart in non-complexified phase space. $(\Xi - \mathrm{i}J\Xi)$ and its complex conjugate span the subspaces of $(\mathbf{\Gamma}_{\mathbb{C}}, J)$ as constructed from the vectors in $\mathbf{\Gamma}$.

In the RHS of eq. (6.8), one has the identification of real spaces and their complex structure with a complex space, as just laid out above. In the LHS one has the complex vector space and its complex structure extended by linearity. Notice how $\Xi \mp \mathrm{i}J\Xi$ are eigenvectors of J with eigenvalues $\pm\mathrm{i}$, meaning $(\mathbf{\Gamma}, J) = \mathbf{S}^+$ and $\overline{(\mathbf{\Gamma}, J)} = \mathbf{S}^-$.

Our original intent was to study the Gaussian states of a quantum field. The expression of canonical coordinates in terms of creation and annihilation operators, as developed in section chapter 4 and in eq. (6.40), stemming from a change of basis, is intimately related to the complex structure.

Example 13. Let $\mathbf{\Gamma} = \mathbb{R}^2$ be the phase space of a harmonic oscillator of mass m and angular frequency ω, with the symplectic and complex structures

$$\Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad J = \begin{pmatrix} 0 & -\frac{1}{\omega} \\ \omega & 0 \end{pmatrix}. \tag{6.9}$$

Let $\Xi = \begin{pmatrix} q & p \end{pmatrix}^{\intercal}$ be the coordinate vector. Writing the components in the normal mode coordinates,

$$q = \frac{1}{\sqrt{2m\omega}} \left(a + a^\dagger\right) \quad \text{and} \quad p = -\mathrm{i}\sqrt{\frac{m\omega}{2}} \left(a - a^\dagger\right), \tag{6.10}$$

diagonalises the complex structure J_0 in $\mathbb{R}^2 \otimes \mathbb{C}$ as

$$\underbrace{\begin{pmatrix} 0 & -\frac{1}{\omega} \\ \omega & 0 \end{pmatrix}}_{\text{canon}} = \frac{1}{2} \begin{pmatrix} (m\omega)^{-\frac{1}{2}} & (m\omega)^{-\frac{1}{2}} \\ -\mathrm{i}(m\omega)^{\frac{1}{2}} & \mathrm{i}(m\omega)^{\frac{1}{2}} \end{pmatrix} \underbrace{\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}}_{\text{mode}} \begin{pmatrix} (m\omega)^{-\frac{1}{2}} & \mathrm{i}(m\omega)^{\frac{1}{2}} \\ (m\omega)^{-\frac{1}{2}} & -\mathrm{i}(m\omega)^{\frac{1}{2}} \end{pmatrix}, \quad (6.11)$$

wherein the LHS indicates J_0 in the canonical basis, whilst the RHS denotes the diagonalised complex structure in the normal mode basis under the change of basis with respect to which the coordinates are defined.

Following from this relation, the reference complex structure has information about the physical state of the system. In fact, the vacuum state of a harmonic oscillator, as defined by $a\,|0\rangle = 0$, can be parametrised by complex structures through its relation with the annihilation operators. In a $2N$-dimensional phase space, consider a general transformation, more so than the one in eq. (6.40),[2]

$$\begin{pmatrix} \vdots \\ \Phi_x \\ \vdots \\ \Pi_x \\ \vdots \end{pmatrix} = \begin{pmatrix} | & & | & | & & | \\ f_{\mathsf{a}1} & \dots & f_{\mathsf{a}N} & \overline{f}_{\mathsf{a}1} & \dots & \overline{f}_{\mathsf{a}N} \\ | & & | & | & & | \end{pmatrix} \begin{pmatrix} \vdots \\ a_\lambda \\ \vdots \\ a_\lambda^\dagger \\ \vdots \end{pmatrix}, \quad (6.12)$$

with mixed indices for N sites x and N modes k, both collected in the $2N$ vector space indices a. The reference complex structure can be written in these terms as[3]

$$J_0 = \begin{pmatrix} | & & | \\ f_{\mathsf{a}1} & \dots & \overline{f}_{\mathsf{a}N} \\ | & & | \end{pmatrix} \begin{pmatrix} \mathrm{i}I & 0 \\ 0 & -\mathrm{i}I \end{pmatrix} \begin{pmatrix} — & \overline{f}_{1\mathsf{b}} & — \\ & \vdots & \\ — & f_{N\mathsf{b}} & — \end{pmatrix} \quad (6.13)$$

Using the resolution of the identity, $\delta^{\mathsf{a}}{}_{\mathsf{b}} = f^{\mathsf{a}}{}_{\mathsf{c}}\overline{f}_{\mathsf{b}}{}^{\mathsf{c}} + \overline{f}^{\mathsf{a}}{}_{\mathsf{c}} f_{\mathsf{b}}{}^{\mathsf{c}}$, we can cook up a projector onto the positive frequency subspace:

$$\begin{aligned} a_\lambda = \Upsilon^\lambda &= f^\lambda{}_{\mathsf{c}}\overline{f}_{\mathsf{b}}{}^{\mathsf{c}}\,\Xi^{\mathsf{b}} \\ &= \frac{1}{2}\left(\delta^\lambda{}_{\mathsf{b}} - \mathrm{i}J_0{}^\lambda{}_{\mathsf{b}}\right)\Xi^{\mathsf{b}}, \end{aligned} \quad (6.14)$$

[2] f_λ form a basis of solutions to the Klein–Gordon equation, as in chapter 4; at the present point, the indices ranging from 1 to N refer to modes. For each mode, the mode basis vectors have components a in phase space.

[3] In index notation, $(J_0)^{\mathsf{a}}{}_{\mathsf{b}} = \mathrm{i}f^{\mathsf{a}}{}_{\mathsf{c}}\overline{f}_{\mathsf{b}}{}^{\mathsf{c}} - \mathrm{i}\overline{f}^{\mathsf{a}}{}_{\mathsf{c}} f_{\mathsf{b}}{}^{\mathsf{c}}$.

wherein we restricted the index a to its first N λ-entries.

Upon quantisation, it is then clear that, given a chosen of basis of normal modes, the definition of the vacuum state is tied to the associated reference structure. To make this explicit, we now write the vacuum state as

$$\forall\lambda\colon a_\lambda \left|J_0\right\rangle = 0. \tag{6.15}$$

A second vacuum, achieved by a unitary transformation, is associated to a second collection of creation and annihilation operators. Let U_γ be the unitary representation of the Bogoliubov matrix $M_\gamma \in \mathrm{Sqz}(J_0)$ such that $J_\gamma = M_\gamma J_0 M_\gamma^{-1}$. It follows that the transformation of modes $\widetilde{\Upsilon}^{\mathsf{a}} = (M_\gamma)^{\mathsf{a}}{}_{\mathsf{b}}\Upsilon^{\mathsf{b}}$ defines a new set of annihilation operators

$$\tilde{a}_\lambda = \sum_{l=1}^{N} \alpha_{\lambda l} a_l + \beta_{\lambda l} a_l^\dagger, \tag{6.16}$$

implementing the *squeeze* unitary operation

$$U_\gamma\colon a_\lambda \mapsto U_\gamma a_\lambda U_\gamma^{-1}, \tag{6.17}$$

that annihilates the *squeezed pure state*

$$\forall\lambda\colon \tilde{a}_\lambda \left|J_\gamma\right\rangle = 0, \tag{6.18}$$

of squeezing parameter γ.

Before moving on to the application of these techniques, we briefly mention that these methods are particularly interesting given the unifying treatment of bosonic and fermionic Gaussian states. In this discussion, focus was placed on the symplectic group, because it describes the kinematics of bosons; fermions, on the other hand, are described by the orthogonal group. Both of them, however, share the property of having their quantum states described by a compatible complex structure.

The final structure to be introduced is a familiar one from other cases, inserting in our vector spaces a inner product. It is related to the previous two structures in a special way.

Definition 19. A positive-definite metric G, on a symplectic vector space with a complex structure, satisfying

$$G_{\mathsf{ab}} = \Omega_{\mathsf{ac}} J^{\mathsf{c}}{}_{\mathsf{b}}, \tag{6.19}$$

is said to be *compatible* with the preceding structures.

The metric compatibility is such that

$$\Omega_{\mathsf{ac}} J^{\mathsf{c}}{}_{\mathsf{b}} \Xi^{\mathsf{a}} \Xi^{\mathsf{b}} > 0, \tag{6.20}$$

for all $\Xi^{\mathsf{a}} \in \mathbf{V}$. This can be demonstrated consistent from antisymmetry of the symplectic form, and its compatibility with the complex structure:

$$\begin{aligned} -\Omega_{\mathsf{ba}} &= \Omega_{\mathsf{ab}} \\ -\Omega_{\mathsf{ba}} J^{\mathsf{a}}{}_{\mathsf{c}} &= \Omega_{\mathsf{ab}} J^{\mathsf{a}}{}_{\mathsf{c}} \\ &= \Omega_{\mathsf{xy}} J^{\mathsf{x}}{}_{\mathsf{a}} J^{\mathsf{y}}{}_{\mathsf{b}} J^{\mathsf{a}}{}_{\mathsf{c}} \\ &= -\Omega_{\mathsf{xy}} \delta^{\mathsf{x}}{}_{\mathsf{c}} J^{\mathsf{y}}{}_{\mathsf{b}} \\ &= -G_{\mathsf{cb}} \\ \implies G_{\mathsf{bc}} &= G_{\mathsf{cb}}. \end{aligned} \tag{6.21}$$

That is, the metric can be represented by a symmetric matrix. These three compatible structures, together, are known as *Kähler structures.*

6.1.1 Linear groups: symplectic, orthogonal and complex

Analogously to the case of the symplectic form, and its symplectic group, both structures have their own preserving group of transformations. For the metric it is the usual orthogonal group of matrices ,

$$\mathrm{O}(\mathbf{V}) \equiv \{O \in \mathrm{GL}(\mathbf{V}) \mid OGO^{\intercal} = G\}. \tag{6.22}$$

For the complex structure, the associated group is that of complex matrices. Let $\mathbf{V}$ be a real vector of dimension $2N$, we may write

$$\mathrm{GL}(N, \mathbb{C}) \subset \mathrm{GL}(\mathbf{V}), \tag{6.23}$$

for $N \times N$ matrices over the complex numbers. This relies on the isomorphism

$$X + \mathrm{i}Y \mapsto \begin{pmatrix} X & -Y \\ Y & X \end{pmatrix}, \tag{6.24}$$

between matrices of complex entries $X + \mathrm{i}Y$, and matrices with real entries of twice the number of columns and rows. A transformation which preserves the complex structure is one that commutes with it:

$$\mathrm{GL}(N, \mathbb{C}) \equiv \{Z \in \mathrm{GL}(\mathbf{V}) \mid JZ = ZJ\}; \tag{6.25}$$

this is case of $X + \mathrm{i}Y$ above.

The fact that the three structures, G, J and Ω can be compatible implies an intersecting region of the three preserving groups of transformation. In fact, one has that they all intersect at the unitary group U:

$$\begin{aligned} \mathrm{U}(N) &= \mathrm{Sp}(2N,\mathbb{R}) \cap \mathrm{O}(2N,\mathbb{R}) \\ &= \mathrm{O}(2N,\mathbb{R}) \cap \mathrm{GL}(N,\mathbb{C}) \\ &= \mathrm{GL}(N,\mathbb{C}) \cap \mathrm{Sp}(2N,\mathbb{R}), \end{aligned} \tag{6.26}$$

wherein we specify the groups by the parameters of their representation spaces. Let us choose standard structures to assess this property:

$$\underset{\Omega}{\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}} \underset{J}{\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}} = \underset{G}{\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}} \tag{6.27}$$

it is enough to verify the intersections by direct computation:

1. $\mathrm{O}(2N,\mathbb{R}) \cap \mathrm{GL}(N,\mathbb{C})$. Let us find out what other properties a matrix such as the one in eq. (6.24) must satisfy in order for it to be orthogonal,

$$\begin{aligned} \begin{pmatrix} X & -Y \\ Y & X \end{pmatrix} \begin{pmatrix} X^\intercal & Y^\intercal \\ -Y^\intercal & X^\intercal \end{pmatrix} &= \begin{pmatrix} XX^\intercal + YY^\intercal & XY^\intercal - YX^\intercal \\ -XY^\intercal + YX^\intercal & XX^\intercal + YY^\intercal \end{pmatrix} \\ &= \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}. \end{aligned} \tag{6.28}$$

2. $\mathrm{GL}(N,\mathbb{C}) \cap \mathrm{Sp}(2N,\mathbb{R})$. Inserting a complex matrix in the definition of a symplectic matrix yields

$$\begin{aligned} \begin{pmatrix} X & -Y \\ Y & X \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} X^\intercal & Y^\intercal \\ -Y^\intercal & X^\intercal \end{pmatrix} &= \begin{pmatrix} YX^\intercal - XY^\intercal & YY^\intercal + XX^\intercal \\ -YX^\intercal + XY^\intercal & -YY^\intercal - XX^\intercal \end{pmatrix} \\ &= \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \end{aligned} \tag{6.29}$$

   which are the same conditions of the first item.

3. $\mathrm{Sp}(2N,\mathbb{R}) \cap \mathrm{O}(2N,\mathbb{R})$. In this case, we prove that symplectic, orthogonal matrices also commute with the complex structure:

$$\begin{aligned} \Omega &= M\Omega M^\intercal \\ &= M\Omega M^{-1} \implies \Omega M = M\Omega. \end{aligned} \tag{6.30}$$

Notice that $\Omega^\intercal = J$, indicating that the transpose of the lower, right-hand above is

$$\begin{aligned} M^\intercal J &= J M^\intercal \\ \implies MJ &= JM. \end{aligned} \tag{6.31}$$

Because M is complex, then from the first two items it is also unitary.

Finally, we prove that the conditions implied by the items above leads to the unitarity of $X + \mathrm{i}Y$:

$$\begin{aligned} (X + \mathrm{i}Y)\,(X - \mathrm{i}Y)^\intercal &= XX^\intercal + YY^\intercal + \mathrm{i}\,(XY^\intercal - YX^\intercal) \\ &= I, \end{aligned} \tag{6.32}$$

hence $X + \mathrm{i}Y$ is unitary.

It is worth noting that the canonical choice of compatible triple in eq. (6.27) is always possible. The *symplectic basis* is the one with respect to which the symplectic form takes that form, and it can always be found (cf. refs. [58, 48]). After the choice of complex structure is made, one finds that the compatible metric yields the standard inner product on a vector space.

The unitary representation of the symplectic group

As a Lie group, the symplectic transformations are generated by a Lie algebra. In fact, the symplectic algebra $\mathfrak{sp}$ is isomorphic to the algebra of quadratic functions on phase space, that also happen to close in its own subalgebra of classical observables. Let a quadratic functions on phase be $\mathcal{K} = K_{\mathsf{ab}}\Xi^{\mathsf{a}}\Xi^{\mathsf{b}}/2$, in which it is enough to consider K_{ab} to be symmetric, because it is contracting with a symmetric tensor. The Poisson brackets yield

$$\begin{aligned} \{\mathcal{K}_1, \mathcal{K}_2\} &= \Omega^{\mathsf{ab}}\partial_{\mathsf{a}}\mathcal{K}_1\partial_{\mathsf{b}}\mathcal{K}_2 \\ &= \Omega^{\mathsf{ab}}(K_1)_{\mathsf{x}\mathsf{y}}\delta^{\mathsf{x}}_{\mathsf{a}}\Xi^{\mathsf{y}}(K_2)_{\mathsf{i}\mathsf{j}}\delta^{\mathsf{i}}_{\mathsf{b}}\Xi^{\mathsf{j}} \\ &= \Omega^{\mathsf{ab}}(K_1)_{\mathsf{a}\mathsf{y}}(K_2)_{\mathsf{b}\mathsf{j}}\Xi^{\mathsf{y}}\Xi^{\mathsf{j}}. \end{aligned} \tag{6.33}$$

The result is once again a quadratic function, with $(K_3)_{\mathsf{y}\mathsf{j}} = \Omega^{\mathsf{ab}}(K_1)_{\mathsf{a}\mathsf{y}}(K_2)_{\mathsf{b}\mathsf{j}}$ symmetric in $\mathsf{y}\mathsf{j}$. To check that these quadratic functions generate the symplectic group, we need to know what are the elements of the symplectic algebra.

Under the exponential map, next to the identity, a symplectic matrix is $M = \exp(\epsilon T)$ with T the generator and $\epsilon \in \mathbb{R}$ parametrises Sp starting from the identity element. It is enough to evaluate what T must obey, to first order:

$$\begin{aligned} \Omega &= \mathrm{e}^{\epsilon T}\Omega\mathrm{e}^{\epsilon T^\intercal} \\ &\approx (1 + \epsilon T)\,\Omega\,(1 + \epsilon T^\intercal) \end{aligned} \tag{6.34}$$

from which follows

$$0 = (T\Omega + \Omega T^{\intercal})\,\epsilon. \tag{6.35}$$

Choosing $T = K\Omega$, for K a symmetric matrix, solves the problem. The explicit Lie algebra isomorphism from the algebra of quadratic functions to the symplectic algebra consists of identifying the symmetric matrix K that parametrises $\mathfrak{sp}$ with the symmetric forms K_{ab} defining the quadratic functions.

The generators of the unitary subgroup can also be found. In order for M to be orthogonal, one must have that $\exp(\epsilon T^{\intercal}) = \exp(-\epsilon T)$; thus, $T = K_{\mathrm{O}}\Omega$ must be antisymmetric. If $K_{\mathrm{O}} = K - \Omega K \Omega$, this is satisfied. K_{O} is still symmetric, and[4]

$$\begin{aligned}(K_{\mathrm{O}}\Omega)^{\intercal} &= \Omega^{\intercal}\,(K - \Omega K\Omega)\\ &= -\Omega K - K\Omega\\ &= (-\Omega K\Omega^{\intercal} - K)\,\Omega\\ &= (\Omega K\Omega - K)\,\Omega\\ &= -K_{\mathrm{O}}\Omega.\end{aligned} \tag{6.36}$$

Finally, we are interested in another subgroup, the $\mathrm{Sqz}(J)$, of transformations that *do not* preserve the complex structure. It can be shown (see appendices of ref. [57]) that the generators of this subgroup are symmetric matrices. In fact, the elements themselves are symmetric: $\exp(\epsilon T)^{\intercal} = \exp(\epsilon T^{\intercal}) = \exp(\epsilon T)$. Similarly to the case above, we have that $K_{\mathrm{Sqz}}\Omega$ must be symmetric, which is the case if $K_{\mathrm{Sqz}} = K + \Omega K \Omega$:

$$\begin{aligned}(K_{\mathrm{Sqz}}\Omega)^{\intercal} &= -\Omega K + K\Omega\\ &= -\Omega K\Omega^{\intercal}\Omega + K\Omega\\ &= (\Omega K\Omega + K)\,\Omega\\ &= K_{\mathrm{Sqz}}\Omega.\end{aligned} \tag{6.37}$$

We have thus identified the symplectic transformations that either preserve or not the complex structure (cf. fig. 6.1). When the vector space aforementioned is the phase space $\mathbf{\Gamma}$, one is dealing with classical mechanics.

The symplectic group is still the same in quantum mechanics, but it must first be represented as unitary transformations (different in principle from the unitary group at the intersection). Exploring the fact that symplectic generators correspond to quadratic functions, and that a self-adjoint representation of linear functions is already known (the Schrödinger representation), we can then construct a unitary representation of the symplectic group [3, 37]. That is

$$U = \exp\Big(-\mathrm{i}\frac{\epsilon}{2} K_{\mathsf{ab}} \Xi^{\mathsf{a}} \Xi^{\mathsf{b}}\Big), \tag{6.38}$$

[4] We are still using the structures chosen above. Verify that $\Omega^{\intercal} = -\Omega = J$.

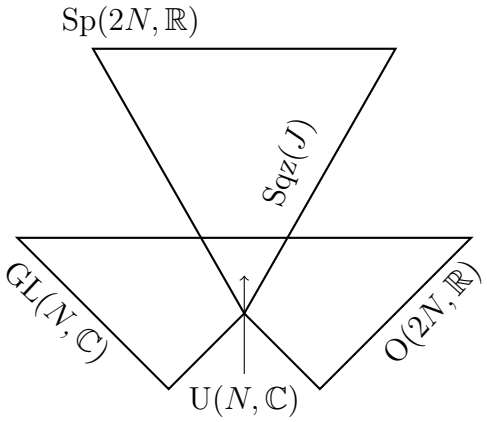

Figure 6.1: A map of the structures inside the symplectic group; the complex, orthogonal and symplectic group meet in a particular way at the unitary group, given a choice of reference triad of compatible structures (G, J, Ω), and the squeeze group of symplectic matrices that do not preserve J are contained outside the region $\mathrm{U}(N, \mathbb{C})$.

for U representing

$$M = \exp\big(\epsilon K_{\mathsf{ac}} \Omega^{\mathsf{cb}}\big). \tag{6.39}$$

In eq. (6.38) the operators are still self-adjoint, ensuring the unitarity of U.

6.2 Entanglement entropy and the covariance matrix

Gaussian states have the property of being completely determined by correlation of the canonical variables. The aforementioned Wick's theorem (theorem 4) is essential in determining this fact. By relying on it, what follows outlines the use of two-point functions in computing entropy, elucidating the role of entanglement entropy as a quantitative measure of quantum correlations. This leads to improved numerical implementation and relies of two steps: firstly, we build a relation between the quantum state and correlations; secondly, we express the correlations in terms of the coupling matrix in the Hamiltonian. Before achieving a general expression in terms of the complex structure, our choices are particular to the case which interests us in section 7.2, based on ref. [59] and reviewed in ref. [40].

In matrix form, we parametrise the transformation from mode basis to canonical

coordinates as

$$\Xi^a = M^{\mathsf{a}}{}_{\mathsf{b}}\, \Upsilon^b \tag{6.40}$$

$$\begin{pmatrix} \Phi \\ \Pi \end{pmatrix} = \begin{pmatrix} u & u \\ \mathrm{i}v & -\mathrm{i}v \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}, \tag{6.41}$$

wherein Φ and Π each denote a vector of configuration and momentum operators; we can take it to be indexed by vertices x of the graph. The same holds for the creation and annihilation operators.

This expansion demands that the real matrices u and v obey

$$2uv^\intercal = -I \tag{6.42}$$

in order to preserve $[\Phi_x, \Pi_y] = \mathrm{i}\delta_{xy}$ (to verify, simply insert eq. (6.40) in the commutator). In components, $2\sum_k u_{xk}v_{ky} = -\delta_{xy}$. This is exactly the mode expansion of earlier sections (chapter 4) meaning it also implies that $\left[a_k, a_l^\dagger\right] = \delta_{kl}$. This is not its most general form, which could include matrices of complex entries, but it is enough for our purposes.

Besides the mode expansion that is done in the global vacuum state, dual to the vertices d.o.f., the following development relies on normal modes of the reduced state, which we posit to be

$$\varrho = \prod_l \left(1 - \mathrm{e}^{-w_l}\right) \exp\left(-\sum_k w_k a_k^\dagger a_k\right), \tag{6.43}$$

wherein $\hat{n}_k = a_k^\dagger a_k$ defines the basis on which the *entangling Hamiltonian* $\sum_k w_k \hat{n}_k$ is diagonalised. This hypothesis relies on a mode expansion such as 6.40.

This density matrix has the aspect of a product of thermal matrices, each pertaining to a possible canonical ensemble of temperature T_k and energy ω_k that could be defined through $w_k = \omega_k/T_k$. In this manner, the normalisation constant would refer to a product of the respective partition functions. This interpretation is not always available and so we will not impose it.

Relying on the "expansion" in thermal states above, valid for any Gaussian state (cf. ref. [60]), and because we are working with bosonic fields, it follows that the associated occupation number $n_k = a_k^\dagger a_k$ has expectation value

$$\langle n_k \rangle = \mathrm{tr}(\varrho \hat{n}_k) = \frac{1}{\mathrm{e}^{w_k} - 1}, \tag{6.44}$$

given by a Bose–Einstein distribution with respect to w_k. The correlation functions for the reduced state can be re-expressed in these terms. That is, $\mathrm{tr}(\varrho \Phi_x \Phi_y)$ and $\mathrm{tr}(\varrho \Pi_x \Pi_y)$ are

$$Q = u \langle n \rangle u^\intercal + u \left(\langle n \rangle + 1\right) u^\intercal \tag{6.45}$$

and

$$P = v\,\langle n\rangle\,v^{\intercal} + v\,(\langle n\rangle + 1)\,v^{\intercal}, \tag{6.46}$$

respectively. We write $\langle n\rangle$ for the diagonal matrix with entries $\langle n_k\rangle$,

$$\langle n\rangle \equiv \begin{pmatrix} \langle n_1\rangle & & & & \\ & \langle n_2\rangle & & & \\ & & \ddots & & \\ & & & \langle n_k\rangle & \\ & & & & \ddots \end{pmatrix}. \tag{6.47}$$

The commutation constraint eq. (6.42) implies $uv^{\intercal} = -I/2$. Inserting this relation in the expressions for Q and P, implies that

$$QP = \frac{1}{4}u(2\,\langle n\rangle + 1)^2 u^{-1}; \tag{6.48}$$

connecting the eigenvalues of QP to those of ϱ.

The matrix u provides a similarity transformation in Equation (6.48), which does not change the eigenvalues of the similar matrices. Therefore, $(2\,\langle n\rangle + 1)^2/4$ is the diagonal form of QP, whose eigenvalues are

$$\begin{aligned} \varsigma_k^2 &= \frac{1}{4}\left(\frac{2}{\mathrm{e}^{w_k} - 1} + 1\right)^2 \\ &= \frac{1}{4}\coth^2\!\left(\frac{w_k}{2}\right). \end{aligned} \tag{6.49}$$

This expression realises the first step outlined at the beginning of the section: the eigenvalues of the covariance matrix is expressed directly in terms of the eigenvalues of the state operator.

Before we move on to the second step, we compute the entanglement entropy explicit in terms of ς_k. To start, we define a different measure of entropy.

Definition 20. The Rényi entropy is

$$\mathcal{S}_r = \frac{1}{1-r}\ln(\operatorname{tr}\varrho^r), \tag{6.50}$$

for integers r.

The Rényi entropy reduces to the von Neumann entropy at the limit $r \to 1$

when r is analytically continued to $\mathbb{R}$. Assuming a normalised state,

$$\begin{aligned}\lim_{r\to 1}\mathcal{S}_r &= \lim_{r\to 1}\frac{1}{1-r}\ln(\operatorname{tr}\varrho^r)\\ &= \lim_{r\to 1}\frac{1}{-\operatorname{tr}\varrho^r}\operatorname{tr}(\varrho^r\ln\varrho)\\ &= -\operatorname{tr}(\varrho\ln\varrho),\end{aligned} \tag{6.51}$$

wherein the second line follows from L'Hôpital's rule (and the fact that ϱ is bounded and Hermitian).

Explicitly, in terms of the eigenvalues,

$$\begin{aligned}\operatorname{tr}\varrho^r &= \prod_l\left(1-\mathrm{e}^{-w_l}\right)^r\prod_k\sum_{\{n_k\}}\mathrm{e}^{-w_k n_k r}\\ &= \prod_k\frac{\left(1-\mathrm{e}^{-w_k}\right)^r}{1-\mathrm{e}^{-rw_k}};\end{aligned} \tag{6.52}$$

inserting the expression for w_k in terms of ς leads to

$$\operatorname{tr}\varrho^r = \prod_k\left[\left(\varsigma_k+\frac{1}{2}\right)^r-\left(\varsigma_k-\frac{1}{2}\right)^r\right]^{-1}. \tag{6.53}$$

The rest of the expression of the entanglement entropy in terms of the Rényi entropy follows straightforwardly,[5]

$$\begin{aligned}\mathcal{S} &= \lim_{r\to 1}\frac{1}{1-r}\ln\left[\prod_k\frac{1}{\left(\varsigma_k+\frac{1}{2}\right)^r-\left(\varsigma_k-\frac{1}{2}\right)^r}\right]\\ &= \lim_{r\to 1}\frac{-1}{1-r}\sum_k\ln\left[\left(\varsigma_k+\frac{1}{2}\right)^r-\left(\varsigma_k-\frac{1}{2}\right)^r\right]\\ &= \lim_{r\to 1}\sum_k\left[\left(\varsigma_k+\frac{1}{2}\right)^r\ln\left(\varsigma_k+\frac{1}{2}\right)-\left(\varsigma_k-\frac{1}{2}\right)^r\ln\left(\varsigma_k-\frac{1}{2}\right)\right],\end{aligned} \tag{6.54}$$

leading to

$$\mathcal{S} = \sum_k\left[\left(\varsigma_k+\frac{1}{2}\right)\ln\left(\varsigma_k+\frac{1}{2}\right)-\left(\varsigma_k-\frac{1}{2}\right)\ln\left(\varsigma_k-\frac{1}{2}\right)\right]. \tag{6.55}$$

The final step in realising the algorithm is to connect the covariance eigenvalues ς to the matrix K_{xy} coupling degrees of freedom in neighbouring vertices. This relies on the fact that K_{xy} is a symmetric positive-definite matrix, and thus diagonalisable.

[5]The $r\to 1$ limit is not regular, returning $0/0$ naïvely. We use L'Hôpital's rule to compute the limit.

In more generality, consider a Hamiltonian form that is block diagonal, including terms coupling different momenta:

$$H = \frac{1}{2}\Xi^{\intercal}\begin{pmatrix} K & 0 \\ 0 & W \end{pmatrix}\Xi. \tag{6.56}$$

We assume that W is also symmetric and positive-definite. Such a matrix can act as a metric in configuration space (*not* the same metric as G_{ab}) and may be used to raise and lower indices indices. We can then rewrite H as

$$H = \frac{1}{2}W_{xy}\left(\Pi_x - \mathrm{i}\left(K^{1/2}\right)_{xi}\Phi_i\right)^{\dagger}\left(\Pi_y - \mathrm{i}\left(K^{1/2}\right)_{yj}\Phi_j\right) + W_{xy}\left(K^{1/2}\right)_{xi}\delta_{iy}, \tag{6.57}$$

wherein the last term comes from using the commutator on $-\mathrm{i}\left(K^{1/2}\right)_{xi}\Phi_i\Pi_y$ in order to cancel a similar contribution with opposite ordering. The first term takes the role of some creation and annihilation opeartors $b^{\dagger}b$ whilst the second takes the role of the ground state energy.

The presence of the W coupling does not modify the Gaussian states of the form found in section 5.3.2, eq. (5.49). This follows from the fact that such Gaussian state is the vacuum corresponding to the annihilation operator defined as

$$b_x\left|0\right\rangle = W_{xy}\left(\Pi_y - \mathrm{i}\left(K^{1/2}\right)_{yj}\Phi_j\right)\left|0\right\rangle = 0. \tag{6.58}$$

One can see from this expression that the presence of W is immaterial in solving for $\left|0\right\rangle$ in configuration basis.

The two point functions follow from eq. (5.49),

$$\varrho(\Phi,\Phi') = \frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}}\exp\left(-\frac{\Phi^{\intercal}K^{1/2}\Phi}{2}\right)\exp\left(-\frac{\Phi'^{\intercal}K^{1/2}\Phi'}{2}\right), \tag{6.59}$$

as

$$\left\langle 0\right|\Phi_x\Phi_y\left|0\right\rangle = \frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}}\int\prod_{i=1}^{N}\mathrm{d}\Phi_i\,\Phi_x\Phi_y\exp\left(-\Phi^{\intercal}K^{1/2}\Phi\right), \tag{6.60}$$

and

$$\left\langle 0\right|\Pi_x\Pi_y\left|0\right\rangle = -\frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}}\int\prod_{i=1}^{N}\mathrm{d}\Phi_i\exp\left(-\frac{\Phi^{\intercal}K^{1/2}\Phi}{2}\right) \frac{\partial}{\partial\Phi_x}\frac{\partial}{\partial\Phi_y}\exp\left(-\frac{\Phi^{\intercal}K^{1/2}\Phi}{2}\right), \tag{6.61}$$

for which we have used the Schrödinger representation $\Pi = -\mathrm{i}\,\partial/\partial\Phi$. Performing the derivations,

$$\langle 0|\Pi_x\Pi_y|0\rangle = \frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}} \int \prod_{i=1}^{N} \mathrm{d}\Phi_i \left(K_{xy}^{1/2} - K_{xi}^{1/2}\Phi_i K_{yj}^{1/2}\Phi_j\right) \exp\bigl(-\Phi^{\intercal} K^{1/2}\Phi\bigr). \tag{6.62}$$

A general solution for these Gaussian integrals is

$$\int \prod_{i=1}^{N} \mathrm{d}\Phi_i\, f(\Phi) \exp\left(-\frac{1}{2}\Phi^{\intercal} A\Phi\right) = \sqrt{\frac{(2\pi)^N}{\det A}} \times \exp\left(\frac{1}{2}\sum_{x,y}(A^{-1})_{xy}\frac{\partial}{\partial\Phi_x}\frac{\partial}{\partial\Phi_y}\right) f(\Phi)\Big|_{\Phi=0}. \tag{6.63}$$

Applying this to the two correlators above yields

$$\begin{aligned}\langle 0|\Phi_x\Phi_y|0\rangle &= \frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}}\sqrt{\frac{(2\pi)^N}{\det 2K^{1/2}}}\exp\left(\frac{1}{4}(K^{-1/2})_{ij}\partial_i\partial_j\right)\Phi_x\Phi_y\Big|_{\Phi=0} \\ &= \frac{1}{2}(K^{-1/2})_{xy}\end{aligned} \tag{6.64}$$

and

$$\begin{aligned}\langle 0|\Pi_x\Pi_y|0\rangle &= \frac{\sqrt{\det K^{1/2}}}{\pi^{N/2}}\sqrt{\frac{(2\pi)^N}{\det 2K^{1/2}}}\Bigg(K_{xy}^{1/2} \\ &\qquad - \exp\left(\frac{1}{4}(K^{-1/2})_{ij}\partial_i\partial_j\right)K_{xa}^{1/2}\Phi_a K_{yb}^{1/2}\Phi_b\Big|_{\Phi=0}\Bigg) \\ &= K_{xy}^{1/2} - \frac{1}{2}K_{xi}^{1/2}(K^{-1/2})_{ij}K_{yj}^{1/2} \\ &= \frac{1}{2}K_{xy}^{1/2}.\end{aligned} \tag{6.65}$$

In summary, we conclude that

$$Q_{xy} = \frac{1}{2}\left(K^{-1/2}\right)_{xy} \tag{6.66}$$

$$P_{xy} = \frac{1}{2}\left(K^{1/2}\right)_{xy}. \tag{6.67}$$

We are interested in finding the entropy for a subregion $\mathtt{X}$. To conclude the algorithm, we restrict the entries to $x, y \in \mathtt{X}$ in Q and P, and proceed to find QP,

$$(QP)_{xy} = \frac{1}{4}\sum_{i=1}^{n}\left(K^{-1/2}\right)_{xi}\left(K^{1/2}\right)_{iy}. \tag{6.68}$$

The eigenvalues of this matrix are ς_k^2, whose square root are to be inserted in formula 6.55. Hence, we have found $\mathcal{S}$. One concludes that the reduced state does not appear as a vacuum because correlations between oscillators at vertices in the complementary regions are being ignored.

The way in which this algorithm is an improvement over the one presented in the previous section, is that the sum over κ and d in eq. (5.58) is bypassed, and only the sum over the modes lk remains, after calculating the mode entropy through eq. (6.55).

Example 14. Consider a lattice with spacing ε, N vertices and a Hamiltonian written in terms of normal modes,

$$H = \sum_k \left(\omega_k b_k^\dagger b_k + \frac{1}{2} \right), \tag{6.69}$$

for some pair of creation/annihilation operators b_k. To achieve this, we express the fields in their Fourier components

$$\Phi_x = \sum_{k=1}^{N} \frac{1}{\sqrt{2\omega_k}} \left(b_k^\dagger \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\mathrm{i}kx\varepsilon} + b_k \mathrm{e}^{-\mathrm{i}\omega t} \mathrm{e}^{\mathrm{i}kx\varepsilon} \right) \tag{6.70}$$

$$\Pi_x = \sum_{k=1}^{N} \mathrm{i}\sqrt{\frac{\omega_k}{2}} \left(b_k^\dagger \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\mathrm{i}kx\varepsilon} - b_k \mathrm{e}^{-\mathrm{i}\omega t} \mathrm{e}^{\mathrm{i}kx\varepsilon} \right). \tag{6.71}$$

From these expressions, the correlator matrices Q_{xy} and P_{xy} are

$$Q_{xy} = \sum_k \frac{1}{2\sqrt{\omega_k}} \mathrm{e}^{-\mathrm{i}k(x-y)\varepsilon} \tag{6.72}$$

$$P_{xy} = \sum_k \frac{\sqrt{\omega_k}}{2} \mathrm{e}^{-\mathrm{i}k(x-y)\varepsilon}. \tag{6.73}$$

6.2.1 Entanglement entropy and covariance from Kähler structures

From the idea that complex structures carry the information in Gaussian states, it follows that the covariance matrix must have a direct connection with this geometric structure. Indeed, we define the covariance matrix in more generality as follows:

Definition 21. Let the $(\Xi^{\mathsf{a}}) = (\Phi, \Pi)$ be the canonical phase space coordinates represented in an algebra of operators. Let ϱ be a state. Then

$$\mathcal{C}^{\mathsf{ab}} \equiv \mathrm{tr}\big(\varrho \Xi^{\mathsf{a}} \Xi^{\mathsf{b}}\big) \tag{6.74}$$

is the covariance matrix of that state.

Take $|J\rangle$ to be the vector in $\mathbf{H}$ associated with a Gaussian state ϱ. From the definition above we can re-express the covariance matrix to establish its relation to the Kähler structures:[6]

$$\begin{aligned}\mathcal{C}^{\mathsf{ab}} &= \langle J|\Xi^{\mathsf{a}}\Xi^{\mathsf{b}}|J\rangle \\ &= \frac{1}{2}\langle J|\left[\Xi^{\mathsf{a}},\Xi^{\mathsf{b}}\right]_{+}+\left[\Xi^{\mathsf{a}},\Xi^{\mathsf{b}}\right]|J\rangle\,,\end{aligned} \tag{6.75}$$

in which the second term yields $\mathrm{i}\Omega^{\mathsf{ab}}$, whilst the second term bears information about the covariance. It is a symmetric and positive-definite tensor. Computing it in the reference vacuum $|J_0\rangle$ returns

$$\begin{aligned}\mathcal{C}^{\mathsf{ab}} &= \langle J_0|\Xi^{\mathsf{a}}\Xi^{\mathsf{b}}|J_0\rangle \\ &= \frac{1}{2}\left(\delta^{\mathsf{ab}}+\mathrm{i}\Omega^{\mathsf{ab}}\right),\end{aligned} \tag{6.76}$$

we see that the symmetric part is the metric compatible to J_0, δ^{ab}.[7]

In terms of covariance, this signifies absence of correlations amongst degrees of freedom but the trivial self-correlations in the diagonal. The non-trivial correlations amongst distinct degrees of freedom, such as the ones encountered in section 6.2, eq. (6.66), for a lattice system, appear after a squeeze of the state $|J_0\rangle$ or, equivalently, a Bogoliubov transformation of J_0.

Under a symplectic transformation M, we can modify the covariance matrix by virtue of the action of M on the metric, $M^{\intercal}GM$. That is,

$$\delta^{\mathsf{cd}}M_{\mathsf{c}}{}^{\mathsf{a}}M_{\mathsf{d}}{}^{\mathsf{b}}=G^{\mathsf{ab}}. \tag{6.77}$$

Simplifying, in matrix notation, to

$$G=M^{\intercal}M. \tag{6.78}$$

It turns out that the covariance matrix takes the form

$$\mathcal{C}^{\mathsf{ab}}=\frac{1}{2}\left(G^{\mathsf{ab}}+\mathrm{i}\Omega^{\mathsf{ab}}\right). \tag{6.79}$$

[6] $[A,B]_{+}\equiv AB+BA$.

[7] A fermionic system, on the other hand, would have the roles of the metric and the symplectic structure reversed: Ω would bear information about correlations since the corresponding algebra product is instead the symmetric anticommutator, given by G. See [61].

In the previous section, what we were referring to as covariance was in fact G, taking the form

$$G = \begin{pmatrix} Q & 0 \\ 0 & P \end{pmatrix} \tag{6.80}$$

for Q and P symmetric. This is a particular case of eq. (6.78) when

$$M^\intercal M = \begin{pmatrix} Q & 0 \\ 0 & P \end{pmatrix}. \tag{6.81}$$

Let

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{6.82}$$

in terms of block matrices. The condition that it is symplectic is

$$\begin{aligned} M^\intercal \Omega M &= \begin{pmatrix} -C^\intercal A + A^\intercal C & -C^\intercal B + A^\intercal D \\ -D^\intercal A + B^\intercal C & -D^\intercal B + B^\intercal D \end{pmatrix} \\ &= \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \end{aligned} \tag{6.83}$$

A solution of this form, satisfying eq. (6.80), can be found by setting $B = C = 0$. This implies that

$$M^\intercal M = \begin{pmatrix} A^\intercal A & 0 \\ 0 & D^\intercal D \end{pmatrix}, \tag{6.84}$$

i.e. A acts as $Q^{1/2}$ and D as $P^{1/2}$, and that

$$\begin{pmatrix} 0 & A^\intercal D \\ -D^\intercal A & 0 \end{pmatrix} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{6.85}$$

meaning that $Q = P^{-1}$. This is precisely what happens in eq. (6.66), ultimately leading to our desired expression for $\mathcal{S}$, eq. (6.55).

Entanglement entropy can be also cast in terms of the complex structure. Resorting to the compatibility of the structures, we can write $G = \Omega J$. The covariance matrix can then be put in the form

$$\mathcal{C}^{\mathsf{ab}} = \frac{\mathrm{i}}{2}\Omega(I - \mathrm{i}J). \tag{6.86}$$

In terms of the complex structure J the entanglement entropy is then rewritten as (see ref. [3])

$$\mathcal{S} = \mathrm{tr}\left[\frac{I - \mathrm{i}J}{2}\log\left(\frac{I - \mathrm{i}J}{2}\right)\right], \tag{6.87}$$

equivalently to the expression in terms of the eigenvalues ς of G^{ab}, as in eq. (6.55).

Chapter 7

Vacuum correlations and entanglement entropy in the Einstein universe

7.1 Vacuum correlations

Let the background be the Einstein $(3+1)$-dimensional spacetime $\mathbb{M}_{\mathrm{E}} = \mathbb{S}^3 \times \mathbb{R}$ with line element

$$\mathrm{d}t^2 - r^2\big[\mathrm{d}\chi^2 + \sin^2\chi\left(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\alpha^2\right)\big]. \tag{7.1}$$

We have the time $t \in \mathbb{R}$, one azimuthal angle $0 < \alpha < 2\pi$ and two polar angles $0 < \theta, \chi < \pi$, supplemented by the coordinate radius r.

A massive Klein-Gordon field $\Phi(t, \chi, \theta, \alpha)$ is described by the Lagrangian

$$\mathcal{L} = \frac{\sqrt{-g}}{2}\left[g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi - \left(m^2 + \xi\mathcal{R}\right)\Phi^2\right]. \tag{7.2}$$

Rigorously, we should use the covariant derivative, but this coincides with the usual derivative in the case of scalar fields, hence we will maintain the use of ∂_μ and its spatial counterpart ∂_i. From hereafter we will also omit the variables dependence of the field to declutter notation.

Varying the action with respect to the scalar field results in the usual Euler–Lagrange equation. In its most general form, applied to this context, we have the Klein–Gordon equation

$$\frac{1}{\sqrt{|g|}}\partial_\mu\Big(\sqrt{|g|}g^{\mu\nu}\partial_\nu\Phi\Big) + \left(m^2 + \xi\mathcal{R}\right)\Phi = 0. \tag{7.3}$$

In $\mathbb{M}_{\mathrm{E}}$ the curvature scalar reduces to $\mathcal{R} = 6/r^2$, but we will only substitute this at the end of the calculations for readability.

7.1.1 Normal modes

In order to compute the correlation function in Eintein's universe, we start by choosing a preferred set of mode functions selected by a condition of invariance under time translations in the given geometry. To achieve this we solve the Klein–Gordon equation, which can be done by separation of variables, generically $\Phi = T(t)X(\chi)Y(\theta,\alpha)$.

Writing the differential operator explicitly on this set-up leads to an equation with the Laplacian of the unit sphere with coordinates (θ,α),[1]

$$\nabla_2\partial^2 + \nabla_3\partial^3 = \frac{1}{r^2\sin^2\chi}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\alpha^2}\right), \tag{7.4}$$

and two more differential operators for t and χ. Multiplying the field equation by $\sin^2\chi$, it becomes

$$\sin^2\chi\left(\frac{\partial^2}{\partial t^2} + m^2 + \xi\mathcal{R}\right)\Phi - \left(\frac{\sin^2\chi}{r^2}\frac{\partial^2}{\partial\chi^2} + \frac{2\sin\chi\cos\chi}{r^2}\frac{\partial}{\partial\chi}\right)\Phi \\ - \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\alpha^2}\right)\Phi = 0. \tag{7.5}$$

Following up with the chosen method immediately yields the solution for the azimuthal and first polar angles. We obtain $Y(\theta,\alpha) = \mathrm{Y}_{lk}(\theta,\alpha)$: the spherical harmonics. The orbital quantum number lies in the interval $l \in \mathbb{N}$, whilst the magnetic quantum number is an integer satisfying $|k| < l$; these intervals will be further restricted by the equation in χ. We have to solve two more equations. The time dependence is easily detachable from χ; dividing by $\sin^2\chi$ plus rearrangement leads to

$$\frac{1}{T(t)}\left[\frac{\partial^2 T}{\partial t^2} + \left(m^2 + \xi\mathcal{R}\right)T(t)\right] = \frac{1}{X(\chi)}\left(\frac{1}{r^2}\frac{\partial^2 X}{\partial\chi^2} + \frac{2\cos\chi}{r^2\sin\chi}\frac{\partial X}{\partial\chi}\right) - \frac{l(l+1)}{r^2\sin^2\chi}. \tag{7.6}$$

We then set each side to equal $-(\lambda^2-1)\,r^{-2}$. The solution for $T(t)$ is attained by identifying its equation as the one for a harmonic oscillator. The solutions are harmonic oscillations $T(t) = \mathrm{e}^{-\mathrm{i}\omega t}$ with frequency

$$\omega_\lambda^2 = m^2 + \xi\mathcal{R} + \frac{(\lambda^2-1)}{r^2}. \tag{7.7}$$

The solution to the remaining equation will determine the values λ can take, fixing the energy spectrum of the theory. The last equation reads

$$\frac{1}{X(\chi)}\left(\frac{\sin^2\chi}{r^2}\frac{\partial^2 X}{\partial\chi^2} + \frac{2\sin\chi\cos\chi}{r^2}\frac{\partial X}{\partial\chi}\right) - \frac{l(l+1)}{r^2} = -\frac{\sin^2\chi}{r^2}\left(\lambda^2-1\right), \tag{7.8}$$

[1] The fact that we can pick apart the θ and α components relies on the metric being diagonal.

once multiplied by $\sin^2\chi$. With simple algebra we arrive at

$$\sin^2\chi\frac{\partial^2 X}{\partial\chi^2}+2\sin\chi\cos\chi\frac{\partial X}{\partial\chi}+\left[(\lambda^2-1)\sin^2\chi-l(l+1)\right]X=0. \tag{7.9}$$

The substitution $X(\chi)=\sin^l\chi C(\cos\chi)$ will transform this equation into a tractable form. By setting $\cos\chi=x$, such that $\mathrm{d}x=-\sin\chi\,\mathrm{d}\chi$ we get

$$\left(1-x^2\right)\frac{\mathrm{d}^2C}{\mathrm{d}x^2}-x\left(2l+3\right)\frac{\mathrm{d}C}{\mathrm{d}x}+\left[\left(\lambda^2-1\right)-l\left(l+2\right)\right]C=0, \tag{7.10}$$

where we can identify the Gegenbauer differential equation. Its general form is

$$(1-x^2)\frac{\mathrm{d}^2C}{\mathrm{d}x^2}-x\left(2\rho+1\right)\frac{\mathrm{d}C}{\mathrm{d}x}+\sigma\left(\sigma+2\rho\right)C=0. \tag{7.11}$$

Setting $\rho=l+1$ and $\sigma=\lambda-l-1$, we return to eq. (7.10). Regular solutions of this equation exist for $\rho>-1/2$, $\rho\neq0$ and $\sigma=0,1,2,3,\ldots$, which implies that λ assumes integer values

$$\lambda=1,2,3,\ldots\quad\text{and}\quad 0\leq l\leq\lambda-1. \tag{7.12}$$

We conclude that $X(\chi)=\sin^l\chi\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)$. We obtain the following solutions to eq. (7.3):

$$f_{\boldsymbol{\kappa}}=\mathrm{n}_{\boldsymbol{\kappa}}\mathrm{e}^{-\mathrm{i}\omega t}\sin^l\chi\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\mathrm{Y}_{lk}(\theta,\alpha), \tag{7.13}$$

indexed by the triple $\boldsymbol{\kappa}\equiv(k,l,\lambda)$ and with $\mathrm{n}_{\boldsymbol{\kappa}}\in\mathbb{C}$ being the normalisation coefficients.

The general solution of eq. (7.3) for the scalar field in the basis $\{f_{\boldsymbol{\kappa}}\}$ is

$$\Phi(x^\mu)=\sum_{\lambda=1}^{\infty}\sum_{l=0}^{\lambda-1}\sum_{k=-l}^{l}z_{\boldsymbol{\kappa}}\mathrm{n}_{\boldsymbol{\kappa}}\mathrm{e}^{-\mathrm{i}\omega t}\sin^l\chi\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\mathrm{Y}_{lk}(\theta,\alpha)+\mathrm{c.c.}, \tag{7.14}$$

wherein $z_{\boldsymbol{\kappa}}$ is the coefficient of expansion.

Let us find the normalisation coefficient. From eq. (4.26), explicitly evaluated for the modes in eq. (7.14),

$$\begin{aligned}\langle f_{\boldsymbol{\kappa}},f_{\boldsymbol{\kappa}'}\rangle=r^3\mathrm{n}_{\boldsymbol{\kappa}}\overline{\mathrm{n}}_{\boldsymbol{\kappa}'}\delta_{ll'}\delta_{kk'}\mathrm{e}^{-\mathrm{i}(\omega-\omega')t}(\omega+\omega')\\ \times\int\mathrm{d}\chi\,(\sin\chi)^{l+l'+2}\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\mathrm{C}^{l'+1}_{\lambda'-l'-1}(\cos\chi),\end{aligned} \tag{7.15}$$

where the normalisation of the spherical harmonics was used (according to the usual 2-norm in function spaces). To further treat this, we need the orthogonalisation condition for Gegenbauer polynomials.

$$\int_1^{-1}\mathrm{d}x\,(1-x^2)^{2\rho-1/2}\mathrm{C}^\rho_\sigma(x)\mathrm{C}^\rho_{\sigma'}(x)=\frac{2\pi\Gamma(\sigma+2\rho)}{4^\rho(\sigma+\rho)[\Gamma(\rho)]^2\Gamma(\sigma+1)}\delta_{\sigma\sigma'}. \tag{7.16}$$

Setting the indices as stated in eq. (7.15) leads to

$$\begin{aligned}\langle f_{\boldsymbol{\kappa}}, f_{\boldsymbol{\kappa}'}\rangle = r^3 \mathrm{n}_{\boldsymbol{\kappa}}\overline{\mathrm{n}}_{\boldsymbol{\kappa}'}\mathrm{e}^{-\mathrm{i}(\omega-\omega')t}(\omega+\omega') \\ \times \frac{2^{-2l-1}\pi\Gamma(\lambda+l+1)}{\lambda[\Gamma(l+1)]^2\Gamma(\lambda-l)}\delta_{\boldsymbol{\kappa}\boldsymbol{\kappa}'}.\end{aligned} \tag{7.17}$$

Equation (4.8a) can only be satisfied, when the set of indices are equal, if

$$2\omega r^3|\mathrm{n}_{\boldsymbol{\kappa}}|^2\frac{2^{-2l-1}\pi\Gamma(\lambda+l+1)}{\lambda[\Gamma(l+1)]^2\Gamma(\lambda-l)} = 1, \tag{7.18}$$

giving

$$\mathrm{n}_{\boldsymbol{\kappa}} = \frac{2^l l!}{r^{3/2}\sqrt{\pi\omega}}\sqrt{\frac{\lambda(\lambda-l-1)!}{(\lambda+l)!}}. \tag{7.19}$$

7.1.2 Two-point function

We described canonical quantisation as the procedure which takes classical observables on phase space with its symplectic structure to an algebra of operators on a Hilbert space of physical states. The equal-time commutation relation

$$\big[\Phi_t\big(x^i\big), \Pi_t\big(y^i\big)\big] = \mathrm{i}\delta\big(x^i - y^i\big) \tag{7.20}$$

defines the algebra of quantum observables. This algebra must be satisfied once the fields are promoted to operator-valued distributions. The operator character of Φ will be represented in eq. (7.14) by the amplitudes $z_{\boldsymbol{\kappa}}$ and its complex conjugate, becoming $a_{\boldsymbol{\kappa}}$ and $a^\dagger_{\boldsymbol{\kappa}}$ in the quantum theory. To realise the representation of observables as operators, it is sufficient to establish a connection between the canonical commutation relation and the normalised inner product as

$$\Big[a_{\boldsymbol{\kappa}}, a^\dagger_{\boldsymbol{\kappa}'}\Big] = \langle f_{\boldsymbol{\kappa}}, \overline{f_{\boldsymbol{\kappa}'}}\rangle \tag{7.21a}$$

$$= \delta_{\mu}(\boldsymbol{\kappa}, \boldsymbol{\kappa}'). \tag{7.21b}$$

To quote the full solution, we have

$$\begin{aligned}\Phi(x^\mu) = \sum_{\lambda=1}^{\infty}\sum_{l=0}^{\lambda-1}\sum_{k=-l}^{l}\Bigg\{\frac{2^l l!}{r^{3/2}\sqrt{\pi\omega_\lambda}}\sqrt{\frac{\lambda(\lambda-l-1)!}{(\lambda+l)!}} \\ \times\Big(a_{\boldsymbol{\kappa}}\mathrm{e}^{-\mathrm{i}\omega t}\sin^l\chi\,\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\mathrm{Y}_{lk}(\theta,\alpha) \\ + a^\dagger_{\boldsymbol{\kappa}}\mathrm{e}^{\mathrm{i}\omega t}\sin^l\chi\,\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\overline{\mathrm{Y}}_{lk}(\theta,\alpha)\Big)\Bigg\},\end{aligned} \tag{7.22}$$

where we now index the frequency with its dependence on λ.

The propagator introduced in section 5.1 can be expressed for the the scalar field in Einstein space through the basis of solutions just outline. Directly from eq. (5.6) it is

$$Q(x,x') = \sum_{\lambda=1}^{\infty}\sum_{l=0}^{\lambda-1}\sum_{k=-l}^{l}\left\{\frac{2^{2l}(l!)^2}{\pi r^3\omega_\lambda}\left[\frac{\lambda(\lambda-l-1)!}{(\lambda+l)!}\right]\right.$$
$$\times \sin^l\chi \mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\sin^l\chi' \mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi')$$
$$\left.\times \mathrm{Y}_{lk}(\theta,\alpha)\overline{\mathrm{Y}}_{lk}(\theta',\alpha')\mathrm{e}^{-\mathrm{i}\omega(t-t')}\right\}. \quad (7.23)$$

First, we address the sum on k by using the addition theorem for spherical harmonics:

$$\sum_{k=-l}^{l}\mathrm{Y}_{lk}(\theta,\alpha)\overline{\mathrm{Y}}_{lk}(\theta',\alpha') =$$
$$\frac{2l+1}{4\pi}\mathrm{P}_l\left(\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\alpha-\alpha')\right), \quad (7.24)$$

for the Legendre polynomial P_l. Then

$$Q = \sum_{\lambda,l}\left\{\frac{2^{2l}(l!)^2(2l+1)}{4\pi^2 r^3\omega_\lambda}\left[\frac{\lambda(\lambda-l-1)!}{(\lambda+l)!}\right]\mathrm{e}^{-\mathrm{i}\omega(t-t')}\right.$$
$$\left.\times \mathrm{P}_l(\cos\eta)\sin^l\chi \mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\sin^l\chi' \mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi')\right\}, \quad (7.25)$$

wherein $\cos\eta = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\alpha-\alpha')$ defines the angle η. This is the angular distance on $\mathbb{S}^2$ parametrised by coordinates (θ,α).

An identity of Legendre polynomials permits us to express it in terms of Gegenbauer polynomials. That is,

$$Q = \sum_{\lambda}\frac{\mathrm{e}^{-\mathrm{i}\omega(t-t')}}{4\pi^2 r^3\omega_\lambda}\sum_{l=0}^{\lambda-1}\left\{2^{2l}(l!)^2(2l+1)\left[\frac{\lambda(\lambda-l-1)!}{(\lambda+l)!}\right]\sin^l\chi\sin^l\chi'\right.$$
$$\left.\times \mathrm{C}^{1/2}_l(\cos\eta)\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi)\mathrm{C}^{l+1}_{\lambda-l-1}(\cos\chi')\right\}. \quad (7.26)$$

Despite the menacing aspect, the sum over l has a simple outcome. It corresponds

to the addition theorem for Gegenbauer polynomials,

$$\begin{aligned}\mathrm{C}_\sigma^\gamma(\cos\chi\cos\chi' + \sin\chi\sin\chi'\cos\eta) = \frac{(2\gamma-2)!}{[(\gamma-1)!]^2}\sum_{\rho=0}^{\sigma} 2^{2\rho}[(\gamma+\rho)!]^2(\sigma-\rho)! \\ \times \frac{(2\gamma+2\rho-1)}{(2\gamma+\sigma+\rho)!}\sin^\rho\chi\sin^\rho\chi' \\ \times \mathrm{C}_\rho^{\gamma-1/2}(\cos\eta)\mathrm{C}_{\sigma-\rho}^{\gamma+\rho}(\cos\chi)\mathrm{C}_{\sigma-\rho}^{\gamma-\rho}(\cos\chi').\end{aligned} \tag{7.27}$$

Upon identifying the indices as

$$\rho = l, \tag{7.28a}$$
$$\sigma = \lambda - 1, \tag{7.28b}$$
$$\gamma = 1, \tag{7.28c}$$

and defining the angle η' through $\cos\eta' = \cos\chi\cos\chi' + \sin\chi\sin\chi'\cos\eta$, the result is

$$Q = \sum_{\lambda=1}^{\infty} \frac{\lambda \mathrm{e}^{-\mathrm{i}\omega_\lambda(t-t')}}{4\pi^2 r^3 \omega_\lambda}\mathrm{C}_{\lambda-1}^1(\cos\eta'). \tag{7.29}$$

This is a general expression of the propagator for the scalar field in the Einstein space. However, by making a choice of interesting physical parameters we can proceed in simplifying and arrive at an explicit form for it. So far we have dealt with a general massive scalar field whose dynamics was defined in eq. (7.2), giving the energy spectrum seen in eq. (7.7). Now we may work with a conformal field by choosing $m = 0$, and $\xi = 1/6$. The computation was put forward without consideration of the actual value for the Ricci scalar in the Einstein spacetime, which is $\mathcal{R} = 6/r^2$. These considerations reduce the energy to $\omega_\lambda = \lambda/r$. This amounts to a correlation function of the form

$$Q = \sum_{\lambda=1}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}\lambda(t-t')/r}}{4\pi^2 r^2}\mathrm{C}_{\lambda-1}^1(\cos\eta'). \tag{7.30}$$

Now, for the last step, the above expression as the generating function for Gegenbauer polynomials,

$$\left(1 - 2xz + z^2\right)^{-\gamma} = \sum_{\sigma=0}^{\infty} \mathrm{C}_\sigma^\gamma(x) z^\sigma. \tag{7.31}$$

We shift summation index $\lambda - 1 = \sigma$ in order to start the sum from zero, which generates an extra $\mathrm{e}^{-\mathrm{i}(t-t')/r}$ term. Equation (7.31) reduces to

$$Q = \mathrm{e}^{-\mathrm{i}(t-t')/r}\sum_{\sigma=0}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}\sigma(t-t')/r}}{4\pi^2 r^2}\mathrm{C}_\sigma^1(\cos\eta'), \tag{7.32}$$

wherein one promptly recognises

$$z = \mathrm{e}^{-\mathrm{i}(t-t')/r}. \tag{7.33}$$

Therefore,

$$\begin{aligned} Q(x,x') &= \mathrm{e}^{-\mathrm{i}(t-t')/r}\left[4\pi^2 r^2\left(1-2\mathrm{e}^{-\mathrm{i}(t-t')/r}\cos\eta'+\mathrm{e}^{-2\mathrm{i}(t-t')/r}\right)\right]^{-1} \\ &= \frac{1}{8\pi^2 r^2}\left[\frac{1}{\cos[(t-t')/r]-\cos\eta'}\right]. \end{aligned} \tag{7.34}$$

7.2 Entanglement entropy in Einstein space

Following our studies of correlation functions in Einstein spacetime, we arrive at the main result of this dissertation: the determination of corrections to the entanglement entropy due to curvature. As we did for flat spacetime, we first discretise the theory and identify degrees of freedom in two spacelike separated regions, whose boundaries are shared and define the *entangling surface*.

The artifice used in this section refers to the Kähler structures of section 6.1, and not on the algorithm laid out by Srednicki and explicated in section 5.3. We follow instead the steps discussed in section 6.2 for the determination of the entanglement entropy directly from the covariance matrix.

In order to compute the entanglement entropy of a spherical region in flat space, we have discretised the corresponding spatial slice. Due to the spherical symmetry of the Einstein universe, we are able to borrow the method used in section 5.3.1 for the flat case, namely, we can decompose the field into a sum of angular normal modes, reducing the coupled degrees of freedom to a one-dimensional manifold which we discretise.

As a result, we have a coupling matrix K_{lk} for each mode, and the algorithm of Casini [59] discussed in section 6.2 can be easily implemented as a Mathematica code. In fact, it is more efficient than what was done in section 5.3 because it relies on fewer steps of matrix diagonalisation, which is computationally demanding.

Before moving on to the use of the covariance matrix in finding the entropy, and its implementation as a numerical problem, we first revise the discretisation procedure as it is applied to the Einstein space and the corresponding scalar field residing in it. Afterwards, we discuss the numerical results and relate them to the literature.

Discretisation and partial mode decomposition

Recall the metric interval of Einstein spacetime, eq. (7.1),

$$\mathrm{d}t^2 - r^2\left[\mathrm{d}\chi^2+\sin^2(\chi)\left(\mathrm{d}\theta^2+\sin^2(\theta)\mathrm{d}\alpha^2\right)\right]. \tag{7.35}$$

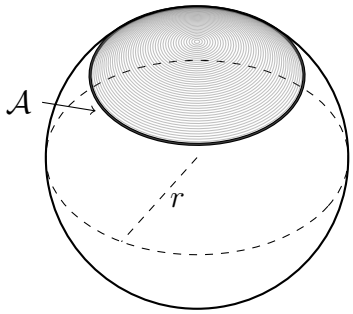

Figure 7.1: In this fictitious two-dimensional spherical space with radius r, an entangling surface of area $\mathcal{A}$ is the circle and its perimeter, as indicated, dividing the surface of the sphere into two regions (the cap on the north pole and everything else southward to it).

To emulate the discretisation done over flat spacetime, we need to exploit the symmetries of the manifold. The natural choice is to explore the spherical symmetry that the Einstein space shares with flat space in defining the two regions into which we want to split space. The codimension 2 manifold on which we model the entangling surface is then again $\mathbb{S}^2$, at t and χ constants.

Fixing t corresponds to picking an $\mathbb{S}^3$ slice, but since the Einstein universe is invariant under time-translations, this choice of instant of time is immaterial. The fixed χ, on the other hand, is responsible for defining the entangling surface itself, and works as the radial coordinate did in flat space. Naming the complementary regions of space as $\mathbb{X}$ and $\mathbb{X}^{\complement}$, their shared boundary is $\partial\mathbb{X} = \mathbb{S}^2$, parametrised by θ and α and with area

$$\mathcal{A} = 4\pi r^2 \sin^2(\chi) \tag{7.36}$$

at physical radius $\boldsymbol{\ell} = r\chi$ in this coordinate chart. In fig. 7.1 we picture the two-dimensional analogue of the Einstein space and its separation into two regions. Discretisation regularises the theory given by the Lagrangian eq. (7.2). Once quantised, its Hamiltonian will be used in the process of finding the entropy of either of the regions $\mathbb{X}$ and $\mathbb{X}^{\complement}$. By the Legendre transform, we find H to be

$$H = \int_{\mathbb{S}^3} \mathrm{d}\chi\, \mathrm{d}\theta\, \mathrm{d}\alpha\, \frac{r^3 \sin^2\chi \sin\theta}{2} \left[\Pi^2 + \partial_i \Phi \partial^i \Phi + \left(m^2 + \frac{6}{r^2}\xi \right) \Phi^2 \right]. \tag{7.37}$$

Exploiting again the spherical symmetry shared by the background and the entangling surface, it is convenient to expand the field into a sum of normal modes lk with well-defined angular momentum. That is,

$$\Phi(x) = \sum_{l=0}^{\infty} \sum_{k=-l}^{l} \frac{\Phi_{lk}(\chi)}{r \sin\chi} \mathrm{Y}_{lk}(\theta, \alpha), \tag{7.38}$$

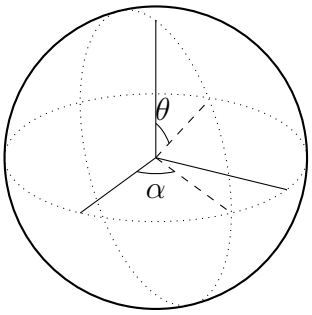

Figure 7.2: Sphere where the spherical harmonics $\mathrm{Y}_{lk}(\theta, \alpha)$ are defined, at some fixed χ.

and

$$\mathit{\Pi}(x) = \sum_{l=0}^{\infty} \sum_{k=-l}^{l} \frac{\mathit{\Pi}_{lk}(\chi)}{r \sin \chi} \mathrm{Y}_{lk}(\theta, \alpha). \tag{7.39}$$

The spherical harmonics $\mathrm{Y}_{lk}(\theta, \alpha)$ once again appear in the partial mode decomposition, now defined on the spheres of constant χ (cf. fig. 7.2).

Inserting equations (7.38) and (7.39) into the Hamiltonian, and using the orthogonality of the spherical harmonics, yields

$$H = \int_0^{\pi} \mathrm{d}\chi \, \frac{r^3 \sin^2 \chi}{2} \sum_{lk} \frac{{\mathit{\Pi}_{lk}}^2}{r^2 \sin^2 \chi} + \frac{1}{r^2} \left[\frac{\partial}{\partial \chi} \left(\frac{\mathit{\Phi}_{lk}}{r \sin \chi} \right) \right]^2 + \left(m^2 + \frac{6}{r^2} \xi + \frac{l(l+1)}{r^2 \sin^2 \chi} \right) \frac{{\mathit{\Phi}_{lk}}^2}{r^2 \sin^2 \chi}, \tag{7.40}$$

wherein $l(l+1)$ is the eigenvalue of the angular part of the Laplacian,

$$\frac{1}{r^2 \sin^2 \chi} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \alpha^2} \right], \tag{7.41}$$

as it acts on Y_{lk}.

By expressing the fields in normal modes we effectively reduce the calculations to a one-dimensional problem on χ. We then assign vertices of a graph to selected values of the angle χ_j. The range of the remaining angle is $0 < \chi < \pi$, allowing us to chop this interval into N parts of value π/N, and identify them with the N edges of the graph. That is, for $j = 0, \ldots, N$ indexing the $N + 1$ vertices, we impose

$$\chi_{j+1} - \chi_j = \frac{\pi}{N}, \tag{7.42}$$

and choose $\chi_0 = 0$. It follows that the other vertices are localised at

$$\chi_j = \frac{\pi j}{N} \quad \text{for} \quad j \geq 1. \tag{7.43}$$

This assignment in coordinate space must correspond to an assignment in space, where the vertices in fact live. Given the radius of curvature r of $\mathbb{S}^3$ and a reference point $\chi = 0$, the physical "radius" along coordinate χ is $\boldsymbol{\ell} = \chi r$, indicating that the maximal possible distance between two points is πr (from north to south poles, see figure fig. 7.3). Conversely, we arrive at a minimal possible physical distance given the discretisation, corresponding to the intervals π/N and equal to

$$\varepsilon = \pi r/N. \tag{7.44}$$

In terms of this minimum, the maximal distance can be expressed as

$$\pi r = N\varepsilon. \tag{7.45}$$

Furthermore, the discretised physical distance from site $j = 0$ to $j \geq 1$ becomes $\boldsymbol{\ell} = j\varepsilon$, or in terms of the radius of curvature,

$$\boldsymbol{\ell} = \frac{\pi r}{N} j. \tag{7.46}$$

Finally, when comparing the curvature of $\mathbb{S}^3$ and its discretisation, it is useful to express the radius in terms of the number of vertices,

$$r = \frac{N\varepsilon}{\pi}. \tag{7.47}$$

The canonical variables are then replaced by discrete versions residing in these sites,

$$\Phi_{lk}(\chi) \rightsquigarrow \Phi_{lkj}, \quad \Pi_{lk}(\chi) \rightsquigarrow \Pi_{lkj}, \tag{7.48}$$

and the integrals and derivatives become sums and finite differences as before,

$$\int \mathrm{d}\chi \rightsquigarrow \frac{\pi}{N} \sum_{j=0}^{N} \tag{7.49}$$

and

$$\left(\frac{\partial}{\partial \chi} \frac{\Phi_{lk}}{r \sin \chi} \right)^2 \rightsquigarrow \frac{2\pi}{N} \left(\frac{\Phi_{lk,j+1}}{\sin[\pi(j+3/2)/N]} - \frac{\Phi_{lkj}}{\sin[\pi(j+1/2)/N]} \right)^2, \tag{7.50}$$

respectively. The choice of evaluating functions of χ at points different to those assigned to the vertex is particularly important in this case due to the symmetries of the problem. The resulting phase space is $\boldsymbol{\Gamma}_{lk} = \mathbb{R}^{2(N+1)}$.

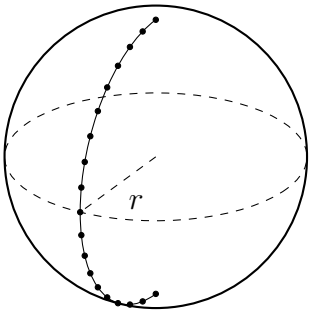

Figure 7.3: By fixing an angle θ, one arrives at a sphere with coordinates (χ, α). The graph vertices span the range $0 < \chi < \pi$. Adjacent vertices are separated by a physical distance of ε.

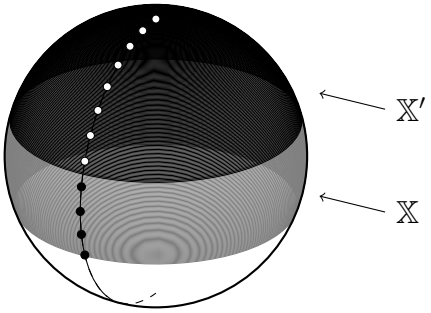

Figure 7.4: Two regions $\mathbb{X}$ (darker, with white vertices) and $\mathbb{X}'$ (lighter, with white *and* black vertices) enclosed by entangling surfaces of equal surface area

On top of the presence of curvature and its effect in the area law for entanglement entropy, Einstein space is naturally compact. Running the algorithm for sites corresponding to χ from 0 to π will lead to repetitions due to the fact that the area for some angle χ will be equal to that of angle $\pi - \chi$.Comparing with the graphs plotted in section 5.3, given the finite size of that lattice, the plot for entanglement entropy in Einstein space will have a doubling of its points since there is a pairing of samples of $\mathcal{S}$ for equal areas. Figure 7.4 demonstrate two entangling surfaces of the same area, opposite to one another considering a reflection across the equator. The entropies of those regions are then equal, relying on the fact that, given such a reflection, the complement of one of the regions is precisely the second one, $\mathbb{X}^{\complement} = \mathbb{X}'$. The equality follows from the third property of entanglement entropy in chapter 3.

We choose to assign the area

$$\mathcal{A} = 4\pi r^2 \sin^2\left(\frac{\pi(j+1/2)}{N}\right) \tag{7.51}$$

to the vertex j. In this way, the first sample of $\mathcal{S}$ correspond to a trace over all sites $j \geq 1$, maintaining a subsystem consisted of site $j = 0$ inside the surface of area $\mathcal{A} = 4\pi r^2 \sin^2(\pi/2N)$. Equivalently, for the last sample we trace out site $j = N$ alone, maintaining the others inside a surface of the same area as before, $\mathcal{A} = 4\pi r^2 \sin^2(\pi - \pi/2N) = 4\pi r^2 \sin^2(\pi/2N)$. The same follows for the other appropriate pairs of vertices.

Once again we arrive at a Hamiltonian of coupled harmonic oscillators,

$$H = \sum_{lk} \left(\sum_{j=0}^{N} \frac{1}{2\varepsilon} \Pi_{lkj}^2 + \sum_{i,j=0}^{N} \Phi_{lki} K_{ij} \Phi_{lkj} \right). \tag{7.52}$$

The matrix K_{ij} is responsible for coupling, through the derivative term, neighbouring vertices i and j. Explicitly, it is

$$\begin{aligned} K_{ij} = \frac{\delta_{ij}}{2\varepsilon} \left(\varepsilon^2 m^2 + \frac{\pi^2 l(l+1)}{N^2 \sin^2\left(\frac{\pi(i+1/2)}{N}\right)} + \frac{\sin^2\left(\frac{\pi(i-1/2)}{N}\right)}{\sin^2\left(\frac{\pi(i+1/2)}{N}\right)} + \frac{6\pi^2 \xi}{N^2} + 1 \right) \\ - \frac{\delta_{i+1,j}}{2\varepsilon} \frac{\sin\left(\frac{\pi(i-1/2)}{N}\right)}{\sin\left(\frac{\pi(i+1/2)}{N}\right)} - \frac{\delta_{i,j+1}}{2\varepsilon} \frac{\sin\left(\frac{\pi(j-1/2)}{N}\right)}{\sin\left(\frac{\pi(j+1/2)}{N}\right)}. \end{aligned} \tag{7.53}$$

From hereafter we write the Hamiltonian as $H = \sum_{lk} H_{lk}$ as was done in section 5.3.1. The indices lk will then be omitted in the canonical variables, whilst derived quantities, such as entanglement entropy, will continue to have them, as they must be distinguished from their mode-independent counterpart, belonging to the full phase space.

Instead of following the methods of section 5.3, consisted of finding the Gaussian state, tracing out degrees of freedom inside the entangling surface, and many other manipulations, we utilise the covariance formalism described in section 6.2 and the formula for entanglement entropy therein, eq. (6.55), which we quote:

$$\mathcal{S}_{lk} = \sum_{i=0}^{N-1} (\varsigma_i + 1/2) \log(\varsigma_i + 1/2) - (\varsigma_i - 1/2) \log(\varsigma_i - 1/2), \tag{7.54}$$

wherein ς_i are the eigenvalues of $\sqrt{QP}$ (essentially containing the symplectic spectrum of $\mathcal{C}$). Entanglement entropy in full follows as $\sum_{lk} \mathcal{S}_{lk} = \sum_l (2l+1) \mathcal{S}_{lk}$, as before.

This method, whilst equivalent to that described in section 5.3, makes it simpler to arrive at $\mathcal{S}_{lk}$ computationally. In contrast to the sum over the infinite eigenvalues of the density matrix, and then over the degrees of freedom pertaining to the

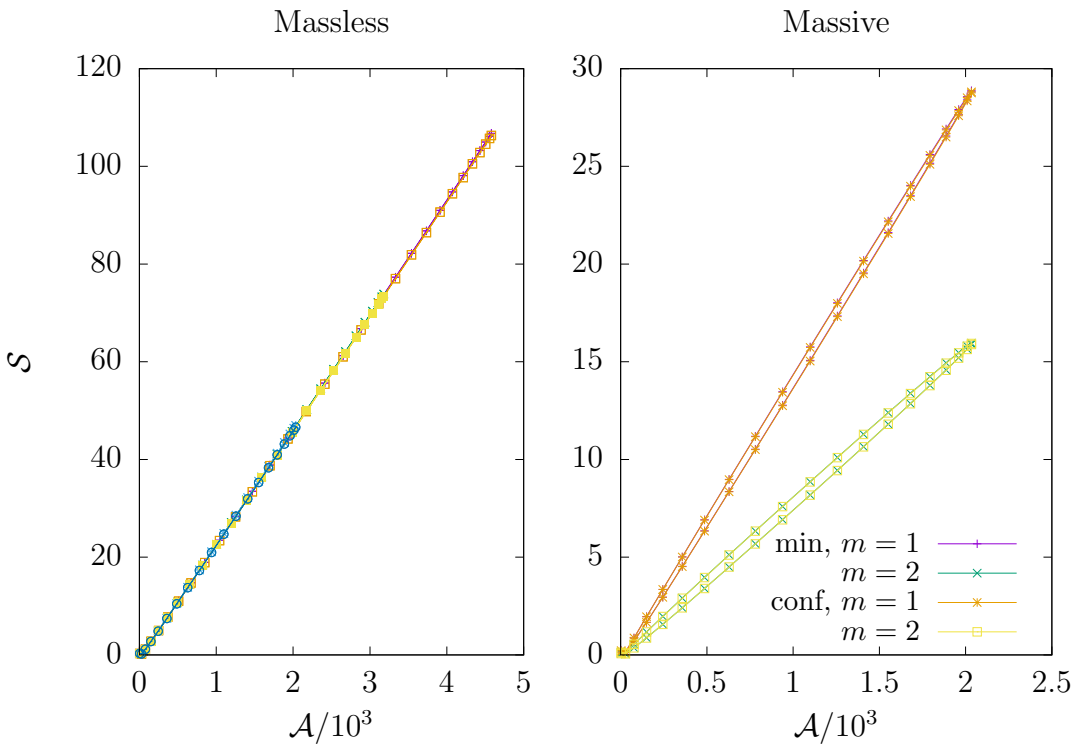

Figure 7.5: Area law of entanglement entropy for minimally and conformally coupled fields in lattices of size $N = 40, 50, 60$. The coefficients of proportionality for the plot of massless fields range within $\pm 2\%$ of the results in ref. [56]. The area law for massive fields have clear dependence on m, being monotonically decreasing for increasing m with overlaps for different curvature couplings.

subregion of space, one only identifies the coupling matrix, and the rest follows from simple linear algebra, as it is shown in listing 7.1, section 7.2.1.

This method allows us to compare the entanglement entropy in Einstein space with that in flat space. In fig. 5.6 we plot the entanglement entropy for both massless and massive fields in the Einstein space, demonstrating an area law behaviour in direct correspondence with the results presented in section 5.3, particularly fig. 5.6 for the massless field. The plot for massive fields also illustrate the mass-dependence of the area law coefficient. This property paves the way for the application of numerical computations in finding both regularisation-independent and curvature corrections to the behaviour of entanglement entropy. These results show the consistency of our code. It is then appropriate to study more refined details of the area law, as it is outlined in the following section.

7.2.1 Universal coefficients of entanglement entropy

The area term is only the dominant contribution to entanglement entropy, arising from the quadratic divergences of the entanglement entropy as $\varepsilon \to 0$. In our choice of natural units, the entropy is dimensionless, which motivates a general expansion in terms of dimensionless combinations of the available quantities: the radius of curvature r, the lattice spacing ε and the correlation length m^{-1}) (see reviews [59] and references therein). That leads to

$$\mathcal{S} = s_2(m, r, \varepsilon)\frac{\mathcal{A}}{\varepsilon^2} + s_1(m, r, \varepsilon)\frac{\boldsymbol{\ell}}{\varepsilon} + s_0(m, r, \varepsilon)\log\left(\frac{\boldsymbol{\ell}}{\varepsilon}\right) + \text{finite terms depending on } m \text{ and } r, \quad (7.55)$$

with the characteristic size of the entangling surface $\boldsymbol{\ell} = \chi r$ acting as a new length scale in the theory; in our case, this scale is the radius of the entangling surface. The first term is the area law, with the coefficient s_2 studied in preceding sections. This expansion is with respect to geometric properties of $\partial\mathbb{X}$ (area, radius, etc.).

The finite contributions in eq. (7.55), that shall be omitted from now on, depend on the choice of regularisation. Morever, it can be shown through analytical methods, that some of the other contributions are *regularisation-independent*, and for this reason also called *universal* [62, 63]. An example is the s_0 term, universal and proportional to the central charge in a conformal field theory in $(1 + 1)$-dimensional spacetime. Appearing in any regularisation scheme, these terms arise from the quantum field theory itself, and not from a possible mechanism of a quantum gravity theory that one expects to naturally justify a choice of scheme.

We are mainly interested in the universal contributions to the area term. As was shown in the last section, massive fields constitute a way to easily study this dependence. In order to follow this practice, it is better to isolate some of the terms present in eq. (7.55). Ref. [64] finds universal contribution in the regime of negligible extrinsic boundary curvature. From the exponential decay of massive correlations, it is enough to consider the boundary $\partial\mathbb{X}$ as flat when $m^{-1} < \boldsymbol{\ell}$, i.e. the correlations accounted in $\mathcal{S}$ are exponentially suppressed at considerable extrinsic curvature of the entangling surface.

The entanglement entropy can be determined analytically in the continuum by exploring a procedure known as the replica trick, which relates it to the derivative of the logarithm of the partition function $\mathcal{Z}$ to some power. Applying heat kernel renormalisation in this method, Hertzberg et al. [64] computes universal contributions to s_2 in a waveguide geometry, which includes a term that is in fact valid in other geometries (precisely because correlations concentrate near the boundary). Relying on the negligible extrinsic curvature of $\partial\mathbb{X}$ condition the entanglement entropy can be expanded in powers of $m\boldsymbol{\ell} > 1$. It is found that

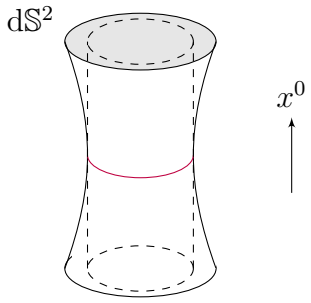

Figure 7.6: Immersed two-dimensional de Sitter space $\mathrm{d}\mathbb{S}^2$ in three-dimensional flat space. The horizontal line is the de Sitter waist, at a choice of time slicing generating $\mathbb{S}^1$. The vertical dashed cylinder represent the Einstein static universe $\mathbb{S}^1 \times \mathbb{R}$ whose radius is that of the de Sitter waist.

accompanying the leading-order divergence there are the following contributions,

$$\frac{s_2(m,\varepsilon)}{\varepsilon^2} = \frac{\sigma_0}{\varepsilon^2} + \sigma_2 m^2 \log(m\varepsilon) + \sigma_2' m^2 + \dots \tag{7.56}$$

For the σ_2 contribution, it was found

$$\sigma_2 = \frac{1}{24\pi}, \tag{7.57}$$

in four-dimensional spacetime. This contribution has been corroborated by numerical computations in a lattice through a dimensional reduction technique in ref. [63].

In refs. [65, 66] Smolkin et al. calculated more corrections, now in curved spaces. They considered a scalar field residing in de Sitter spacetime, and computed the entanglement entropy for spherical regions near the region known as *de Sitter waist*. Figure 7.6 shows an immersion of de Sitter space $\mathrm{d}\mathbb{S}$ in a fictitious ambient flat space of one higher dimension.[2]

This is a *maximally symmetric spacetime*, in contrast to the maximally symmetric *spaces* introduced in chapter 2. In fact, different choices of foliation of $\mathrm{d}\mathbb{S}$ lead to the three FLRW geometries, eq. (2.54), introduced in that section [53]. In particular, the spherical space $\mathbb{S}^3$ of varying radius $R(t)$ is recovered by choosing slices of constant time corresponding to horizontal circles in fig. 7.6.

Refs. [65, 66] provide two conflicting versions of the term s_2 in de Sitter space obtained in different treatments of the heat kernel for spherical geometries. The

[2] In standard Cartesian coordinates of the ambient space, with the x^0 axis pointing up, de Sitter is the hyperboloid $(x^0)^2 - \sum_i (x^i)^2 = L^2$.

resulting corrections to s_2 at the de Sitter waist are

$$\frac{s_2(m,r)}{\varepsilon^2} = \left[\frac{(1-6\xi)}{24\pi}m^2 + \left(\frac{1}{360\pi} - \frac{(1-6\xi)^2}{72\pi}\right)\frac{1}{r^2}\right]\log(m\varepsilon) + \dots \tag{7.58}$$

and

$$\frac{s_2(m,r)}{\varepsilon^2} = \left[\frac{m^2}{24\pi} + \left(\frac{1}{360\pi} - \frac{(1-6\xi)}{72\pi}\right)\frac{1}{r^2}\right]\log(m\varepsilon) + \dots \tag{7.59}$$

The second expression reproduce the $1/24\pi$ factor found in ref. [64], but the present only does so in the case for minimal coupling. The presence of the extra coefficient $1-6\xi$ in eq. (7.58) has important implications, namely that entanglement entropy differs in flat space for minimally and conformally coupled scalar fields.

Motivated by eqs. (7.58) and (7.59), and including the finite term, proportional to $\mathcal{A}$ that accompanies the logarithmic universal contribution in eq. (7.56), our ansatz for the coefficient s_2 is

$$\frac{s_2(m,r)}{\varepsilon^2} = \frac{\sigma_0}{\varepsilon^2} + \sigma_2' m^2 + \sigma_2 m^2 \log(m\varepsilon) + \tilde{\sigma}_0 \frac{\log(m\varepsilon)}{r^2} + \dots \tag{7.60}$$

The curvature coupling ξ is dimensionless, so the coefficients σ can be expected to depend on it, but not through a predictable form.

On top of the universality of the contributions, the discussion that follows studies the validity of eqs. (7.58) and (7.59). These expressions, computed in de Sitter space, contain explicit curvature dependence with which we can compare numerical results in the lattice. Our setup, on the other hand, relies on the the Einstein universe, which has constant curvature $\mathcal{R} = 6/r^2$; in fig. 7.6, this would be analogous to a cylinder.[3] Because computations in refs. [65, 66] were restricted to the de Sitter waist, we expect to simulate these calculations in the lattice by approximating an infinitesimal region around the waist by a spherical universe whose radius at that region coincide with the de Sitter radius.

The global coordinates discussed, that slices de Sitter spacetime in $\mathbb{S}^3$ foliations of time-dependent radius, endows the manifold with metric

$$\mathrm{d}t^2 - r^2\cosh^2(t/r)\left[\mathrm{d}\chi^2 + \sin^2(\chi)\left(\mathrm{d}\theta^2 + \sin^2(\theta)\mathrm{d}\alpha^2\right)\right], \tag{7.61}$$

corresponding to a closed FLRW cosmological model with scale factor

$$R^2(t) = r^2\cosh^2(t/r) \tag{7.62}$$

[3]The analogy should not be taken too far, however, because the cylinder has no intrinsic curvature, whilst $\mathbb{S}^3 \times \mathbb{R}$ does.

This choice of scale factor is appropriate for our comparison. Recall from section 2.2 that the curvature scalar in the closed universe, whose curvature is positive, is

$$\mathcal{R} = 6\left[\frac{1}{R}\frac{\mathrm{d}^2 R}{\mathrm{d}t^2} + \frac{1}{R^2}\left(\frac{\mathrm{d}R}{\mathrm{d}t}\right)^2 + \frac{1}{R^2}\right] \tag{7.63a}$$

resulting in

$$= \frac{12}{r^2}. \tag{7.63b}$$

7.2.2 Results

In order to exploit the approximations given, we need to allow for appropriate ranges of values in the numerical implementation. In summary, the length scales of a massive field theory in the Einstein universe and a choice of entangling surface of characteristic length $\boldsymbol{\ell}$ are, in the continuum,

$$\varepsilon < m^{-1} < \boldsymbol{\ell} < \pi r. \tag{7.64}$$

This can be translated to lattice parameters. The length $\boldsymbol{\ell}$ will be appointed a specific size n as was done in section 5.3. Setting $\varepsilon = 1$, it is

$$1 < m^{-1} < n < N, \tag{7.65}$$

with m^{-1} now being measured in multiples of ε.

The Mathematica code implements the covariance approach to finding the entanglement entropy from section 6.2. Having already determined the Hamiltonian and the coupling matrix K_{ij}, eq. (7.53), the code follows in listing 7.1 at the end of this section.[4]

To avoid numerical artefacts appearing at the borders, $n = 0$ and $n = N$, we restrict the range n for which the entanglement entropy will be evaluated to a subset of values such that eq. (7.65) is still satisfied and that will be appropriately sensitive to the background geometry. Given a choice of $N = 100$, we have picked the range

$$40 < n < 60, \tag{7.66}$$

in which the effects of the curvature will be most prominent at $n = 50$. This means that we have 21 samples for an entropy-area plot. Under the conditions imposed by eq. (7.65) the mass range is chosen as

$$0.030 < m < 0.100, \tag{7.67}$$

[4]Note that in the code our definition of site indexing and lattice size is different from the one used in this text (r is the vertex index and R the lattice size).

corresponding to correlation lengths $33 > m^{-1} > 10$. The numerical calculation is evaluated for values of l up to 3000.

Finally, the last parameter that needs to be specified is the curvature coupling, which will be our usual minimal and conformal ones, $\xi = 0$ and $\xi = 1/6$ respectively. Evaluating the expected parameters in eq. (7.58) for the given radius of curvature $r = 100/pi$ yields

$$\sigma_2 = \frac{1}{24\pi}, \tag{7.68}$$

$$\tilde{\sigma}_2 = -\frac{\pi}{90 \times 100}, \tag{7.69}$$

for minimal coupling (with contributions unchaged from flat space), and

$$\sigma_2 = 0, \tag{7.70}$$

$$\tilde{\sigma}_2 = -\frac{\pi}{360 \times 100^2}, \tag{7.71}$$

for conformal coupling. Now, looking at eq. (7.59), one has the same minimal coupling corrections but

$$\sigma_2 = \frac{1}{24\pi}, \tag{7.72}$$

$$\tilde{\sigma}_2 = -\frac{\pi}{360 \times 100^2}, \tag{7.73}$$

for conformal coupling, with the flat space contribution present once again.

The strategy to find the universal massive contributions and its curvature corrections is to analyse it under the light of eqs. (7.55) and (7.60). We can extract s_2 through a simple linear plot $\mathcal{S} = s_2\mathcal{A} + b$, in which we accumulate lesser divergences in b and that will recover slightly different values $0.0234 \gtrsim s_2(m, r)$ for different masses. Each of these points serve in a second fit, modelled over the function $s_2 = \sigma_0 + \sigma_2 m^2 \log m + \tilde{\sigma}_0 \log(m)/r + \sigma_2' m^2$.

In fig. 7.7 we plot the results for the parameters just discussed. The decrease in the value of the coefficient of proportionality of the linear plot is noticeable directly from the vertical offset of the lines. The differences are minute and to study them we need to follow with the second fit.

From the data set generated by Mathematica the second fit follows promptly. We use the acquired values of s_2 and their corresponding m and arrive at tables 7.1 and 7.2 after fitting with the conflicting eqs. (7.58) and (7.59). The contributions attributed to the minimal coupling does not change between the references. We plot the data set and the fitted function in fig. 7.8.

Our results indicate, however, that the fitting eq. (7.58) for conformal coupling leads to a disagreement, and the $\tilde{\sigma}_2$ is not recovered. This is opposite to the fitting

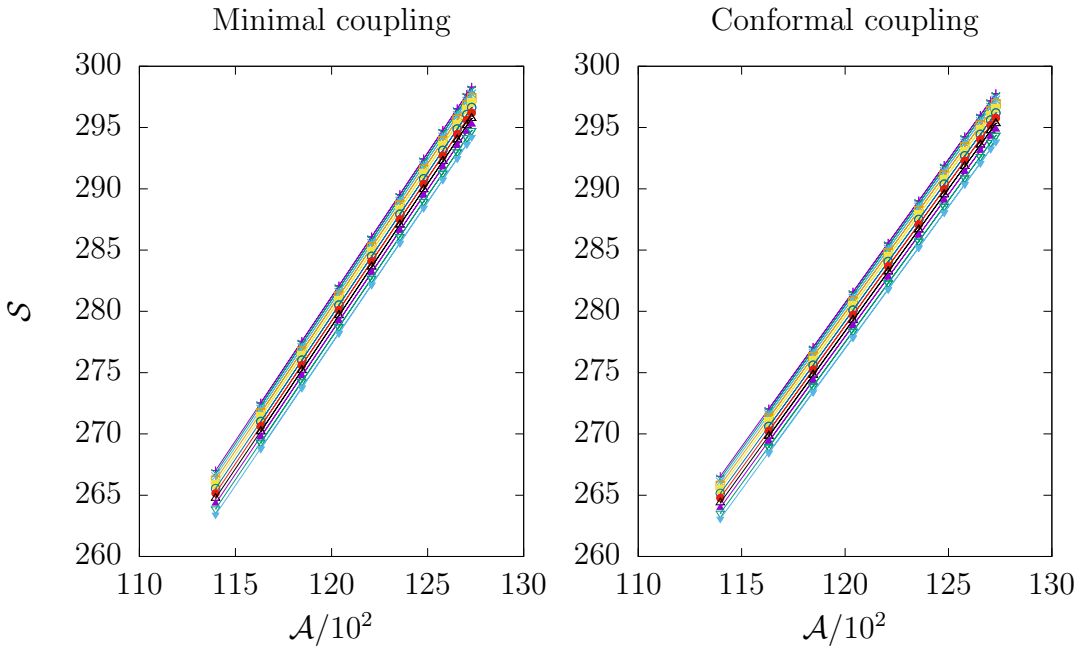

Figure 7.7: Linear plot for the entropy-area relation for massive fields in both curvature couplings. The range of masses is $0.030 < m < 0.100$ in increments of 0.007, totalling 10 points in the intermediate range $40 < n < 60$ of the total 100 sites.

Minimal coupling

Method	σ_2	$\tilde{\sigma}_2$
Numerical	0.0126 ± 0.0033	$(-9.01 \pm 11.57) \times 10^{-6}$
Analytical	$0.0133 \sim 1/24\pi$	$-3.490\,66 \times 10^{-6} \sim -1/90\pi r^2$

Table 7.1: Fit for the slopes of fig. 7.7 versus their corresponding mass and either one of eqs. (7.58) and (7.59), which are equal for the present case of $\xi = 0$.

Conformal coupling

Method	Coefficients in ref. [66]	
	σ_2	$\tilde{\sigma}_2$
Numerical	—	$(-4.182\,13 \pm 0.427\,00) \times 10^{-5}$
Analytical	—	$8.726\,65 \times 10^{-7} \sim 1/360\pi r^2$
	Coefficients in ref. [65]	
	σ_2	$\tilde{\sigma}_2$
Numerical	$0.013\,33 \pm 0.003\,20$	$(3.81 \pm 11.14) \times 10^{-6}$
Analytical	$0.013\,26 \sim 1/24\pi$	$8.726\,65 \times 10^{-7} \sim 1/360\pi r^2$

Table 7.2: Comparison between the values fitted over equations eqs. (7.58) and (7.59) respectively in the case of $\xi = 1/6$. The conflict between the fitted value and the expectation found in ref. [66] is apparent, whilst still being within the error bar for the result in ref. [65].

which includes the same contribution already appearing in flat space, σ_2 due to ref. [65]; in this case, the value found for σ_2 is accurate to within 1%. Still assuming [65], the expectations of $\tilde{\sigma}_2$ for both couplings are found to lie inside the margin of error of the calculations.

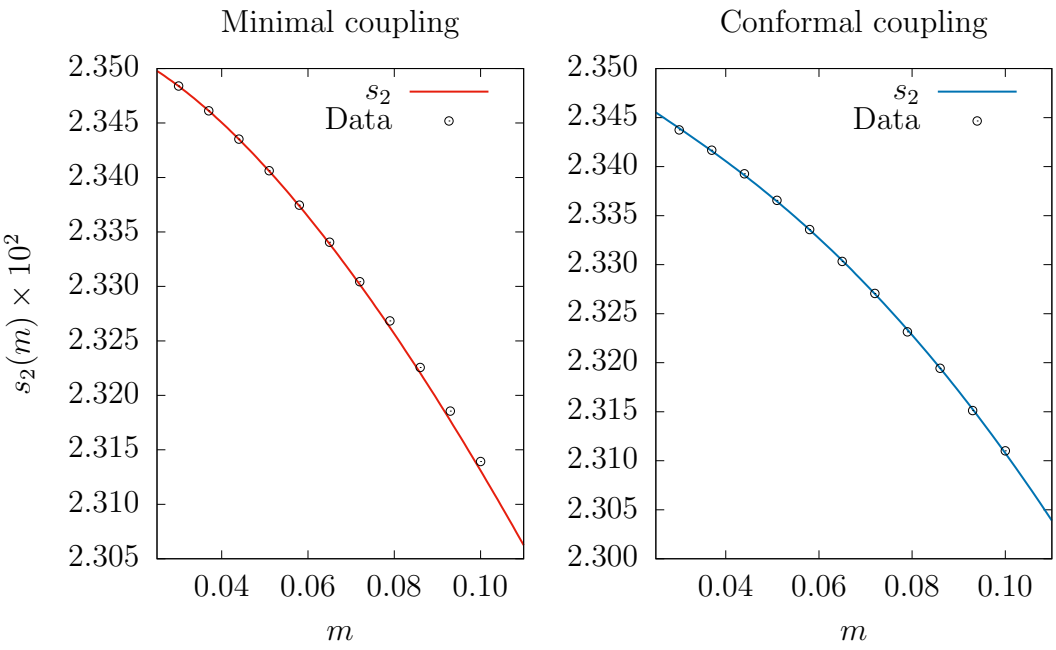

Figure 7.8: Entropy area-density s_2 plotted as a function of the mass m for both $\xi = 0$ and $\xi = 1/6$. In the conformal case the fitting is based on coefficients of ref. [65].

Listing 7.1: Entanglement entropy through the covariance matrix formalism in the Einstein universe

```
(*Defines the symmetric coupling matrix*)
couplingK[l_] :=
  N@(0.5/a) Table[((
        l*(l + 1)*\[Pi]^2)/((R)^2*Sin[\[Pi]*(i + 0.5)/(R)
           ]^2) +
        Sin[\[Pi]*(i - 0.5)/(R)]^2/Sin[\[Pi]*(i + 0.5)/(R)
           ]^2 +
        1. + \[Pi]^2/(R)^2 6. \[Xi] + a^2 m^2)
           KroneckerDelta[i, j] -
      Sin[\[Pi]*(j - 0.5)/(R)]/
       Sin[\[Pi]*(j + 0.5)/(R)] KroneckerDelta[i, j + 1] -
      Sin[\[Pi]*(i - 0.5)/(R)]/
       Sin[\[Pi]*(i + 0.5)/(R)] KroneckerDelta[i + 1, j], {i
          , 0,
      R}, {j, 0, R}];
(*Coupling matrix*)
(**)
(*Extracts the eigenvalues and eigenvectors \
of the coupling matrix*)

eigenvalK[l_] := eigenvalK[l] = Eigenvalues@couplingK[l];
eigenvecK[l_] :=
  eigenvecK[l] =
   Map[Normalize, Eigenvectors[couplingK[l]]]\[Transpose];
(*Spectrum of coupling matrix*)
(**)
(*Defines the correlation block \
matrices Q and P*)

Xmat[l_] :=
  Xmat[l] = (1/2) eigenvecK[l].DiagonalMatrix[
      eigenvalK[l]^(-1/2)].Inverse[eigenvecK[l]];
Pmat[l_] :=
  Pmat[l] = (1/2) eigenvecK[l].DiagonalMatrix[eigenvalK[l
     ]^(
      1/2)].Inverse[eigenvecK[l]];
(*Correlation block matrices*)
```

```
(**)
(*Extracts the subregion \
correlations*)
Xreduce[r_, l_] := Xmat[l][[;; r + 1, ;; r + 1]];
Preduce[r_, l_] := Pmat[l][[;; r + 1, ;; r + 1]];
(*Reduced correlations*)
(**)
(*Computes the symplectic spectrum of \
the covariance matrix*)

eigenvalC[r_, l_] := (Eigenvalues[Xreduce[r, l].Preduce[r,
    l]])^(
  1/2);
(**)
(*Computes the per-mode entanglement entropy*)

modeEntropy[r_, l_] :=
  modeEntropy[r, l] =
   Table[If[Abs[eigenvalC[r, l][[i]] - 0.5] < 10^-10,
     0, (eigenvalC[r, l][[i]] + 0.5) Log[
       eigenvalC[r, l][[i]] + 0.5] - (eigenvalC[r, l][[i
          ]] -
        0.5) Log[eigenvalC[r, l][[i]] - 0.5]], {i, r +
        1}] //
    Total;
(**)
(*Sum the per-mode entropies to find the full entanglement
   \
entropy*)
areaLaw[lmax_] :=
 Monitor[Table[{r,
   Sum[(2 l + 1) Re[modeEntropy[r, l]], {l, 0, lmax}]}, {r
     , rmin,
    rmax}], {r, l}]
```

Chapter 8

Conclusion

We have seen throughout this dissertation how the formalisms of general relativity and quantum field theory interplay in the investigation of the area law of entanglement entropy of quantum fields in curved spacetime. We studied the entanglement entropy of scalar fields in the Einstein universe and its dependence on the parameters of the system. In order to achieve this we first reviewed a variety of techniques for computing the entanglement entropy of quantum fields in flat space and the theoretical underpinnings of the theory of quantum fields in curved spaces. We were then able to adapt the techniques developed in the flat case to the curved Einstein spacetime by exploring its high degree of symmetry.

In chapters 2 to 4 we presented the basics of each framework. In section 2.2 we motivate our choice of background based on the symmetry arguments. The von Neumann entropy is then introduced in section 3.2 and serves as our choice of entropy measure, to be used on the study of the canonically quantised scalar fields in the chosen background.

Concluding chapter 4 we discussed the Unruh effect which demonstrated the non-trivial behaviour of the quantum vacuum: similarly to the appearance of fictitious forces in non-inertial reference frames, the particle content of a theory is coordinate dependent. The vacuum is attached to a choice of basis of solutions to the classical field equations, and a preferred choice may therefore be nonexistent, especially in curved spacetimes.

Starting chapter 5 we introduced the correlations of the quantum vacuum. A review of the Reeh–Schlieder theorem in section 5.1.1 followed, measuring the amount of entanglement in the vacuum by indicating that operators localised in finite regions of space are sufficient to reproduce to arbitrary accuracy any physical state of the system. An explicit formula of the two-point functions for a massless scalar field in flat spacetime is found in section 5.1, for which the rigorous definition of quantum fields as operator-valued distributions is realised. The last subsection in chapter 5 reviews the numerical method due to Srednicki [2] for computing the

entanglement entropy of a scalar field. The theory is simplified by redefining it as a one-dimensional problem after a decomposition into angular normal modes, followed by discretisation. The vacuum is a Gaussian state, which facilitates the calculation of the trace, resulting in an explicit numerical value for the von Neumann entropy, confirming the expected area law behaviour.

A more abstract analysis of the representation of Gaussian states in phase space is carried out in chapter 6. We first introduce the compatible triad of metric, symplectic and complex structures with which to equip a finite-dimensional phase space. Secondly, the symplectic, orthogonal and complex groups preserving each structure are introduced, culminating in the unitary group located at their intersection. Section 6.2 reframes the entanglement entropy in terms of the covariance matrix, further linking it to the compatible triple in a more general setting as the Gaussian states are no longer treated with respect to a choice of basis. A more efficient algorithm for finding the entanglement entropy in these terms is then elaborated, based on ref. [59].

In the final chapter we repeat our investigation of vacuum correlations, but now in the maximally symmetric space of the Einstein universe. We find solutions to the classical equations of motion for the scalar field and, after quantising it, we compute the two-point functions in the Einstein space, which assumes a simple form in the case of massless fields minimally coupled to the curvature. In section 7.2 we apply the algorithm for numerically computing the entanglement entropy of scalar fields in the Einstein universe by exploiting its symmetries, allowing again for a decomposition into angular normal modes and discretisation into a one-dimensional lattice. The area law is recovered for minimally and conformally coupled fields, and we study it further by identifying curvature and universal corrections to it by varying the mass and the size of the lattice.

There is a controversy in the literature regarding a universal contribution to entanglement entropy that is curvature-independent but surprisingly determined by the choice of coupling of the field to the curvature [66, 65]. In our results we do not observe this behaviour, and instead they indicate a universal contribution that is also coupling-independent and equal to the flat space result as our intuition suggests, supporting ref. [65] in contrast to what is predicted in ref. [66].

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