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Particle Creation, Adiabatic Regularization and Entropy in Expanding Universes

Master's Dissertation in Physics

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“*I know the road is long, but you gotta carry on*”

Tyler Marenyi

“*May these pages find readers who will put them to use.*”

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Abstract

We investigate the thermodynamics of particle creation in expanding universes, focusing on entropy production and the emergence of thermal behavior from unitary evolution. Using an asymptotically flat FLRW toy model, we show that the initial vacuum evolves into a two-mode squeezed state, with particle pairs created in correlated momentum modes. To quantify the irreversible loss of phase information, we compute the diagonal entropy from the density matrix in the instantaneous energy eigenbasis. The resulting diagonal elements exhibit a thermal-like distribution, allowing us to assign an effective temperature to each mode.

Extending this analysis to de Sitter spacetime requires regularization of ultraviolet divergences. We construct an adiabatic vacuum via second-order WKB approximation and use it as a reference state to extract regularized Bogoliubov coefficients. For a conformally coupled massive scalar field, we compute the particle number spectrum, diagonal entropy, and effective temperature for two representative masses: the critical mass, $m = H/2$ and a heavy mass, $m = H$.

Our results reveal that thermalization is mass dependent. For $m = H$, the effective temperature of super-horizon modes asymptotically approaches the Gibbons-Hawking temperature, $T = H/2\pi$ indicating that principal series fields (for which $m \geq H$ thermalize at the horizon temperature. On the other hand, the critical mass exhibits a logarithmic infrared divergence, leading to a divergent effective temperature. We conclude that thermalization in de Sitter space is not a universal feature, but it depends sensitively on the field's mass.

Keywords: Quantum field theory in curved spacetime; General Relativity; Quantum thermodynamics; Quantum statistical mechanics; Adiabatic Regularization; de Sitter spacetime;

Resumo

Investigamos a termodinâmica da criação de partículas em universos em expansão, com foco na produção de entropia e no surgimento de comportamento térmico a partir de uma evolução unitária. Usando um modelo FLRW simplificado, assintoticamente plano, mostramos que o vácuo inicial evolui para um estado comprimido de dois modos, com pares de partículas criados em modos de momento correlacionados. Para quantificar a perda irreversível de informação de fase, calculamos a entropia diagonal a partir da matriz densidade na base instantânea dos autovetores de energia. Os elementos diagonais resultantes exibem uma distribuição semelhante à térmica, permitindo-nos atribuir uma temperatura efetiva a cada modo.

Estender essa análise ao espaço-tempo de Sitter requer a regularização de divergências ultravioleta. Para isso, construímos um vácuo adiabático por meio da aproximação WKB de segunda ordem e o utilizamos como estado de referência para extrair coeficientes de Bogoliubov regularizados. Para um campo escalar massivo com acoplamento conforme, calculamos o espectro de número de partículas, a entropia diagonal e a temperatura efetiva para duas massas representativas: a massa crítica, $m = H/2$, e uma massa pesada, $m = H$.

Nossos resultados revelam que a termalização depende da massa. Para $m = H$, a temperatura efetiva dos modos super-horizonte se aproxima assintoticamente da temperatura de Gibbons-Hawking, $T = H/2\pi$, indicando que os campos da série principal (para os quais $m \geq H$) termalizam na temperatura do horizonte. Por outro lado, a massa crítica exibe uma divergência infravermelha logarítmica, levando a uma temperatura efetiva divergente. Concluímos que a termalização no espaço de Sitter não é uma característica universal, mas depende fortemente da massa do campo.

Palavras-Chave Teoria quântica de campos em espaço-tempo curvo; Relatividade Geral; Termodinâmica quântica; Mecânica estatística quântica; Regularização adiabática; Espaço-tempo de Sitter;

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Chapter 1

Introduction

Quantum field theory (QFT) and general relativity (GR) are two great pillars upon which modern theoretical physics is built. On one hand, QFT constitutes the successfully tested framework that accurately describes the quantum dynamics of matter and non-gravitational interactions, incorporating locality, causality, and the principles of special relativity within Minkowski spacetime [1–3]. Conversely, general relativity is a geometrical description of gravitation in which spacetime is described as a smooth and differentiable manifold, and its curvature is sourced by energy and momentum [4–6]. In its structure, these two theories are very distinct: in QFT, spacetime is fixed and serves as a background on which quantum fields propagate, whereas in GR, the background itself becomes a dynamical entity governed by the Einstein field equations.

Tensions between these frameworks emerged soon after the birth of quantum mechanics. In 1929, Heisenberg and Pauli's work on quantum electrodynamics revealed divergent self-energies in perturbative calculations [7]. Pauli thought that including gravity might cure these divergences, prompting his assistant Léon Rosenfeld at ETH Zurich to attempt the first quantization of linearized gravity in 1930 [8]. By 1939, Fierz and Pauli had shown that linearized gravity in flat spacetime reduces to the equations of a massless spin-2 field, identifying the graviton as its associated particle [9].

The subsequent progress of perturbative quantum field theory in the mid-20th century raised optimism that gravity could eventually be integrated in the same framework. Those was short lived, as the results of Hooft and Veltman [10], followed by the two-loop computations by Goroff and Sagnotti [11] proved that perturbative quantum gravity requires an infinite number of counterterms to cancel the ultraviolet divergences. While viable as an effective field theory below the Planck scale, direct quantization of the Einstein–Hilbert action cannot yield a UV-complete theory of gravity.

Faced with this dead end, a different approach gained traction. A full theory of quantum gravity remained seemingly out of reach, but one could follow a path similar to that of early quantum electrodynamics, where matter was quantized while the electromagnetic field was treated classically [12], By analogy, quantum fields could be studied on a classical gravitational background. This semiclassical theory is known as quantum field theory in curved spacetime.

An important advance in this framework was made by Leonard Parker in the late 1960's and early 1970's. Studying quantum fields in Friedmann–Lemaître–Robertson-Walker (FLRW) cosmologies, Parker discovered that cosmic expansion inevitably creates particles from the vacuum. Using Bogoliubov transformations [13, 14] to relate mode solutions at different times, he proved that the dynamical gravitational background mixes positive- and negative-frequency modes as defined by a comoving observer. This mixing produces the phenomenon now known as gravitational particle creation [15–20]: even when a field begins in its vacuum state, the expectation value of the particle number operator becomes nonzero as the universe expands.

Parallel to the advancements in quantum field theory in curved spacetime, another major development arose in the latter half of the twentieth century: the understanding that quantum entanglement and information-theoretic measures are essential for understanding the thermodynamic behavior of quantum systems [21, 22]. Phenomena like Hawking radiation and the Unruh effect [23, 24], for instance, exhibit thermal spectra, suggesting that gravity endows quantum fields with a thermodynamic character [25]. However, taking into account that these effects originate from pure quantum states that evolve unitarily, the question of how thermal behavior can emerge from an underlying pure state must be addressed.

A clue for explaining this behavior came from the realization that the phenomenon of gravitational particle creation inherently produces entanglement [26, 27]. When a dynamic spacetime amplifies vacuum fluctuations, particles are generated in correlated pairs with opposite momenta, $(k, -k)$ [28, 29]. The global quantum state of the field (for example, the vacuum state) remains pure; however, if one considers only a subset of modes, such as tracing over partner modes that propagate outside an observer's causal horizon, the reduced density matrix becomes a mixed state. The entropy associated with this reduced state is the entanglement entropy [30, 31], not a classical thermodynamic entropy; yet, it plays a similar quantitative role.

As the areas of quantum thermodynamics and nonequilibrium quantum statistical mechanics have matured, the connection between the thermodynamic properties of quantum fields emerging from the underlying gravitational field has become increasingly clear. An important development was the introduction of the concept of microscopic diagonal entropy in the early 2010's [32–34]. The diagonal entropy is defined by restricting the density matrix to its diagonal part in the instantaneous energy eigenbasis. It measures the number of accessible microstates consistent with the energy distribution when a system is driven far from equilibrium, a condition analogous to that encountered in an expanding cosmological background.

In this work, we investigate the thermodynamic aspects and entropy production due to gravitational particle creation in an expanding universe. We will first examine a simple toy model, consisting in a free, real and massive scalar field propagating in a $1+1$ asymptotically flat FLRW spacetime. The study of this kind of cosmological model is motivated by the fact that it facilitates the formulation of particle creation. In a universe that undergoes expansion at all times, such as our own, there is no natural definition of positive and negative-frequency modes throughout the entire evolution, in contrast to an asymptotically flat spacetime, where well defined vacuum states exist.

Following the analysis of an asymptotically flat Friedmann-Lemaître-Robertson-Walker (FLRW) universe, this work employs the method of **adiabatic regularization** [15, 35–38] to investigate particle production and its associated thermodynamic properties within a de Sitter spacetime. Adiabatic regularization is necessary to eliminate the ultraviolet divergences that inevitably happen in the computation of the particle number density and other observables in expanding backgrounds.

Chapter 2 is the theoretical foundation of the quantum field theory of scalar fields in curved spacetime. We begin by formulating the classical dynamics of the field propagating in a general gravitational background. This includes the derivation of the covariant Klein-Gordon equation and the associated energy-momentum tensor from the action principle. To ensure a well-posed initial value problem and causal wave propagation, we emphasize the hyperbolic character of the field's equation of motion and discuss the necessity of global hyperbolicity for the causal structure of spacetime. Then, we utilize the classical phase space defined by the invariant Klein-Gordon inner product and proceed to canonically quantize the field. We introduce the mode expansion alongside the corresponding creation and annihilation operators that construct the Fock space. A central focus of this chapter is the inherent ambiguity in defining a unique, observer-independent vacuum state in generic curved spacetimes, a difficulty that arises directly from the absence of a global timelike Killing vector field. Finally, the chapter introduces the formalism of Bogoliubov transformations, which is the linear transformation that relates inequivalent mode decompositions and their respective vacuum states. We demonstrate that the Bogoliubov transformation relating the modes induces a transformation of the ladder operators, and with this, we formally define the particle number operator.

In Chapter 3, we apply the formalism developed in the previous chapter to a $1+1$

spatially flat FLRW spacetime with asymptotically static regions. We analytically determine the Bogoliubov coefficients relating these regions, explicitly demonstrating that particle creation occurs as a direct consequence of the spacetime expansion. In sequence, we show that the initial vacuum state evolves into a highly entangled, two-mode squeezed state in the late-time basis, where particles are generated in correlated momentum pairs. To quantify the thermodynamic of this (unitary) evolution, we provide a brief discussion on the problem of irreversibility in physics, and use it to introduce the concept of diagonal entropy. By focusing on the diagonal elements of the density matrix in the instantaneous energy eigenbasis, this quantity serves as a consistent measure of irreversibility. It captures the effective loss of accessible information inherent to the system due to the rapid dephasing of unobservable quantum coherences. Finally, by calculating the diagonal entropy for the created particle distribution, we reveal the emergent thermodynamic behavior of the field, which ends with the identification of a thermal-like spectrum and an effective temperature associated with each field mode.

Chapter 4 is a brief but necessary chapter, devoted to introducing the tools to deal with the problem of the divergences that arise when calculating physical observables, such as the particle number and energy density in spacetimes that are not asymptotically flat. To obtain physically meaningful and finite results, we introduce the method of adiabatic regularization. We begin by reviewing the Wentzel-Kramers-Brillouin (WKB) approximation, a semiclassical method for obtaining approximate solutions to second-order ordinary differential equations. This mathematical tool is applied to the field's mode equations, allowing us to define the adiabatic vacuum state order-by-order. This adiabatic vacuum will serve as the reference state that will be used to characterize the particle content of the quantum field as the universe expands. By comparing the exact modes that defines the vacuum state of the field to the modes that define the adiabatic vacuum, we can extract the Bogoliubov coefficients that eliminates the divergences.

Chapter 5 extends the investigation of cosmological particle creation to a more realistic and cosmologically relevant background: four-dimensional de Sitter spacetime. We begin by reviewing the geometric properties of the de Sitter manifold, focusing specifically on the Poincaré coordinate patch, which effectively models an exponentially expanding, spatially flat universe. Within this spacetime, we analyze the dynamics of a massive, conformally coupled real scalar field.

As discussed in the previous chapters, in spacetimes such as de Sitter, where asymptotically flat regions do not exist, there is no way to naturally define particle states. To address this, we identify and select the Bunch-Davies vacuum as our preferred initial state. This choice is motivated by the fact that it recovers the standard Minkowski positive-frequency behavior in the deeply sub-horizon limit (when $\eta \to -\infty$, we expect the modes of all wavelengths to be inside the horizon).

After selecting the exact mode functions and the initial vacuum state, we apply the method of adiabatic regularization developed in Chapter 4. By tracking the mode evolution as it crosses the cosmological horizon, we define the physical particle content through a direct comparison between the exact field modes and the adiabatic reference state. We then utilize the regularized spectrum of the particle number to write the time evolution of the diagonal entropy per mode of the created particles of different masses, and demonstrate that thermalization is mass dependent.

Chapter 2

Quantum Field Theory in Curved Spacetime

Quantum field theory in curved spacetime (QFTCS) is the theory that describes the propagation of a quantum field that exists in a classical, curved (fixed or dynamic) background, $(\mathcal{M}, g_{\mu\nu})$, as in the framework of general relativity [39, 40]. Because the metric is treated classically, QFTCS is not regarded as a fundamental theory of nature; in fact, it is expected to break down when the spacetime curvature approaches Planck scales. Regardless, QFTCS is likely to provide a good description of quantum processes within its domain of validity, which includes a variety of phenomena such as Hawking radiation, trace anomalies, backreaction of $\langle T_{\mu\nu} \rangle$, and of central relevance to this work, the creation of particles by time-dependent gravitational backgrounds.

One of the greatest difficulties in transitioning from QFT in Minkowski spacetime to QFTCS is the absence of *Poincaré invariance*, which is heavily relied upon when dealing with quantum fields within a flat background. Indeed, many of the familiar symmetries we are accustomed to are not even well-defined in the context of a curved spacetime. For instance, the lack of a global timelike *Killing vector* implies that it is no longer possible to guarantee both energy conservation and the canonical decomposition of field modes into positive and negative frequencies; therefore, one cannot define a unique vacuum state, and the interpretation of particles becomes ambiguous. Different observers will generally disagree on what constitutes a vacuum, leading to inequivalent Fock representations and, ultimately, no preferred notion of particle number [41].

The goal of this chapter to present a consistent formulation of quantum field theory in curved spacetime regarding a real scalar field. We begin by formulating the dynamics of a real scalar field on a general curved background with metric $g_{\mu\nu}$, introducing the covariant action, the associated stress–momentum tensor, and the covariant Klein–Gordon equation, with a brief review of the theory of second-order partial differential equations being necessary to highlight the hyperbolic character of the field's equation of motion. The role of global hyperbolicity of the spacetime structure will also be discussed, ensuring a well-posed initial value problem. The Klein–Gordon inner product is then defined as the structure underlying the normalization of field modes and the construction of the classical phase space. Following from these results, the canonical quantization procedure is presented, including the mode expansion of the field, the introduction of creation and annihilation operators, and the construction of a Fock space, where we will address the inherent ambiguity in defining a unique vacuum state. Finally, we develop the formalism of Bogoliubov transformations, which relate different choices of mode decompositions and vacuum states, and introduce the particle number operator as a tool for characterizing particle creation in time-dependent gravitational backgrounds.

2.1 Real Scalar Fields in Curved Backgrounds

2.1.1 The Action and the Energy-Momentum Tensor

Let $\mathcal{M}$ be a manifold that is assumed to be smooth, 4-dimensional, and equipped with a Lorentzian metric g with signature $(+---)$. This defines the curved spacetime that will be denoted $(\mathcal{M}, g)$.

Let us consider a real scalar field ϕ propagating in this manifold. The Lagrangian density is

$$\mathcal{L}(x) = \frac{1}{2}\sqrt{-g}\left[g^{\mu\nu}(x)\nabla_\mu\phi(x)\nabla_\nu\phi(x) - (m^2 + \xi R(x))\phi^2(x)\right], \tag{2.1}$$

where ∇_μ denotes the covariant derivative, g is the determinant of the metric (we explain in Appendix A.1 why the quantity $\sqrt{-g}$ appears), and ξ is a numerical factor that couples the scalar field to gravity, represented by the Ricci scalar $R(x)$.

Regarding the coupling constant ξ, there are two values of great interest in the literature: the minimally coupled case, where $\xi = 0$, and the conformally coupled case, where $\xi = \frac{d-2}{4(d-1)}$ for a d-dimensional spacetime. In two dimensions, conformal coupling yields $\xi = 0$, coinciding with the minimal coupling prescription. In four dimensions, conformal coupling gives $\xi = 1/6$.

The resulting action functional is obtained by the integration of (2.1) over all of $\mathcal{M}$:

$$S[\phi] = \frac{1}{2}\int d^4x\sqrt{-g}[g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - (m^2 + \xi R)\phi^2]. \tag{2.2}$$

Variation of the action with respect to $g_{\mu\nu}$ yields the energy-momentum tensor:

$$T_{\mu\nu}(x) = -\frac{2}{\sqrt{-g}}\frac{\delta S}{\delta g_{\mu\nu}}; \tag{2.3}$$

making use of the following identities

$$\begin{aligned}\delta(\sqrt{-g}) &= \frac{1}{2}\sqrt{-g}g^{\mu\nu}\delta g_{\mu\nu},\\ \delta g^{\mu\nu} &= -g^{\mu\alpha}g^{\nu\beta}\delta g_{\alpha\beta},\end{aligned} \tag{2.4}$$

we obtain

$$\begin{aligned}T_{\mu\nu} = \nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\left(g^{\alpha\beta}\nabla_\alpha\phi\nabla_\beta\phi - m^2\phi^2\right)\\ +\xi\left(G_{\mu\nu} + g_{\mu\nu}\Box_g - \nabla_\mu\nabla_\nu\right)\phi^2,\end{aligned} \tag{2.5}$$

where $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R$ is the Einstein tensor.

The energy-momentum tensor $T_{\mu\nu}$ characterizes the local distribution and flux of energy and momentum carried by the field. In general relativity, $T_{\mu\nu}$ acts as the source of the Einstein-Field equations, which describe how energy and momentum influence the geometry of spacetime. In quantum field theory in curved spacetime, the expectation value $\langle T_{\mu\nu}\rangle$ determines the backreaction, which is the modification of the geometry induced by the quantum field through

$$G_{\mu\nu} = 8\pi G\langle T_{\mu\nu}\rangle. \tag{2.6}$$

In this work, however, the backreaction is neglected. We will focus instead on the dynamics of scalar fields in curved spacetime and on the physical consequences of particle creation.

2.1.2 Equation of Motion and Global Hyperbolicity

Having written the action functional (2.2), and given that, for a scalar $\nabla_\mu = \partial_\mu$, the equation of motion for the field is obtained via Hamilton's principle $\delta S = 0$:

$$\begin{aligned}\delta S &= \frac{1}{2}\int d^4x\sqrt{-g}\left[g^{\mu\nu}\delta(\partial_\mu\phi\partial_\nu\phi) - (m^2+\xi R)\delta(\phi^2)\right]\\ &= \int d^4x\sqrt{-g}\left[g^{\mu\nu}\partial_\mu(\delta\phi)\partial_\nu\phi - (m^2+\xi R)\phi\delta\phi\right]\\ &= \int d^4x\left[-\partial_\mu(\sqrt{-g}\,g^{\mu\nu}\partial_\nu\phi) - \sqrt{-g}(m^2+\xi R)\phi\right]\delta\phi\\ &= 0,\end{aligned} \tag{2.7}$$

leading us to the covariant Klein-Gordon equation

$$(\Box_g + m^2 + \xi R)\phi = 0, \tag{2.8}$$

where $\Box_g \phi = \frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}\, g^{\mu\nu}\partial_\nu\phi)$ defines the covariant d'Alembertian operator.

Before studying the explicit solutions of (2.8), we briefly review some general aspects of partial differential equation theory related to its classification. This discussion is necessary for us to identify the properties associated with the hyperbolic character of the equation and its implications, in particular, those concerning causal propagation and the spacetime structure.

The Klein-Gordon equation is a second-order PDE. Equations of this type receives a special classification determined by the coefficients of their highest-order derivative terms. In analogy with the classification of conic sections via the discriminant of a quadratic form, second-order PDEs are classified as **hyperbolic**, **parabolic**, or **elliptic**.

To make this distinction precise, consider a general second-order PDE for a scalar function $f(x)$ on $\mathbb{R}^{n+1}$ of the form

$$Df = g^{\mu\nu}(x)\partial_\mu\partial_\nu f + b^\mu(x)\partial_\mu f + c(x)f. \tag{2.9}$$

The principal part of the operator D is defined as

$$D_0 f = g^{\mu\nu}(x)\partial_\mu\partial_\nu f, \tag{2.10}$$

and the classification of the PDE is formulated in terms of the principal symbol, defined as

$$p(x,k) = g^{\mu\nu}(x)k_\mu k_\nu, \tag{2.11}$$

where $k = (k_0, ..., k_n)$. In local coordinates, the principal symbol may be regarded as a polynomial:

$$p(x,(k_0,\vec{k})) = ak_0^2 + bk_0 + c, \tag{2.12}$$

with coefficients depending on x and $\vec{k}$.

If we fix the coordinate x^0 to play the role of time, and if for every nonzero spatial $\vec{k}$, the equation

$$p(x,(k_0,\vec{k})) = 0 \tag{2.13}$$

admits only real and distinct solutions, the corresponding PDE is said to be **hyperbolic with respect to** x^0. This condition is equivalent to requiring that the discriminant $\Delta(x,\vec{k}) = b^2 - 4ac$ is strictly positive.

In contrast, if $\Delta(x,\vec{k}) = 0$, the polynomial has a single real root with multiplicity two, and the PDE is classified as **parabolic**. Finally, if $\Delta(x,\vec{k}) < 0$, the polynomial has no real roots, and the PDE is said to be **elliptic**.

To illustrate these definitions, let us consider the Klein-Gordon equation. Expanding $\Box_g$, we obtain

$$\Box_g = \frac{1}{\sqrt{-g}} \left[(\partial_\mu \sqrt{-g}\, g^{\mu\nu})(\partial_\nu \phi) + \sqrt{-g}\, g^{\mu\nu} \partial_\mu (\partial_\nu \phi) \right] . \tag{2.14}$$

Now, we look for the highest-order derivatives, which appear in the term involving $g^{\mu\nu}\partial_\mu(\partial_\nu\phi)$. Provided that the metric is Lorentzian, $\Delta(x, \vec{k})$ is always positive, rendering equation (2.8) a hyperbolic equation.

The relevance of these notions lies in their implications for the initial value problem associated with the Klein–Gordon equation. Hyperbolicity is a necessary condition for formulating a Cauchy problem with finite propagation speed; unlike parabolic or elliptic equations (such as the heat equation and Poisson's equation), which allow disturbances to propagate with infinite speed across space as a consequence of *strong maximum principles*, [42] hyperbolic differential equations describe wave-like phenomena where information travels at a finite speed. The principal part of $\Box_g$ (the term with second derivatives) determines the characteristic surface propagation; because the metric is Lorentzian, these characteristics coincide exactly with the null light cones of spacetime. This constraint ensures that the field respects causality: a disturbance at a given spacetime point can only influence events within its future light cone, and conversely, the state of the field at any point is determined uniquely by the information encoded in its causal past [43].

While the hyperbolic nature of wave equations make so that the propagation speed of the wave is finite and guarantee a local well-posedness, it is not sufficient to guarantee the existence of globally well-behaved solutions for the initial value problem. An arbitrary Lorentzian spacetime could present causal pathologies, such as closed timelike curves or incomplete causal domains, which may obstruct the existence or uniqueness of solutions defined on the entire manifold. To prevent these kinds of problems, additional conditions are needed on the spacetime structure, which leads to the requirement of **global hyperbolicity**:

Definition 1. *A spacetime $(\mathcal{M}, g_{\mu\nu})$ is said to be globally hyperbolic if it possesses a Cauchy surface Σ, a spacelike hypersurface that every inextensible causal curve intersects exactly once, so that the state of the field at any point in the manifold is uniquely determined by the initial data specified on Σ.*

Every spacetime considered in this work shall be globally hyperbolic.

2.1.3 Klein-Gordon Inner Product and Canonical Momentum

In order to define a conserved notion of norm, it is necessary to introduce an appropriate inner product. For a spacelike hypersurface Σ with a future-directed unit normal vector n^μ, the Klein-Gordon inner product of a pair of solutions is defined as

$$(\phi_1, \phi_2) = -i \int_\Sigma d\Sigma^\mu \left(\phi_1 \partial_\mu \phi_2^* - \phi_2^* \partial_\mu \phi_1\right) \ . \tag{2.15}$$

Provided that the spacetime is globally hyperbolic, the hypersurface is taken to be a Cauchy surface. Moreover, the inner product is independent of the choice of Σ:

$$(\phi_1, \phi_2)_{\Sigma_1} = (\phi_1, \phi_2)_{\Sigma_2}. \tag{2.16}$$

This surface independence is proven by the use of Gauss' theorem: let V be the four-volume bounded by Σ_1 and Σ_2, and, if necessary, assume timelike boundaries on which $\phi_1 = \phi_2 = 0$. Assuming that the solutions of (2.8) vanish at spatial infinity, we may write

$$\begin{aligned}(\phi_1, \phi_2)_{\Sigma_2} - (\phi_1, \phi_2)_{\Sigma_1} &= -i \oint_{\partial V} d\Sigma^\mu \left(\phi_1 \partial_\mu \phi_2^* - \phi_2^* \partial_\mu \phi_1\right) \\ &= -i \int_V \nabla^\mu \left(\phi_1 \partial_\mu \phi_2^* - \phi_2^* \partial_\mu \phi_1\right) \, dV.\end{aligned} \tag{2.17}$$

Furthermore, expanding the integrand, we obtain

$$\phi_1 \Box_g \phi_2^* - \phi_2^* \Box_g \phi_1 = 0, \tag{2.18}$$

proving equation (2.16).

The solutions of the Klein-Gordon equation span a complex vector space, denoted by $\mathcal{S}$, which admits a decomposition into subspaces $\mathcal{S}^+$ and $\mathcal{S}^-$ of positive- and negative-norm solutions; i.e., there exists a complete set of complex **mode solutions** $u_i(x)$ that is orthonormal with respect to (2.15):

$$(u_i, u_j) = \delta_{ij}, \quad (u_i^*, u_j^*) = -\delta_{ij}, \quad (u_i, u_j^*) = 0, \tag{2.19}$$

where the index i is just a schematic representation of the set of quantities necessary to label the modes. In generic curved spacetimes, however, this decomposition is not unique, as different choices of mode bases lead to distinct splittings of $\mathcal{S}$. This non-uniqueness will be explored in detail in the following sections.

With the choice of mode bases made, a general solution $\phi \in \mathcal{S}$ can be expanded as

$$\phi(x) = \sum \left(a_i u_i(x) + b_i u_i^*(x)\right), \tag{2.20}$$

with complex coefficients a_i and b_i. Finally, since the field is real, $\phi(x) = \phi^*(x)$, which implies $b_i = a_i^*$.

The Klein–Gordon inner product provides a covariant characterization of the space of classical solutions and underlies the mode decomposition of the field; however, the formalism of canonical quantization developed in the next section requires the introduction of a phase space structure defined on spacelike hypersurfaces. In particular, a set of canonical variables needs to be identified. These are the field ϕ and its conjugate momentum, which will be denoted by π. This construction necessarily breaks the manifest covariance of the theory since a specific coordinate system must be chosen.

Let $\{\Sigma_t\}$ be a foliation of spacetime by spacelike Cauchy hypersurfaces labeled by a time function t. Each Σ_t has a future-directed unit normal vector n^μ. The canonical momentum is obtained by

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial(\partial_t \phi)}, \tag{2.21}$$

which, for the Lagrangian density (2.1), yields

$$\pi = \sqrt{-g}\,(g^{00}\partial_t\phi + g^{0i}\partial_i\phi). \tag{2.22}$$

In spacetimes where the metric is diagonal with respect to the chosen foliation—such as the FLRW metrics—the mixed components g^{i0} vanish. In this case, the canonical momentum simplifies to

$$\pi = \sqrt{-g}\,g^{00}\partial_t\phi. \tag{2.23}$$

2.2 Canonical Quantization

2.2.1 Equal-Time Commutators and Mode Expansion

Building on the classical formulation developed in the previous sections, the theory is quantized using the canonical quantization formalism, in which the field $\phi(x)$ and its conjugate momentum $\pi(x)$ are promoted to Hermitian operator-valued distributions acting on a Hilbert space of quantum states. The algebraic structure of the quantum theory is defined by imposing the equal-time commutation relations:

$$\begin{aligned}
&[\phi(\vec{x},t), \phi(\vec{x}',t)] = 0 \\
&[\pi(\vec{x},t), \pi(\vec{x}',t)] = 0 \\
&[\phi(\vec{x},t), \pi(\vec{x}',t)] = i\delta^{(3)}(\vec{x}-\vec{x}').
\end{aligned} \tag{2.24}$$

Here, a specific foliation $\{\Sigma_t\}$ has been chosen, where $\delta^{(3)}(\vec{x}-\vec{x}')$ denotes the Dirac delta distribution on Σ_t with the usual property of

$$\int d\Sigma\, \delta^{(3)}(\vec{x}-\vec{x}') = 1. \tag{2.25}$$

Let $\{u_i\}$ be an arbitrary complete set of positive-norm solutions of the Klein–Gordon equation, with respect to the Klein–Gordon inner product, and $\{u_j^*\}$ the corresponding negative norm-modes. Then, the field operator ϕ may be expanded as

$$\phi(x) = \sum_i \left(a_i u_i(x) + a_i^\dagger u_i^*(x)\right). \tag{2.26}$$

The coefficients a_i and $a_i^\dagger$ have the interpretation of creation and annihilation operators and obey

$$\begin{aligned}
[a_i, a_j] &= 0 \\
[a_i^\dagger, a_j^\dagger] &= 0 \\
[a_i, a_j^\dagger] &= \delta_{ij},
\end{aligned} \tag{2.27}$$

as a direct consequence of (2.24).

There will be a normalized ground state, the **vacuum state**, denoted by $|0\rangle$, defined by the condition that it is annihilated by every annihilation operator:

$$a_i\,|0\rangle = 0, \qquad \forall\, i; \tag{2.28}$$

physically, the vacuum is the state that does not contain any field quanta. It is normalized as $\langle 0|0\rangle = 1$.

The one-particle Hilbert space is defined by the one-particle state $|1_i\rangle$ obtained by applying the creation operators $a_i^\dagger$ to the vacuum state

$$|1_i\rangle = a_i^\dagger\,|0\rangle\,. \tag{2.29}$$

Similarly, a many-particle state is constructed by

$$|1_{i_1}, 1_{i_2}, ..., 1_{i_n}\rangle = a_{i_1}^\dagger a_{i_2}^\dagger ... a_{i_n}^\dagger\,|0\rangle\,. \tag{2.30}$$

If the state has two or more quanta per mode, then

$$|n_{i_1}, n_{i_2}, ...n_{i_r}\rangle = (n_{i_i}! n_{i_2}!, ..., n_{i_r}!)^{-\frac{1}{2}} (a_{i_1}^\dagger)^{n_1} (a_{i_2}^\dagger)^{n_2} ... (a_{i_r}^\dagger)^{n_j}\,|0\rangle\,, \tag{2.31}$$

where the $n!$ terms are necessary due to the Bose-Einstein statistics of identical particles; equation (2.31) defines the complete Fock space.

The creation and annihilation operators act on a particle-state as

$$\begin{aligned} a_i^\dagger \left| n_i \right\rangle &= (n_i + 1)^{\frac{1}{2}} \left| (n_i + 1) \right\rangle \\ a_i \left| n_i \right\rangle &= n_i^{\frac{1}{2}} \left| (n - 1) \right\rangle . \end{aligned} \tag{2.32}$$

The number operator for each i is defined by

$$N_i = a_i^\dagger a_i, \tag{2.33}$$

such that

$$N_i \left| n_1, ..., n_i, ..., n_j \right\rangle = n_i \left| n_1, ..., n_i, ..., n_j \right\rangle . \tag{2.34}$$

States that obey (2.34), i.e., eigenstates of the number operator, are the basis vectors for the entire Fock space. The normalization is given by

$$\left\langle n_{i_1}, n_{i_2}, ..., n_{i_r} \middle| m_{i'_1}, m_{i'_2}, ..., m_{i'_s} \right\rangle = \prod_\alpha \delta_{n_{i_\alpha} m_{i'_\alpha}} . \tag{2.35}$$

2.2.2 The Problem of the Unique Vacuum State

In Minkowski spacetime, there is a natural, unique set of modes chosen by all inertial observers. These modes are closely related to the natural cartesian coordinates $(\vec{x}, t)$, and these coordinates are, in turn, associated with the Poincaré group of boosts, rotations and translations. The notion of particles is defined through the decomposition of field modes into positive- and negative-frequency components. This classification is determined by the existence of a global timelike Killing vector field, $K^\mu = (\partial_t)^\mu$, which generates time translations and allows one to define frequency with respect to a preferred time coordinate.

Formally, the differential operator $\mathcal{L}_K$ is defined with respect to K^μ, and the mode solutions may be taken as its eigenfunctions. This differential operator is called the *Lie derivative*. The action of $\mathcal{L}_K$ on the scalar field ϕ gives $\mathcal{L}_K \phi = K^\mu \partial_\mu \phi$. For the modes $u(x)$ in Minkowski spacetime, the eigenvalue equation is

$$\begin{aligned} \mathcal{L}_K u(x) &= K^\mu \partial_\mu u(x) \\ &= \partial_t u(x) \\ &= -i\omega u(x). \end{aligned} \tag{2.36}$$

Similarly, applying $\mathcal{L}_K$ to its complex conjugate:

$$\begin{aligned}\mathcal{L}_K u^*(x) &= K^\mu \partial_\mu u^*(x) \\ &= \partial_t u^*(x) \\ &= +i\omega u^*(x).\end{aligned} \tag{2.37}$$

The $u(x)$ modes are said to be of positive frequency with respect to the time coordinate t, meaning that they obey (2.36), while the $u^*(x)$ modes are said to be of negative frequency with respect to t, satisfying (2.37). This construction leads to a unique and observer-independent decomposition of the field in flat spacetime, ensuring that the associated vacuum state is unambiguously defined.

This construction no longer applies in generic curved spacetimes. Global time-like Killing vector fields do not necessarily exist, and in their absence, there is no preferred notion of time translation with respect to which frequency can be defined. As a consequence, the decomposition of field solutions into positive- and negative-frequency modes becomes non-unique and depends on the choice of observer or on the particular foliation of spacetime. As briefly discussed in section 2.1.3, different choices of mode bases lead to inequivalent definitions of annihilation and creation operators, and hence to distinct vacuum states.

To illustrate this feature, let us consider an alternative set of mode solutions $\{\bar{u}_i(x)\}$ that satisfy the Klein-Gordon inner product (2.15). The field operator can, therefore, be expanded with respect to these new modes:

$$\phi(x) = \sum_i \left(b_i \bar{u}_i(x) + b_i^\dagger \bar{u}_i^*(x) \right). \tag{2.38}$$

The operators b_i and $b_i^\dagger$ obey the commutation relations

$$\begin{aligned}[b_i, b_j] &= 0 \\ [b_i^\dagger, b_j^\dagger] &= 0 \\ [b_i, b_j^\dagger] &= \delta_{ij},\end{aligned} \tag{2.39}$$

and the vacuum state with respect to the $\{\bar{u}_i(x)\}$ modes is $|\bar{0}\rangle$, such that

$$b_i |\bar{0}\rangle = 0, \quad \forall\, i. \tag{2.40}$$

The corresponding ladder operators define a new number operator:

$$N_{\bar{u}_i} = b_i^\dagger b_i, \tag{2.41}$$

and the associated Fock space is built by repeated application of $b^\dagger$ on $|\bar{0}\rangle$.

2.3 Bogoliubov Transformations

Bogoliubov transformations were originally introduced in the context of many-body quantum theory by Nikolai Bogoliubov [13] in the late 1940s, in his seminal work on interacting Bose systems and superfluidity. The relevance of Bogoliubov transformations to quantum field theory in curved spacetime, however, was first recognized in the late 1960s and early 1970s, most notably in the work of Leonard Parker on particle creation in expanding universes. Parker proved that time-dependent gravitational backgrounds naturally induce a mixing between positive- and negative-frequency modes, which is precisely captured by a Bogoliubov transformation.

This section is dedicated to introducing the Bogoliubov formalism and studying how two complete sets of Klein–Gordon modes are connected by linear transformations that preserve the Klein–Gordon inner product. We then analyze the induced transformations between the associated creation and annihilation operators.

2.3.1 Bogoliubov Coefficients and Normalization

Let us consider two distinct sets of modes, $\{u_i\}$ and $\bar{u}_i$, each normalized with respect to (2.15). Both sets are complete, and they can be related by the Bogoliubov transformations

$$\begin{aligned} \bar{u}_j &= \sum_i (\alpha_{ji} u_i + \beta_{ji} u_i^*) \\ u_j &= \sum_i (\alpha_{ji}^* \bar{u}_i - \beta_{ji} \bar{u}_i^*). \end{aligned} \tag{2.42}$$

The complex coefficients α_{ij} and β_{ij} are the **Bogoliubov coefficients**, and can be obtained by means of the Klein-Gordon inner product:

$$\begin{aligned} \alpha_{ij} &= (\bar{u}_i, u_j) \\ \beta_{ij} &= -(\bar{u}_i, u_j^*). \end{aligned} \tag{2.43}$$

The transformation between the two sets of modes induces a transformation between the creation and annihilation operators associated with each set of modes. By substituting the transformation (2.42) into the field operator written in the $\{\bar{u}_i\}$

basis, as given by equation (2.38), we obtain

$$\begin{aligned}\phi &= \sum_j \left\{ b_j \left(\sum_i \alpha_{ji} u_i + \beta_{ji} u_i^* \right) + b_j^\dagger \left(\sum_i \alpha_{ji}^* u_i^* + \beta_{ji}^* u_i \right) \right\} \\ &= \sum_{ji} \alpha_{ji} b_j u_i + \beta_{ji} b_j u_i^* + \alpha_{ji}^* b_j^\dagger u_i^* + \beta_{ji}^* b_j^\dagger u_i^* \\ &= \sum_{ji} \left\{ \left(\alpha_{ji} b_j + \beta_{ji}^* b_j^\dagger \right) u_i + \left(\alpha_{ji}^* b_j^\dagger + \beta_{ji} b_j \right) u_i^* \right\}.\end{aligned} \tag{2.44}$$

Comparison with (2.26) yields the relation between the ladder operators

$$\begin{aligned}a_i &= \sum_j \left(\alpha_{ji} b_j + \beta_{ji}^* b_j^\dagger \right) \\ a_i^\dagger &= \sum_j \left(\alpha_{ji}^* b_j^\dagger + \beta_{ji} b_j \right),\end{aligned} \tag{2.45}$$

while the inverse transformation can be written as

$$\begin{aligned}b_i &= \sum_j \left(\alpha_{ji}^* a_j - \beta_{ji}^* a_j^\dagger \right) \\ b_i^\dagger &= \sum_j \left(\alpha_{ji} a_j^\dagger - \beta_{ji} a_j \right).\end{aligned} \tag{2.46}$$

Consistency requires that the set of operators $\{b, b^\dagger\}$ satisfies the same canonical commutation relation as the set $\{a, a^\dagger\}$, as stated by (2.27) and (2.39). This imposes a constraint on the Bogoliubov coefficients:

$$\begin{aligned}[b_i, b_j^\dagger] &= \sum_{kj} \{ \alpha_{ji}^* \alpha_{kj} [a_j, a_k^\dagger] - \beta_{ji}^* \beta_{kj} [a_k, a_j^\dagger] \} \\ &= \sum_k (\alpha_{ki}^* \alpha_{kj} - \beta_{ki}^* \beta_{kj}),\end{aligned} \tag{2.47}$$

and

$$\begin{aligned}[b_i, b_j] &= \sum_{kj} \{ \beta_{kj}^* \alpha_{ji}^* [a_k^\dagger, a_j] + \alpha_{kj}^* \beta_{ji}^* [a_k, a_j^\dagger] \} \\ &= \sum_k (\alpha_{kj}^* \beta_{ki}^* - \alpha_{ki}^* \beta_{kj}^*).\end{aligned} \tag{2.48}$$

It follows that

$$\begin{aligned}\sum_k (\alpha_{ki} \alpha_{kj}^* - \beta_{ki} \beta_{kj}^*) &= \delta_{ij} \\ \sum_k (\alpha_{kj} \beta_{ki} - \alpha_{ki} \beta_{jk}) &= 0.\end{aligned} \tag{2.49}$$

2.3.2 Number Operator and Particle Interpretation

From (2.45) and (2.46), it is clear that the Fock spaces based on the choices of modes $\{u_i\}$ or $\{\bar{u}_i\}$ are different, provided that none of the Bogoliubov coefficients β_{ji} vanish. For instance, consider the Fock space constructed by defining the vacuum with respect to the annihilation operators associated $\{a_i\}$, associated with the $\{u_i\}$ modes. It should not be a surprise that the vacuum defined with respect to the $\{b_i\}$ operators, associated with the $\{\bar{u}_i\}$ modes, is not annihilated by a_i:

$$\begin{aligned} a_i \left|\bar{0}\right\rangle &= \sum_j (\alpha_{ji} b_j + \beta^*_{ji} b^\dagger_j) \left|\bar{0}\right\rangle \\ &= \sum_j \beta^*_{ji} \left|1_{g_j}\right\rangle \\ &\neq 0. \end{aligned} \tag{2.50}$$

The expectation value of the number operator defined with respect to the $\{u_i\}$ modes, $N_{u_i} = a^\dagger_i a_i$ in the $|\bar{0}\rangle$ state is

$$\begin{aligned} \langle\bar{0}| a^\dagger_i a_i |\bar{0}\rangle &= \sum_{jk} \langle\bar{0}| [(\alpha^*_{ji} b^\dagger_j + \beta_{ji} b_j)(\alpha_{ki} b_k + \beta^*_{ki} b^\dagger_k)] |\bar{0}\rangle \\ &= \sum_{jk} \beta_{ji}\beta^*_{ki} \langle\bar{0}| b_j b^\dagger_k |\bar{0}\rangle , \end{aligned}$$

and using (2.39), we get

$$\langle\bar{0}| a^\dagger_i a_i |\bar{0}\rangle = \sum_j |\beta_{ji}|^2, \tag{2.51}$$

which can be interpreted as the vacuum in the $\{g_i\}$ basis containing $\sum_j |\beta_{ji}|^2$ particles in the u_i mode.

With the formalism now developed, we discovered that the notion of particles in curved spacetime is completely dependent on the choice of mode decomposition used to define the Fock representation. The nonvanishing expectation value $\langle\bar{0}| a^\dagger_i a_i |\bar{0}\rangle$ reflects the "conflict" between two possible definitions of what positive-frequency is. With time translation symmetry absent, different observers (here represented by different choices of time slicing) lead to inequivalent particle interpretations related by the Bogoliubov transformations. The particle number does not represent a fundamental, observer-independent observable; instead, it represents an effective and representation-dependent concept. Despite all of this, it remains a useful diagnostic tool for characterizing physical processes in time-dependent or curved backgrounds, provided its limited and contextual nature is kept in mind.

Chapter 3

Particle Creation in an Asymptotically Flat Expanding Universe

We begin this chapter exploring the class of metrics known as the **FLRW metrics**, which describes expanding universes. After this, we will consider a $1+1$ dimensional asymptotically static spacetime. In such a spacetime, the cosmic expansion is confined to a finite time interval, and the geometry reduces to that of Minkowski spacetime in the remote past and future, which we will denote as the *in* and *out* regions, respectively. This choice is made because we can define a unique vacuum state in the asymptotic regions and relate them through Bogoliubov transformations that provide a finite and meaningful result for the measurement of the total particle number.

We will also demonstrate that the process of particle creation from an initial vacuum state generates quantum correlations. The particles are created in pairs with correlated momenta $(k, -k)$. To quantify the statistical properties of this state, we will calculate the **diagonal entropy**, obtained from the diagonal entries of the density matrix in the energy basis. This quantity captures the effective loss of accessible information due to the loss of access to quantum coherence due to dephasing, and gives a measure of the emergent thermodynamic behavior of the system. From the resulting distribution, we identify that the spectrum is indeed thermal-like, and an effective temperature associated with each mode is introduced.

Of course, a $1+1$ FLRW universe is not realistic at all. It is a simple toy model for us to study some aspects of particle production and the thermodynamic associated with this system. Observation has shown that the stage of the universe in which we live is one where the expansion is still taking place. In such a spacetime, there is not an **in** or *out* regions where a unique vacuum state, and consequently, the notion of particles can be well defined. In a spacetime where the expansion always taking place, a naive calculation of the number of particles present at an arbitrary time t, using a time-dependent number operator, leads to UV divergences [35]. In this scenario, to obtain a physically sensible and finite particle number density, the method of *adiabatic regularization* must be employed. This will be addressed in the following chapters.

3.1 Asymptotically Flat Spacetimes

3.1.1 The FLRW Metric

Expanding spacetimes are described by the metric known as the Friedmann-Lemaître-Robertson-Walker (FLRW) metric [5, 44–48]. The FLRW metric is actually a class of three distinct metrics corresponding to the three different possible geometries of the spatial section, and we will devote this subsection to the study of these metrics.

The FLRW metric can be derived from two fundamental assumptions about the nature of the universe, which comprise the **cosmological principle**. The first assumption is the **homogeneity of space**, the notion that we do not occupy a privileged position in the universe; i.e., the spacetime in which we live "looks" the same from all points in space. More precisely, we say that the spacetime is spatially homogeneous if there exists a family of spacelike hypersurfaces Σ_t that foliates all spacetime, such that for each t, there exists an isometry of $g_{\mu\nu}$ that takes an arbitrary point $p \in \Sigma_t$ to another arbitrary point $q \in \Sigma_t$. The second assumption is that of the **isotropy of space**, meaning that there is no preferred direction, which translates to invariance under spatial rotations. Formally, there exists a congruence of timelike curves with tangent vectors u^μ, vectors s_1^μ, and s_2^μ that are orthogonal to u^μ (spatial tangent vectors) at any point p, and an isometry of $g_{\mu\nu}$ that leaves p and u^μ fixed but rotates one of the spatial vectors into the other

The significance of these assumptions is that each three-dimensional spatial slice of the spacetime is maximally symmetric. We therefore consider our spacetime manifold to be $\mathcal{M} = \mathbb{R} \times \Sigma_t$, with $\mathbb{R}$ representing the time direction and Σ_t as the maximally symmetric spatial submanifold. The spacetime interval takes the form

$$\mathrm{d}s^2 = \mathrm{d}t^2 - a^2(t)\mathrm{d}\sigma^2 \tag{3.1}$$

where $\mathrm{d}\sigma^2$ is the space interval on the spatial submanifold, and $a(t)$ the *scale factor* is a smooth function that expresses the time dependence of physical spatial distances. The space interval $\mathrm{d}\sigma^2$ can be expressed as

$$\mathrm{d}\sigma^2 = \gamma_{ij}\mathrm{d}v^i\mathrm{d}v^j, \tag{3.2}$$

where the v^i are coordinates on Σ, and γ_{ij} is a maximally-symmetric three-dimensional metric.

The coordinates used here for the full spacetime are called **comoving coordinates**. An observer who stays at a constant v^i is a **comoving observer**. It is worth stressing that comoving observers are an idealization that works very well for the large-scale, homogeneous expansion described by the metric above. In particular, neither the Earth nor the Solar System follows an exactly comoving worldline. Gravitationally bound systems are not coupled to the cosmological expansion: their internal dynamics are dominated by local gravitational forces rather than by the global expansion given by $a(t)$. Nevertheless, we shall adopt the idealized description in terms of comoving coordinates since these gravitationally bound systems are not significant for what will be developed throughout this work.

The Riemann tensor for a maximally symmetric space (see A.2) is given by

$$R_{ijkl} = k(\gamma_{ik}\gamma_{jl} - \gamma_{il}\gamma_{jk}), \tag{3.3}$$

where $k = R/6$ and the Ricci tensor is

$$R_{jl} = 2k\gamma_{jl}. \tag{3.4}$$

It is convenient to express the spatial metric $\mathrm{d}\sigma^2$ as

$$\mathrm{d}\sigma^2 = e^{2\beta(r)}\mathrm{d}r^2 + r^2\mathrm{d}\Omega^2, \tag{3.5}$$

where r is the radial coordinate and $\mathrm{d}\Omega^2 = \mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\phi^2$. The nonvanishing components of the Ricci tensor reads

$$\begin{aligned} R_{rr} &= \frac{2}{r}\partial_r\beta \\ R_{\theta\theta} &= e^{-2\beta}(r\partial_r\beta - 1) + 1 \\ R_{\phi\phi} &= [e^{-2\beta}(r\partial_r\beta - 1) + 1]\sin^2\theta. \end{aligned} \tag{3.6}$$

Using (3.4), one obtains

$$\beta = -\frac{1}{2}(1 - kr^2), \tag{3.7}$$

yielding, for the metric on Σ_t:

$$\mathrm{d}\sigma^2 = \frac{\mathrm{d}r^2}{1 - kr^2} + r^2\mathrm{d}\Omega^2. \tag{3.8}$$

Since $k \propto R$, it sets the curvature of the spatial section. It is usual to normalize this, so

$$k \in \{-1, 0, +1\}. \tag{3.9}$$

The $k = -1$ case is associated to negative curvature on Σ_t, called **open** or **hyperbolic**; $k = 0$ corresponds to no curvature on Σ_t, called **flat**; at last, the $k = +1$ case corresponds to positive curvature on Σ_t, called **closed**. Notice that we are only considering cases where the topology is simply connected, meaning that there are no "holes" in Σ_t.

Finally, the line element on the full spacetime manifold $\mathcal{M}$ is then

$$\mathrm{d}s^2 = \mathrm{d}t^2 - a^2(t) \begin{cases} \frac{\mathrm{d}r^2}{1+r^2} + r^2\mathrm{d}\Omega^2 \\ \mathrm{d}r^2 \quad + r^2\mathrm{d}\Omega^2 \\ \frac{\mathrm{d}r^2}{1-r^2} \ + r^2\mathrm{d}\Omega^2 \end{cases} \tag{3.10}$$

corresponding to the three FLRW metrics.

3.1.2 Equation of Motion and Asymptotic Vacua

We will work in an asymptotically flat FLRW spacetime in order to make precise the notions of in and out vacuum states. These backgrounds are characterized by an early and a late-time regime (the so called *in* and *out* regions, respectively), in which the geometry approaches that of Minkowski spacetime, allowing for an unambiguous definition of positive-frequency modes. We begin by deriving the field equation in a conformally flat representation of the spacetime and by analyzing the asymptotic properties of the Minkowski-like regions, which will serve as the basis for defining the corresponding vacuum states.

Let us consider a conformally coupled (note that minimal coupling and conformal coupling are equivalent in two dimensions), real scalar field propagating in a 1+1 *spatially flat* FLRW spacetime $g_{\mu\nu} = \text{diag}(1, -a^2(t))$, which, in rectangular coordinates, corresponds to the spacetime interval

$$\mathrm{d}s^2 = \mathrm{d}t^2 - a^2(t)\mathrm{d}x^2. \tag{3.11}$$

To obtain a conformally flat representation of the spacetime, we perform a conformal transformation (see appendix A.3) by introducing a new time coordinate η, which is called *conformal time*. This new coordinate is related to the comoving time t by the relation $d\eta = dt/a(t)$. In the literature, it is standard to define $C(\eta) = a(\eta)^2$. The function $C(\eta)$ is the *conformal factor*, and its role is similar to that of the scale factor. The metric becomes $g_{\mu\nu} \to \tilde{g}_{\mu\nu} = C(\eta)\text{diag}(1, -1)$, which corresponds to

$$ds^2 = C(\eta)(d\eta^2 - dx^2). \tag{3.12}$$

As we previously discussed, spatial translation invariance is a symmetry in this spacetime (the space is homogeneous), allowing for functions $u_k(x, \eta)$ that obey the Klein-Gordon equation to be expressed as a product of separate variables:

$$u_k(x, \eta) = \frac{e^{ikx}}{(2\pi)^{1/2}} \chi_k(\eta). \tag{3.13}$$

It can be immediately verified that for this metric, we have $\sqrt{-g} = C(\eta)$, and using equation (2.8), one can readily find that (3.13) solves the Klein-Gordon equation if the time-dependent function $\chi_k(\eta)$ solves

$$\chi_k''(\eta) + \omega_k^2(\eta)\chi_k(\eta) = 0, \tag{3.14}$$

where the prime denotes the derivative with respect to the conformal time, $d/d\eta$, and the effective frequency is given by

$$\omega_k^2(\eta) = k^2 + C(\eta)m^2. \tag{3.15}$$

Note that (3.14) resembles the equation of motion for a simple harmonic oscillator with a time-dependent frequency. In the massless limit $m = 0$, the frequency becomes time independent: $\omega = k$, and the mode equation reduces exactly to that of a free field in flat spacetime. This reflects the conformal invariance of a massive scalar field in 1+1 dimensions and implies the absence of particle creation in this case.

Since the spacetime is asymptotically flat, the conformal factor approaches constant values in these regions

$$C(\eta) \to \begin{cases} C_1, & \eta \to -\infty \\ C_2, & \eta \to +\infty, \end{cases} \tag{3.16}$$

as illustrated in figure 3.1. The frequencies $\omega(\eta)$ then take the following asymptotic values:

$$\omega(\eta) \to \begin{cases} \omega_{\text{in}} = \sqrt{k^2 + C_1 m^2}, & \eta \to -\infty \\ \omega_{\text{out}} = \sqrt{k^2 + C_2 m^2}, & \eta \to +\infty. \end{cases} \tag{3.17}$$

The Minkowski character of the spacetime in the asymptotic regions allows for the definition of natural and unique vacuum states corresponding to the mode bases

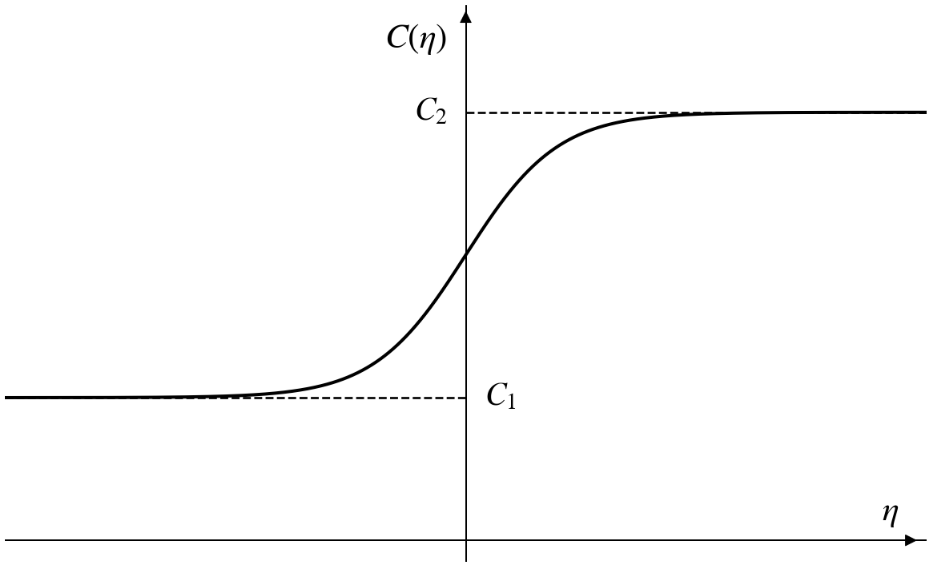

FIGURE 3.1: Evolution of the conformal factor $C(\eta)$ for a $1+1$ asymptotically static universe.

$\{u_k^{in}\}$ and $\{u_k^{out}\}$. These vacua are defined, respectively, by the annihilation conditions:

$$\begin{aligned} a_k \left|0\right\rangle_{in} &= 0 \\ b_k \left|0\right\rangle_{out} &= 0 \end{aligned} \tag{3.18}$$

where $\{a_k\}$ are the annihilation operators associated with $\{u_k^{in}\}$, and $\{b_k\}$ are the annihilation operators associated with $\{u_k^{out}\}$.

The temporal functions $\chi_k^{\text{in}}(\eta)$ and $\chi_k^{\text{out}}(\eta)$ satisfy the Klein-Gordon equation in flat spacetime in the asymptotic regions and are normalized to exhibit positive frequency behavior. Explicitly, they obey the asymptotic conditions

$$\begin{aligned} \chi_k^{\text{in}}(\eta) &\to \frac{e^{-i\omega_{\text{in}}\eta}}{(2\omega_{\text{in}})^{1/2}}, \qquad \eta \to -\infty \\ \chi_k^{\text{out}}(\eta) &\to \frac{e^{-i\omega_{\text{out}}\eta}}{(2\omega_{\text{out}})^{1/2}}, \qquad \eta \to +\infty, \end{aligned} \tag{3.19}$$

where ω_{in} and ω_{out} are the constant asymptotic frequencies.

Although both sets of modes are defined with respect to their asymptotic properties in different regions, they are solutions of the Klein-Gordon equation throughout the entirety of spacetime; thus, they are related by a Bogoliubov transformation:

$$u_k^{in} = \sum_{k'} (\alpha_{kk'}\, u_{k'}^{out} + \beta_{kk'}\, u_{k'}^{out\,*}). \tag{3.20}$$

Since the modes in the asymptotic regions are required to be plane waves, the $\alpha_{kk'}$ and $\beta_{kk'}$ coefficients are proportional to $\delta_{kk'}$ and $\delta_{k,-k'}$, respectively, and we have

$$\begin{aligned} \alpha_{kk'} &= \alpha_k \, \delta_{kk'} \\ \beta_{kk'} &= \beta_k \, \delta_{k,-k'} . \end{aligned} \tag{3.21}$$

The Bogoliubov transformation, therefore, simplifies to:

$$u_k^{in} = \alpha_k \, u_k^{out} + \beta_k \, u_{-k}^{out\,*} . \tag{3.22}$$

The first constraint in (2.49) becomes

$$|\alpha_k|^2 - |\beta_k|^2 = 1, \tag{3.23}$$

guarantying the preservation of the Klein–Gordon inner product and, equivalently, of the canonical commutation relations.

3.1.3 Exact Solution for the Mode Functions

A particular model that has an exact solution is one that was studied by Bernard and Duncan in 1977 [49] in the context of regularization and renormalization in curved spacetimes, and it illustrates the effect of nonzero mass in a minimally coupled theory.

Consider the specific choice

$$C(\eta) = A + B \tanh{(\rho\eta)}, \tag{3.24}$$

where $A > B > 0$, so that $C(\eta) \to (A \pm B)$ as $\eta \to \pm\infty$. These conditions are necessary to ensure that the universe expands ($C'(\eta) = B \text{sech}^2 \rho\eta > 0$) and to preserve the oscillatory behavior of modes in the *in* region. The number ρ is a parameter that controls the timescale of the expansion; in the limit $\rho \to 0$, the evolution is arbitrarily slow, and the effects of particle production are negligible, whereas when $\rho \to +\infty$, the expansion becomes strongly nonadiabatic, leading to significant particle creation.

For this choice of conformal factor, the equation of motion (3.14) takes the form

$$\chi_k''(\eta) + \left[k^2 + (A + B \tanh{(\rho\eta)}) m^2\right] \chi_k(\eta) = 0, \tag{3.25}$$

with asymptotic frequencies defined by

$$\begin{aligned} \omega_{in} &= \left[k^2 + (A - B)m^2\right]^{1/2} \\ \omega_{out} &= [k^2 + (A + B)m^2]^{1/2}, \end{aligned} \tag{3.26}$$

characterizing the flat regions in the distant past and future, respectively.

The solutions for the equation (3.25) are given in terms of hypergeometric functions [41, 49] ${}_2F_1(a, b; c; z)$. It is found that the normalized spacetime modes that behave as positive-frequency Minkowski modes in the *in* region are

$$\begin{aligned} u_k^{in}(x, \eta) = &\frac{1}{(4\pi\omega_{in})^{1/2}} \exp\{ikx - i\omega_+\eta - (i\omega_-/\rho) \ln[2\cosh(\rho\eta)]\} \\ &\times {}_2F_1\left(1 + (i\omega_-/\rho), i\omega_-/\rho; 1 - (i\omega_{in}/\rho); \frac{1}{2}(1 + \tanh(\rho\eta))\right), \end{aligned} \tag{3.27}$$

where we have defined $\omega_\pm = \frac{1}{2}(\omega_{out} \pm \omega_{in})$. In the asymptotic past, these modes satisfy

$$u_k^{in}(x, \eta) \xrightarrow[\eta \to -\infty]{} \frac{e^{ikx - i\omega_{in}\eta}}{(4\pi\omega_{in})^{1/2}}, \tag{3.28}$$

in agreement with the first condition in equation (3.19).

Similarly, the normalized modes that behave as positive-frequency Minkowski modes in the *out* region are:

$$\begin{aligned} u_k^{out}(x, \eta) = &\frac{1}{(4\pi\omega_{out})^{1/2}} \exp\{ikx - i\omega_+\eta - (i\omega_-/\rho) \ln[2\cosh(\rho\eta)]\} \\ &\times {}_2F_1\left(1 + (i\omega_-/\rho), i\omega_-/\rho; 1 + (i\omega_{out}/\rho); \frac{1}{2}(1 - \tanh(\rho\eta))\right), \end{aligned} \tag{3.29}$$

satisfying in the asymptotic future

$$u_k^{out}(x, \eta) \xrightarrow[\eta \to +\infty]{} \frac{e^{ikx - i\omega_{out}\eta}}{(4\pi\omega_{out})^{1/2}}, \tag{3.30}$$

in accordance with the second condition in (3.19).

3.2 Particle Production During the Period of Expansion

3.2.1 Determination of the Bogoliubov Coefficients

Since the *in* and *out* mode functions are defined by distinct asymptotic conditions, we have $u_k^{in} \neq u_k^{out}$, and a nontrivial Bogoliubov transformation relating the two bases exists. Explicitly, the Bogoliubov coefficients α_k and β_k can be determined analytically by using the linear transformation properties of hypergeometric functions. In particular, we make use of the identity[50]

$$\begin{aligned} {}_2F_1(a,b;c;z) = &\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \\ &\times {}_2F_1(a,b;a+b-c+1;1-z) \\ &+ (1-z)^{(c-a-b)}\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} \\ &\times {}_2F_1(c-a,c-b;c-a-b+1;1-z) \end{aligned} \tag{3.31}$$

to relate u_k^{in} and u_k^{out}.

For the ${}_2F_1(a,b;c;z)$ on the u_k^{in} mode, we have

$$\begin{cases} a = 1 + i\omega_-/\rho \\ b = i\omega_-/\rho \\ c = 1 - i\omega_{in}/\rho \\ z = \dfrac{1}{2}(1+\tanh\rho\eta). \end{cases} \tag{3.32}$$

Applying the transformation (3.31) and comparing with

$$u_k^{in} = \alpha_k u_k^{out} + \beta_k u_{-k}^{out\,*}, \tag{3.33}$$

one finds that the Bogoliubov coefficients can be expressed in terms of Gamma functions as

$$\alpha_k = \left(\frac{\omega_{out}}{\omega_{in}}\right)^{1/2} \frac{\Gamma(1-i\omega_{in}/\rho)\Gamma(-i\omega_{out}/\rho)}{\Gamma(-i\omega_+/\rho)\Gamma(1-i\omega_+/\rho)} \tag{3.34}$$

$$\beta_k = \left(\frac{\omega_{out}}{\omega_{in}}\right)^{1/2} \frac{\Gamma(1-i\omega_{in}/\rho)\Gamma(i\omega_{out}/\rho)}{\Gamma(i\omega_-/\rho)\Gamma(1+i\omega_-/\rho)}. \tag{3.35}$$

Taking into account the translational invariance of the asymptotic regions, the Bogoliubov coefficients are diagonal in momentum space and take the form

$$\begin{aligned} \alpha_{kk'} &= \alpha_k \delta_{kk'} \\ \beta_{kk'} &= \beta_k \delta_{k,-k'}, \end{aligned} \tag{3.36}$$

in accordance with the general structure discussed in section 3.1.2.

Using the following identity for Gamma functions

$$|\Gamma(1\pm ix)|^2 = \frac{\pi x}{\sinh(\pi x)}, \tag{3.37}$$

together with

$$\left|\frac{\Gamma(ix)}{\Gamma(iy)}\right|^2 = \frac{y\sinh(\pi y)}{x\sinh(\pi x)}, \tag{3.38}$$

it is readily found that

$$|\alpha_k|^2 = \frac{\sinh^2(\pi\omega_+/\rho)}{\sinh(\pi\omega_{in}/\rho)\sinh(\pi\omega_{out}/\rho)} \tag{3.39}$$

$$|\beta_k|^2 = \frac{\sinh^2(\pi\omega_-/\rho)}{\sinh(\pi\omega_{in}/\rho)\sinh(\pi\omega_{out}/\rho)}, \tag{3.40}$$

from which the normalization condition (3.23) follows immediately.

3.2.2 Number Density of Created Particles

Substituting (3.21) into equation (2.51), we obtain the mean particle number in the *in* vacuum for each mode: $n_k = |\beta_k|^2$, that is

$$n_k = \frac{\sinh^2(\pi\omega_-/\rho)}{\sinh(\pi\omega_{in}/\rho)\sinh(\pi\omega_{out}/\rho)}. \tag{3.41}$$

The particle number per unit comoving length is then given by

$$n = \frac{1}{2\pi}\int_0^\infty dk\; n_k, \tag{3.42}$$

and the physical number per unit physical length is

$$n_{phys} = \frac{n}{\sqrt{C_2}}, \tag{3.43}$$

where $C_2 = A + B$. For (3.41), when $k \to \infty$, the integrand in the density (3.42) becomes the exponential decay $|\beta_k|^2 \sim e^{-2\pi k/\rho}$, so the integral converges.

We can set $A = 1.5$, $B = 0.5$, $m = 1$, and plot n_k vs k to illustrate the decay of n_k in two regimes: first, when the rapidity of the expansion is slow, i.e., $\rho \ll \omega_k$, and second, when the expansion is sudden, i.e., $\rho \gg \omega_k$. The graphics are given in figures 3.2 and 3.3.

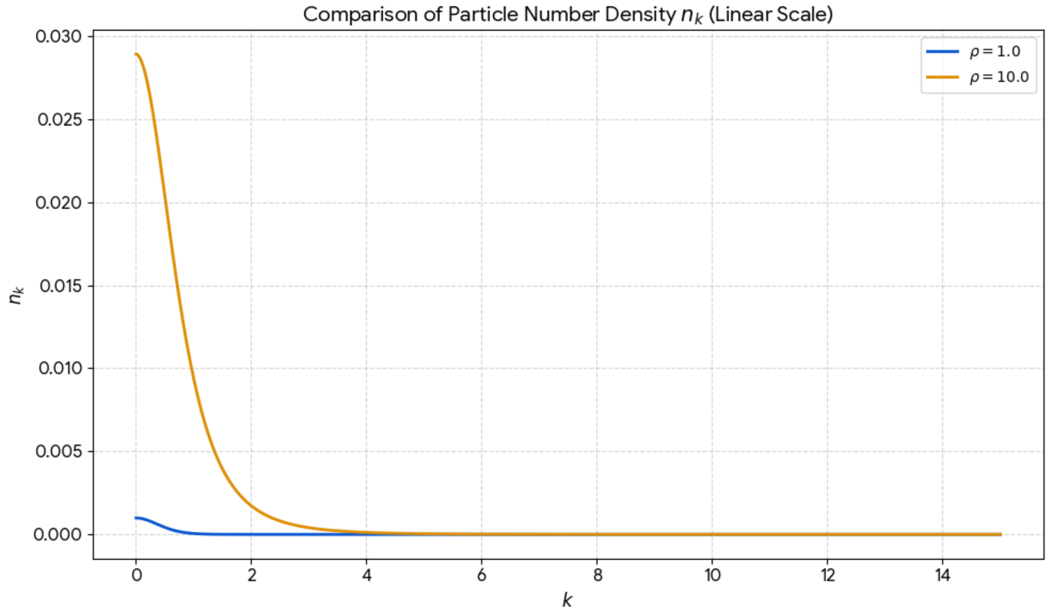

FIGURE 3.2: Mean particle number per mode, linear scale.

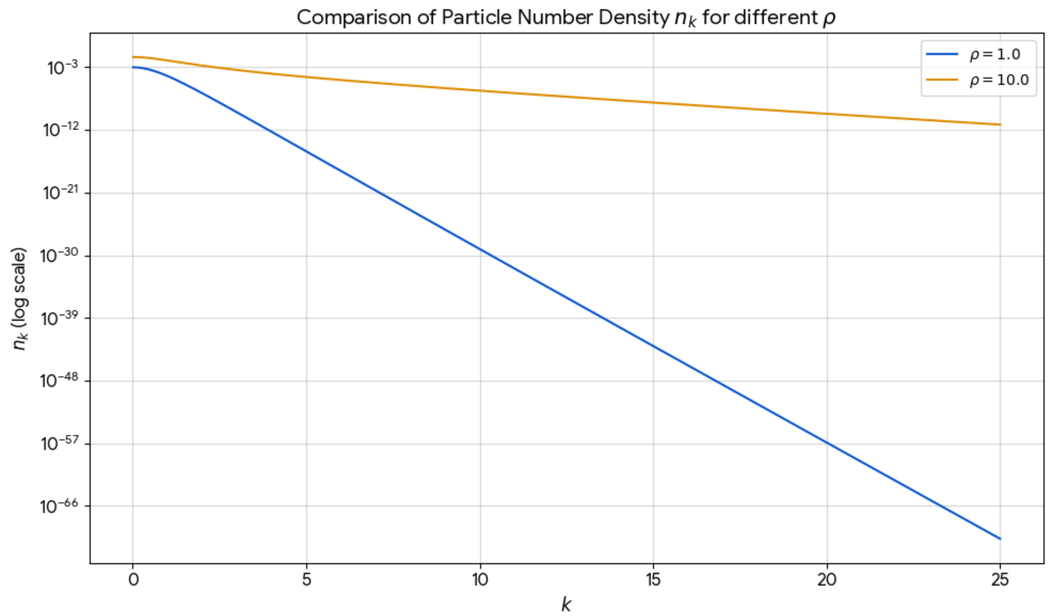

FIGURE 3.3: Mean particle number per mode, logarithmic scale.

3.2.3 Squeezed Vacuum

Now, let's pause for a moment and consider the vacuum state defined in the remote past, $|0\rangle_{in}$, which is annihilated by all $\{a_k\}$, i.e., the annihilation operators associated with the modes $\{u_k^{in}\}$. Our goal is to understand how this state (which is the state of the field at all times) is perceived by an observer in the *out* region, whose notion of particles is defined with respect to the modes $\{u_k^{out}\}$. Until now, we have demonstrated that time dependent backgrounds typically mix positive- and negative-frequency modes (which also leads to the mixing of the ladder operators of each asymptotic region, as expressed in 2.3.1 and 3.2.2), changing the notion that the state of the field is "empty" of excitations. This subsection is dedicated to demonstrating that this vacuum state acquires the characteristic structure of a two-mode squeezed state.

The field operator may be expanded in terms of either of the two sets of modes:

$$\begin{aligned} \phi &= \sum_k \left(a_k u_k^{in} + a_k^\dagger u_k^{in\,*} \right) \\ \phi &= \sum_k \left(b_k u_k^{out} + b_k^\dagger u_k^{out\,*} \right). \end{aligned} \tag{3.44}$$

The Bogoliubov transformation between the ladder operators is found by direct substitution of (3.22) into the field expansion in terms of $\{u_k^{in}\}$,

$$\phi = \sum_k \left[a_k(\alpha_k\, u_k^{out} + \beta_k\, u_{-k}^{out\,*}) + a_k^\dagger(\alpha_k^*\, u_k^{out*} + \beta_k^*\, u_{-k}^{out}) \right]. \tag{3.45}$$

Changing the dummy index $\sum a_k^\dagger \beta_k^* u_{-k}^{out} \rightarrow \sum a_{-k}^\dagger \beta_{-k}^* u_k^{out}$, we match the coefficients of u_k^{out} and obtain the transformation

$$b_k = \alpha_k a_k + \beta_k^* a_{-k}^\dagger, \tag{3.46}$$

where $\beta_{-k}^* = \beta_k^*$ because of isotropy. The inverse transformation is then given by

$$a_k = \alpha_k^* b_k - \beta_k^* b_{-k}^\dagger. \tag{3.47}$$

The annihilation condition of the *in* vacuum state in terms of the ladder operators associated with the *out* region reads

$$\begin{aligned} a_k \left|0\right\rangle_{in} &= \left(\alpha_k^* b_k - \beta_k^* b_{-k}^\dagger \right) \left|0\right\rangle_{in} \\ &= 0. \end{aligned} \tag{3.48}$$

We can rearrange this equation to

$$b_k \left|0\right\rangle_{in} = \frac{\beta_k^*}{\alpha_k^*} b_{-k}^\dagger \left|0\right\rangle_{in}, \tag{3.49}$$

showing explicitly that $\left|0\right\rangle_{in}$ contains correlated $(k, -k)$ pairs.

Since the momenta k and $-k$ are linked, we write an ansatz for the *in* vacuum as a two-mode squeezed state [51] of the form

$$|0\rangle_{in} = N \exp\left\{ \frac{1}{2} \sum_{q} \lambda_q^* b_q^\dagger b_{-q}^\dagger \right\} |0\rangle_{out} , \tag{3.50}$$

where N is obtained through normalization.

To determine the coefficient λ_q^*, we will make use of the annihilation condition given by (3.49). Acting b_k on (3.50), and using the identity $\left[b_k, f(b^\dagger)\right] |0\rangle_{out} = b_k f(b^\dagger) |0\rangle_{out}$, we may write

$$b_k |0\rangle_{in} = N \left[b_k, \exp\left\{ \frac{1}{2} \sum \lambda_q^* b_q^\dagger b_{-q}^\dagger \right\} \right] |0\rangle_{out} . \tag{3.51}$$

Now, let $A = b_k$ and $B = \frac{1}{2} \sum \lambda_q^* b_q^\dagger b_{-q}^\dagger$. Provided that $[[A, B], B] = 0$, we may write $[A, \mathrm{e}^B] = [A, B]\mathrm{e}^B$. In fact,

$$\begin{aligned} [b_k, B] &= \frac{1}{2} \sum_q \lambda_q^* [b_k, b_q^\dagger b_{-q}^\dagger] \\ &= \frac{1}{2} \sum_q 2\delta_{kq} \lambda_q^* b_{-q}^\dagger \\ &= \lambda_k^* b_{-k}^\dagger \end{aligned} \tag{3.52}$$

and obviously

$$\lambda_k^* [b_{-k}^\dagger, B] = 0, \tag{3.53}$$

so we might rewrite (3.51) as:

$$b_k |0\rangle_{in} = \lambda_k^* b_{-k}^\dagger N \mathrm{e}^B |0\rangle_{out} . \tag{3.54}$$

Comparison with (3.49) leads us to $\lambda_k^* = \beta_k^* / \alpha_k^*$, so that

$$|0\rangle_{in} = N \exp\left\{ \sum_{k>0} \frac{\beta_k^*}{\alpha_k^*} b_k^\dagger b_{-k}^\dagger \right\} |0\rangle_{out} , \tag{3.55}$$

where the sum was restricted to only positive values of k to eliminate the symmetry factor $\frac{1}{2}$.

To make this expression clearer, we may use the fact that the $b^\dagger$ operators for different momenta commute, allowing us to break the exponential of the sum into the product

$$\exp\left\{ \sum_{k>0} \frac{\beta_k^*}{\alpha_k^*} b_k^\dagger b_{-k}^\dagger \right\} = \prod_{k>0} \exp\left\{ \frac{\beta_k^*}{\alpha_k^*} b_k^\dagger b_{-k}^\dagger \right\}, \tag{3.56}$$

so we can write the state while focusing on a single mode pair $(k, -k)$

$$|0\rangle_{in}^{(k,-k)} = \exp\left\{ \frac{\beta_k^*}{\alpha_k^*} b_k^\dagger b_{-k}^\dagger \right\} |0_k, 0_{-k}\rangle_{out} . \tag{3.57}$$

Using the Taylor formula $\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!}$, together with $|n\rangle = \frac{(b_k^\dagger)^n}{\sqrt{n!}}$, we obtain

$$|0\rangle_{in}^{(k,-k)} = N_k \sum_{n=0}^{\infty} \left(\frac{\beta_k^*}{\alpha_k^*} \right)^n |n_k, n_{-k}\rangle . \tag{3.58}$$

Finally, to determine the normalization coefficients N_k, one simply uses the condition $\langle 0|0\rangle = 1$ to write

$$|N_k|^2 \sum_{n=0}^{\infty} \left| \frac{\beta_k}{\alpha_k} \right|^{2n} = |N_k|^2 \frac{1}{1 - |\beta_k/\alpha_k|^2} = 1, \tag{3.59}$$

thus

$$N_k = \sqrt{1 - \left| \frac{\beta_k}{\alpha_k} \right|^2} . \tag{3.60}$$

Since different pairs factorize, we can finally write the full product obtained for the *in* vacuum in terms of the *out* basis. Doing so, we find that the vacuum state of the field in the remote past has the following form in the far future:

$$|0\rangle_{in} = \bigotimes_k \sqrt{1 - \left| \frac{\beta_k}{\alpha_k} \right|^2} \sum_{n=0}^{\infty} \left(\frac{\beta_k^*}{\alpha_k^*} \right)^n |n_k, n_{-k}\rangle_{out} . \tag{3.61}$$

This expression shows that the in-region vacuum state evolves into an entangled state in the asymptotic future. The mixing between creation and annihilation operators leads to correlated particle production in the $(k, -k)$ sectors, with the squeezing parameter being "controlled" by the ratio $\lambda_k = \beta_k/\alpha_k$. What this really means is that, when expressed in the out basis, the *in*-vacuum is represented as a superposition of multiparticle excitations, despite being defined as empty in the asymptotic past.

3.3 Diagonal Entropy

This section is dedicated to first delineating the problem of irreversibility in physics, exploring how this has been historically tackled in the context of thermodynamics and statistical mechanics. We then provide the definition of **diagonal entropy**, which is defined within the instantaneous energy eigenbasis of the system. Finally, the properties and the arguments for the introduction of diagonal entropy are explored.

3.3.1 The Problem of Irreversibility

The problem of irreversibility manifests itself when one considers the conflict between the time-symmetric nature of the laws of microscopic physics and the observation of macroscopic thermodynamic processes, which are irreversible. This conflict, often referred to as Loschmidt's paradox, questions how an arrow of time emerges from fundamental equations, such as Newton's laws or the Schrödinger equation, which possess no intrinsic or preferred direction of time.

In classical statistical mechanics, Ludwig Boltzmann attempted to resolve this by introducing a probabilistic interpretation of entropy associated with the number of microstates of an ideal gas, compatible with a macrostate of such gas [52–54]. It takes the functional form $S = \ln \Omega$ ($k_b = 1$ in natural units), where Ω is the total number of microstates.

In quantum mechanics, the most natural candidate for a microscopic entropy, due to its enormous success mainly in information theory, is the von-Neumann entropy S_{vN} [30], defined as

$$S_{vN} = -\mathrm{Tr}\{\rho \ln \rho\}, \tag{3.62}$$

where ρ is the state (density operator) of the system.

There are some caveats regarding the von-Neumann entropy that must be addressed. Consider, for instance, an isolated quantum system (such as a free scalar field in a curved spacetime) that evolves according to

$$\frac{d\rho(t)}{dt} = -i\left[H(t), \rho(t)\right]. \tag{3.63}$$

The formal solution for this equation is $U(t)\rho(0)U^{\dagger}(t)$, where $U(t)$ is a unitary operator. One main property of unitary evolution is the preservation of the spectrum of the density operator, which translates to the affirmation that the von-Neumann entropy remains **strictly** invariant over time, meaning that $S_{vN}(t) = S_{vN}(0)$ for any closed system. To make a clear connection to this work, consider the expansion of the universe; physical intuition and observational evidence suggest that the system heats up and entropy increases as vacuum fluctuations are amplified into real particles. If one were to strictly interpret the von Neumann entropy as the thermodynamic entropy, one would be forced to conclude that the universe undergoes an isentropic process regardless of the rapidity of the expansion. This is, of course, in direct contradiction to the second law of thermodynamics, which demands entropy production for non-adiabatic processes.

Another postulate of thermodynamics that is violated by S_{vN} is that the entropy is unique as a function of energy. Again, this violation occurs in isolated systems, where S_{vN} must vanish in any cyclic process, even if there is a non-zero change in the system's energy. All of these properties of S_{vN} must, at the very least, show us that we must be cautious when interpreting it as an honest thermodynamic entropy.

The solution to this problem, particularly for isolated quantum systems driven out of equilibrium, was solidified with the introduction of the diagonal entropy by Anatoli Polkovnikov in 2011. This measure posits that in generic Hamiltonian systems, the "natural" coarse-graining is dictated by the system's own energy eigenbasis. By focusing on the diagonal elements of the density matrix in the instantaneous energy basis, Polkovnikov provided a quantity that satisfies the fundamental thermodynamic relations, respects the adiabatic theorem, and serves as a unique measure of irreversibility without relying on external heat baths or arbitrary partitions.

3.3.2 The Definition of Diagonal Entropy

Let us introduce the concept of diagonal entropy. Originally proposed in reference [32] in the context of non-equilibrium quantum thermodynamics, the diagonal entropy is defined from the diagonal elements of the full density operator in the energy eigenbasis, as

$$S_d = -\sum \rho_{nn} \ln \rho_{nn}. \tag{3.64}$$

The motivation to define the diagonal entropy is justified by several arguments made by Polkovnikov. Here, we outline the main ones.

In general, the information relevant for time-averaged observables, namely, those accessible in thermodynamic measurements is within exclusively the diagonal elements of the density operator. This becomes evident when considering sufficiently complex quantum systems that evolve toward a steady state after a process occurring in the remote past. In such a situation, the density operator may be written as

$$\rho(t) = \sum_{mn} \rho_{mn} e^{-i(E_m - E_n)t} \left| m \right\rangle \left\langle n \right|, \tag{3.65}$$

where the energy eigenstates satisfy the time independent Schrödinger equation $H \left| n \right\rangle = E_n \left| n \right\rangle$, with H being the final, time independent Hamiltonian. Assuming that isolated quantum systems display ergodic behavior, the long-time average of a thermodynamic observable O is expected to coincide with its equilibrium ensemble value. The time average is defined as

$$\overline{\langle O(t)\rangle} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt\langle O(t)\rangle, \tag{3.66}$$

with $\langle O(t)\rangle = \mathrm{Tr}\{\rho(t)O\}$. Substituting the above form of $\rho(t)$, one finds

$$\overline{\langle O(t)\rangle} = \sum_{m,n}\rho_{mn}O_{nm}\overline{e^{-i(E_m-E_n)t}}, \tag{3.67}$$

where $O_{nm} = \langle n|O|m\rangle$ are the matrix elements of the observable in the energy eigenbasis. If the Hamiltonian spectrum is non-degenerate, the long-time average of the oscillatory factor satisfies

$$\overline{e^{-i(E_m-E_n)t}} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt\, e^{-i(E_m-E_n)t} = \delta_{mn}. \tag{3.68}$$

Consequently, the time-averaged expectation value reduces to

$$\overline{\langle O(t)\rangle} = \sum_{n}\rho_{nn}O_{nn}. \tag{3.69}$$

A second argument supporting the relevance of the diagonal elements ρ_{nn} follows from the adiabatic theorem of quantum mechanics [55]. For a slowly varying Hamiltonian $H(t)$, satisfying

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle, \tag{3.70}$$

the theorem states that transitions between instantaneous energy eigenstates are suppressed in the quasi-static limit.

Consider a general solution of the time-dependent Schrödinger equation expanded in the instantaneous eigenbasis, given by $|\Psi(t)\rangle = \sum_n c_n(t)|n(t)\rangle$. If the Hamiltonian varies sufficiently slowly, the amplitudes evolve according to

$$c_n(t) = c_n(0)\exp\left\{-i\int_0^t\left[E_n(t') - i\langle n(t')|\frac{\partial}{\partial t'}|n(t')\rangle\right]dt'\right\}. \tag{3.71}$$

Because equation (3.71) relates $c_n(t)$ to $c_n(0)$ only by a global phase factor, an immediate consequence is the conservation of the occupation probabilities, $|c_n(t)|^2 = |c_n(0)|^2$. Thus, a system initially prepared in an eigenstate of $H(0)$ remains in the corresponding instantaneous eigenstate of $H(t)$, up to a time-dependent phase. In density-operator language, the diagonal elements in the instantaneous energy basis, $\rho_{nn}(t) = |c_n(t)|^2$, remain constant during any quasi-static evolution.

If heat is identified microscopically with energy changes arising from transitions between different energy levels [56], quasi-static processes correspond to thermodynamic adiabatic transformations. Consequently, any entropy functional that depends exclusively on ρ_{nn}, such as S_d, must be conserved under adiabatic processes, in agreement with thermodynamic expectations.

3.4 Results and Thermodynamics

3.4.1 D-Entropy of the Field in the Asymptotic Spacetime

Up until now, we have shown how the expansion of the universe induces mixing between positive and negative-frequency modes, leading to particle creation through the Bogoliubov transformation between the *in* and *out* vacua. The vacuum state defined at early times evolves into a two-mode squeezed state when expressed in terms of the *out* basis, coupling modes of opposite momenta. This entanglement between the momentum pairs represents the quantum origin of cosmological particle production.

Although the particles are generated in correlated pairs, the global quantum state of the field remains pure and therefore, as previously discussed, possesses zero von Neumann entropy [30]. Nevertheless, observers who are restricted to a subset of modes perceive an effective loss of information, which is manifested as an increase in entropy. This apparent irreversibility is usually captured by the entanglement entropy, obtained from the reduced density matrix after tracing over the inaccessible partner modes. However, this quantity does not suffice to quantify the informational content of the process; it measures quantum correlations between subsystems, but it does not account for the redistribution of populations among the instantaneous energy eigenstates that accompany non-equilibrium evolution.

Let us proceed to compute S_d for the system of created particles due to the expansion of the universe. From the squeezed vacuum representation (3.61), we can immediately construct the corresponding density operator of the field in the out-Fock basis. For a single momentum pair $(k, -k)$, we have

$$|0\rangle_{in}^{(k,-k)} = \sqrt{1 - \left|\frac{\beta_k}{\alpha_k}\right|^2} \sum_{n=0}^{\infty} \left(\frac{\beta_k^*}{\alpha_k^*}\right)^n |n_k, n_{-k}\rangle_{out} . \tag{3.72}$$

The density operator for that pair is, therefore:

$$\rho^{(k)} = \left(1 - \left|\frac{\beta_k}{\alpha_k}\right|^2\right) \sum_{n,m}^{\infty} \left(\frac{\beta_k^*}{\alpha_k^*}\right)^n \left(\frac{\beta_k}{\alpha_k}\right)^m |n_k, n_{-k}\rangle_{out} \langle m_k, m_{-k}| . \tag{3.73}$$

The diagonal elements of this operator in the energy basis are

$$\begin{aligned}\rho_{nn}^{(k)} &= \langle n_k, n_{-k}| \, \rho^{(k)} \, |n_k, n_{-k}\rangle \\ &= \left(1 - \left|\frac{\beta_k}{\alpha_k}\right|^2\right) \sum_{n',m}^{\infty} \left(\frac{\beta_k^*}{\alpha_k^*}\right)^{n'} \left(\frac{\beta_k}{\alpha_k}\right)^{m} \delta_{nn'}\delta_{mn} \\ &= \left(1 - \left|\frac{\beta_k}{\alpha_k}\right|^2\right) \left|\frac{\beta_k}{\alpha_k}\right|^{2n}.\end{aligned} \tag{3.74}$$

We can use the quantity $\lambda_k = |\beta_k/\alpha_k|^2$ and write (3.74) as

$$\rho_{nn}^{(k)} = (1 - \lambda_k)\lambda_k^n. \tag{3.75}$$

These diagonal entries form a properly normalized probability distribution, $\sum_n (1-\lambda_k)\lambda_k^n = 1$, and quantify the population of the instantaneous energy eigenstates of the two-mode sector. The diagonal entropy for the pair is then obtained by applying the formula (3.64). Substituting $\rho_{nn}^{(k)} = (1 - \lambda_k)\lambda_k^n$ and evaluating the sum, we obtain

$$S_d^{(k)} = -\ln(1 - \lambda_k) - \frac{\lambda_k}{1 - \lambda_k} \ln(\lambda_k). \tag{3.76}$$

It is convenient to express the above result in terms of the mean occupation number in a mode k. Using the fact that $|\alpha_k|^2 - |\beta_k|^2 = 1$, we can write

$$\left|\frac{\beta_k}{\alpha_k}\right|^2 = \frac{|\beta_k|^2}{1 + |\beta_k|^2}, \tag{3.77}$$

and since $\lambda_k = |\beta_k/\alpha_k|^2$ and $n_k = |\beta_k|^2$, we obtain

$$S_d^{(k)} = (1 + n_k)\ln(1 + n_k) - n_k \ln(n_k). \tag{3.78}$$

This is the diagonal entropy associated with the occupation distribution of mode k. The total diagonal entropy of the field is simply the sum of the diagonal entropies of each mode:

$$S_d = \sum_k \left[(1 + n_k)\ln(1 + n_k) - n_k \ln(n_k)\right]. \tag{3.79}$$

3.4.2 Effective Temperature Derivation

Let us restrict our attention to the form of the diagonal elements given by (3.75). This is exactly the expression of the occupation probabilities of a single bosonic mode in thermal equilibrium with a reservoir at a temperature T_k. The density operator of a harmonic oscillator of frequency ω_k in the canonical ensemble [53, 57] is given by

$$\rho = \sum \frac{e^{-(n+\frac{1}{2})\omega_k/T_k}}{Z} |n\rangle \langle n| , \tag{3.80}$$

where $e^{-(n+\frac{1}{2})\omega_k/T_k}/Z = p_n$ are the normalized probabilities, and Z is the partition function, given by

$$Z = \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})\omega_k/T_k}. \tag{3.81}$$

Evaluating the sum, we obtain

$$Z = \frac{e^{-\omega_k/2T_k}}{1 - e^{-\omega_k/T_k}}, \tag{3.82}$$

so that the probabilities p_n are given by

$$p_n = (1 - e^{-\omega_k/T_k})e^{-n\omega_k/T_k}. \tag{3.83}$$

Comparing (3.83) with (3.75), we clearly see that the diagonal entries ρ^k_{nn} can be interpreted as a thermal distribution. One can identify

$$\lambda_k = e^{-\omega_k/T_k}, \tag{3.84}$$

which, by inverting this expression, an **effective temperature** for each mode can be defined:

$$T^{(k)}_{\text{eff}} = \frac{\omega_k}{\ln{(1/\lambda_k)}}, \tag{3.85}$$

where ω_k is the frequency of the created particles. Equivalently, in terms of the mean occupation number:

$$T^{(k)}_{\text{eff}} = \frac{\omega_k}{\ln{(1 + \frac{1}{n_k})}}. \tag{3.86}$$

It is important to stress that, this effective temperature **does not** correspond to a physical heat bath, but rather to the reallocation of energy among field modes caused by the evolution of the spacetime background. The Bogoliubov coefficient β_k acts as a dynamical source of excitations, and the degree of squeezing, given by the ratio $\lambda_k = |\beta_k/\alpha_k|^2$, determines how "hot" each mode appears to be.

This interpretation provides a thermodynamical language for the phenomenon of gravitational particle creation: each mode behaves as if it were in a thermal state at temperature $T^{(k)}_{\text{eff}}$, with the associated diagonal entropy $S^{(k)}_d$ in the role of the corresponding thermodynamical entropy. The diagonal entropy quantifies the redistribution of excitations among energy levels and the uncertainty associated with occupations probabilities in the energy eigenbasis, while also providing a relation between quantum field theory in curved spacetime and the more familiar framework of statistical mechanics.

Chapter 4

Adiabatic Vacuum and Adiabatic Regularization

4.1 The WKB Approximation

Before defining the adiabatic vacuum and discussing the ultraviolet divergences that appear when we deal with certain types of spacetimes, and how to eliminate them, it will be useful to briefly recall an important mathematical tool that is widely used in wave propagation physics, especially in quantum mechanics, namely, the Wentzel–Kramers–Brillouin (WKB) approximation.

Essentially, the WKB approximation is a semiclassical method for obtaining approximate solutions of second-order ODEs of the form

$$\frac{d^2y}{dx^2} + p^2(x)y(x) = 0, \tag{4.1}$$

where $p(x)$ is a smooth function. This type of ODE is very common in quantum mechanics when the potential V depends on the position x. For instance, the (one-dimensional) Schrödinger equation for the wave function $\psi(x)$ of such a system can be written as:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0, \tag{4.2}$$

where we can identify $p(x) = \sqrt{2m\hbar^{-2}(E - V(x))}$ (just for this section, we have restored the $\hbar$'s).

When the potential $V(x)$ is exactly constant, the p term is constant, and the exact solutions are simply plane waves of the form $\psi(x) = A\exp(\pm ipx/\hbar)$. When $p(x)$ varies slowly compared with the local wavelength of the solution, one may introduce the ansatz

$$\psi(x) = \exp\left(\frac{i}{\hbar}S(x)\right). \tag{4.3}$$

Substituting this ansatz into the Schrödinger equation yields the nonlinear equation

$$i\hbar S''(x) - [S'(x)]^2 + p^2(x) = 0. \tag{4.4}$$

We may expand $S(x)$ as a power series in $\hbar$, which acts as the small parameter controlling the semiclassical limit ($\hbar \to 0$):

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \mathcal{O}(\hbar^3)\ldots \tag{4.5}$$

By substituting this expansion back into the differential equation and equating terms of the same order in $\hbar$, one can solve for the functions $S_n(x)$ iteratively. The zeroth-order equation gives $(S_0')^2 = p^2(x)$, which implies $S_0(x) = \pm\int p(x)dx$. The first-order equation yields $iS_0'' - 2S_0'S_1' = 0$, leading to $iS_1(x) = -\frac{1}{2}\ln p(x)$. Combining these leading terms, we can reconstruct the wavefunction to this order of approximation:

$$\psi(x) = \exp\left[\frac{i}{\hbar}\left(S_0 + \hbar S_1 + \mathcal{O}(\hbar^2)\right)\right] \simeq \exp\left(\frac{i}{\hbar}S_0\right)\exp\left(iS_1\right). \tag{4.6}$$

The above expression leads us to

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}}\exp\left(\pm\frac{i}{\hbar}\int^x p(x')dx'\right), \tag{4.7}$$

where C is a normalization constant. For this approximation to be valid, the terms dropped in the expansion must be negligible. Physically, this requires that the local de Broglie wavelength, $\lambda(x) = h/p(x)$, must change very slowly (adiabatically) over a distance of one wavelength. Mathematically, this adiabatic condition is expressed as:

$$\left|\frac{d\lambda}{dx}\right| \ll 1. \tag{4.8}$$

When this condition is met, the system's properties vary adiabatically, allowing the wave to adjust its wavelength and amplitude continuously.

A more convenient formulation for the WKB approximation is just to consider the ansatz (adapted to normalization conditions) for a differential equation of the form (4.1) as:

$$y(x) = \frac{1}{\sqrt{2W(x)}}\exp\left\{i\int^x W(x')dx'\right\}. \tag{4.9}$$

A nonlinear equation for the functions $W(x)$ is obtained by substituting the ansatz into the differential equation:

$$W^2(x) = p^2(x) - \frac{1}{2}\left(\frac{W''}{W} - \frac{3}{2}\frac{W^2}{W}\right), \tag{4.10}$$

and can be solved iteratively by expanding $W(x)$ in powers of derivatives of $p^2(x)$.

4.2 The Need for Adiabatic Regularization

In the previous chapter, we demonstrated how cosmological particle creation is unambiguously defined when the spacetime possesses asymptotically flat *in* and *out* regions. For this, we defined stable *in* and *out* vacuum states and related them via Bogoliubov transformations. However, if the creation of particles is attributed to the dynamics of the spacetime geometry, it is only logical to conclude that the particles are actively being created during the period of expansion itself. But there lies the problem: in the intermediate region, there is no natural, unique definition of particle states.

One might attempt to bypass this by identifying particles with the excitations of a particle detector carried by a preferred comoving observer, who sees the universe as isotropic. Even then, the particle number is not a constant of motion. Any physical measurement of it requires a finite time interval Δt. If A is the average rate of particle creation, a precise measurement demands $|A|\Delta t \ll 1$. Also, the energy-time Heisenberg uncertainty principle tells us that there is an inherent uncertainty in the particle number. Since $\Delta E \approx m\Delta N$, the particle number has an uncertainty of the form $(m\Delta t)^{-1}$. Then, the total uncertainty in the particle number is bounded by $\Delta N \geq (m\Delta t)^{-1} + |A|\Delta t$, demonstrating that an exact, instantaneous measurement is constrained by quantum uncertainty [15, 17, 35, 41].

Beyond these measurement uncertainties, we are faced with a far more severe problem when attempting to compute expectation values for physical observables, such as the particle number density or the stress-energy tensor $\langle T_{\mu\nu}\rangle$ at an arbitrary time during the expansion. If we calculate the Bogoliubov coefficients using the instantaneous vacuum as the reference state, the resulting momentum distribution fails to decouple from the high-frequency vacuum fluctuations. The ultraviolet tail of the particle spectrum, $|\beta_k|^2$, does not decay sufficiently fast at high momenta, leading to a divergence when integrated over all modes to find the total particle number density. This divergence then propagates into the thermodynamic observables of the system. Because the total diagonal entropy of the field is constructed from the mode-by-mode particle distribution, where the contribution of each mode is given by $S_d^{(k)} = (1 + |\beta_k|^2)\ln(1 + |\beta_k|^2) - |\beta_k|^2 \ln(|\beta_k|^2)$, an unregularized, divergent particle spectrum inevitably yields an infinite total diagonal entropy. This divergence renders the measure of thermodynamic irreversibility meaningless, emphasizing the necessity of a better definition of the local reference state.

To obtain finite predictions from the theory, these artificial divergences need to be eliminated with a regularization scheme, namely the adiabatic regularization scheme [35, 37, 38, 58]. Our approach is to redefine the local reference state. By employing the WKB approximation, we can construct an instantaneous state, that is, the adiabatic vacuum, that matches the exact short-distance singularity structure of the field, absorbing all the unphysical vacuum polarization effects. By defining the Bogoliubov transformation directly with respect to this adiabatic vacuum, we can extract a β_k that yields a finite particle number density and total diagonal entropy.

4.3 The Adiabatic Vacuum

4.3.1 UV Divergences

To see how the UV divergences described above explicitly appear, let us examine the formal expressions for the physical observables of the scalar field. The two main quantities of interest for characterizing the thermodynamic state and the backreaction of the created particles are the total particle number density, n, and the energy density, u (where $u = \langle T_{00} \rangle$).[1]

For a spatially flat four-dimensional expanding universe, the total particle number density is obtained by integrating the momentum distribution over all comoving modes, divided by the physical volume, is

$$n(\eta) = \frac{1}{2\pi^2 a(\eta)^3} \int dk\, k^2\, |\beta_k(\eta)|^2, \tag{4.11}$$

where $a(\eta)$ is the scale factor in terms of the conformal time. Similarly, the energy density of the created particles is given by

$$u(\eta) = \frac{1}{2\pi^2 a(\eta)^4} \int dk\, k^2 \omega_k(\eta) |\beta_k(\eta)|^2. \tag{4.12}$$

To evaluate these integrals at an arbitrary time η, one must determine the Bogoliubov coefficient $\beta_k(\eta)$. As seen in Chapter 2, this coefficient is obtained by taking the Klein-Gordon inner product between the exact mode $\bar{u}_{\vec{k}}(\vec{x}, \eta)$ of the field

[1] Although we are not delving into the backreaction problem in this work, it is important to mention it briefly since it constitutes one of the main reasons why the method of adiabatic regularization was developed.

and the negative-frequency mode of the chosen reference vacuum, $u_{\vec{k}}(\vec{x},\eta)$ (see equation (2.43)). This is equivalent to imposing to the temporal parts of the modes the Wronskian-type of condition:

$$\beta_k(\eta) = -i\left[\bar{\chi}_k(\partial_\eta \chi_k) - (\partial_\eta \bar{\chi}_k)\chi_k\right]. \tag{4.13}$$

If one naively attempts to define the local vacuum state using the "instantaneous Minkowski vacuum" (corresponding to the zeroth-order WKB approximation), the reference mode would be defined by: $\chi_k^{(\text{Minkowski})}(\eta) = (2\omega_k)^{-1/2}\exp\bigl(-i\int \omega_k d\eta\bigr)$ $\equiv (2\omega_k)^{-1/2}\exp(-i\omega_k\eta)$. The UV divergences come directly from how the exact mode χ_k behaves in the high-momentum limit when it is projected against this reference state.

In the short-distance regime, the exact field modes are highly oscillatory and can be asymptotically expanded using the WKB method. However, because the spacetime is dynamic, the exact WKB phase incorporates higher-order derivatives of the scale factor (such as a' and a''), causing the exact effective frequency $W_k(\eta)$ to deviate from the simple classical frequency $\omega_k(\eta)$.

When the exact WKB expansion for $\bar{\chi}_k$ is substituted into the Klein-Gordon inner product alongside the zeroth-order reference mode χ_k^*, the frequency mismatch $(W_k - \omega_k)$ prevents the two states from perfectly orthogonalizing. An asymptotic expansion of this inner product reveals that the high-frequency modes retain a non-vanishing excitation amplitude. Then, the leading surviving terms in the squared Bogoliubov coefficient decay as a power law:

$$|\beta_k^{(unreg)}|^2 \sim \mathcal{O}\left(\frac{1}{k^4}\right) \quad \text{as} \quad k \to \infty. \tag{4.14}$$

This rate of decay is very slow. Because the density of states in three-dimensional momentum space grows as $k^2 dk$, substituting this high-k tail back into the integral for the particle number density yields:

$$n^{(unreg)} \sim \int^{\infty} k^2 \left(\frac{1}{k^4}\right) dk = \int^{\infty} \frac{dk}{k} \to \infty. \tag{4.15}$$

This represents a logarithmic ultraviolet divergence. The choice of the zeroth-order vacuum implies the spontaneous creation of an infinite number of high-energy particles.

The situation is a lot worse for the energy density, where the integrand carries an additional factor of $\omega_k \sim k$ in the UV limit:

$$u^{(unreg)} \sim \int^{\infty} k^2(k)\left(\frac{1}{k^4}\right) dk = \int^{\infty} dk \to \infty, \tag{4.16}$$

resulting in a quadratic ultraviolet divergence, making the energy-momentum tensor physically meaningless.

4.3.2 Defining the Vacuum Order-by-Order

To kill the UV divergences, we need to construct our regularization scheme, and to do that, we need to define the concept of **adiabatic vacuum**, that is, the state defined by the modes that, in some sense, come "closest" to the Minkowski spacetime limit. This will be our reference state, and from the Bogoliubov transformation between the exact modes and the modes defining the adiabatic vacuum, we will extract the Bogoliubov coefficient β_k that will render our observables finite. As we are working with cosmological models, let us restrict our construction to FLRW metrics. As we saw, the line element of a FLRW metric in 3+1 dimensions is given by

$$\mathrm{d}s^2 = C(\eta)[\mathrm{d}\eta^2 - \mathrm{d}x^2 - \mathrm{d}y^2 - \mathrm{d}z^2]. \tag{4.17}$$

The spatial sections are homogeneous, so the mode solutions are separable:

$$u_{\vec{k}} \propto e^{i\vec{k}\cdot\vec{x}}\chi_k(\eta). \tag{4.18}$$

If the field is conformally coupled, the temporal mode satisfies: [41]

$$\chi_k''(\eta) + \omega_k^2(\eta)\chi_k(\eta) = 0, \tag{4.19}$$

where

$$\omega_k^2 = k^2 + C(\eta)m^2. \tag{4.20}$$

The formal solution to equation (4.19) is a WKB-type solution:

$$\chi_k(\eta) = \frac{1}{\sqrt{2W_k}} \exp\left[-i\int^{\eta} W_k(\eta')d\eta'\right], \tag{4.21}$$

where W_k satisfies

$$W_k^2(\eta) = \omega_k^2(\eta) - \frac{1}{2}\left(\frac{W_k''}{W_k} - \frac{3}{2}\frac{W_k'^2}{W_k^2}\right). \tag{4.22}$$

There is a phase factor that is implicit in equation (4.21) which is specified by choosing a lower limit for the integral. Since this is a global phase, it is irrelevant to the physics, and we can just compute the primitive of the integral and evaluate it at η.

If the spacetime is varying slowly, W_k' and W_k'' will be negligible compared to ω_k^2 in equation (4.22), so a zeroth order approximation is to substitute

$$W_k^{(0)}(\eta) \equiv \omega_k(\eta) \tag{4.23}$$

in (4.21). Of course, when $C(\eta) \to \text{constant}$, $\omega_k(\eta)$ also becomes constant, and this solution reduces (as expected) to the standard Minkowski spacetime modes. This is the zeroth adiabatic order.

Now, the next iteration yields

$$W_k^{(2)}(\eta) = \sqrt{\omega_k^2(\eta) - \frac{1}{2}\left(\frac{\omega_k''}{\omega_k} - \frac{3}{2}\frac{\omega_k'^2}{\omega_k^2}\right)}. \tag{4.24}$$

Expanding to the second order, we obtain

$$W_k^{(2)} = \omega_k(\eta) + \frac{1}{2\omega_k}\left[\frac{3}{4}\left(\frac{\omega_k'}{\omega_k}\right)^2 - \frac{1}{2}\frac{\omega_k''}{\omega_k}\right]. \tag{4.25}$$

Substituting this into (4.21), we obtain the second order adiabatic temporal modes, which define the second order adiabatic vacuum. The second adiabatic order is the minimal order necessary to regularize the particle number, so we shall stop here. But for the regularization of other quantities, such as the energy-momentum tensor, one would need the fourth order approximation.

We shall denote the Ath order adiabatic approximation to the temporal modes χ_k by $\chi_k^{(A)}$, and the associated "full" modes (4.18) as $u_{\vec{k}}^{(A)}$. These modes define the Ath order adiabatic vacuum.

In general, there exists the relation [41]

$$u_k = \alpha_k^{(A)}(\eta)u_k^{(A)} + \beta_k^{(A)}(\eta)u_k^{(A)*}, \tag{4.26}$$

that defines an exact mode solution for the field equation in terms of the adiabatic approximation $u_k^{(A)}$.

Chapter 5

Particle Creation and Entropy Production in de Sitter Spacetime

5.1 The de Sitter Geometry

Now that we developed the formalism of adiabatic regularization, we now apply it to a more realistic and cosmologically significant scenario: de Sitter spacetime. Unlike the asymptotically flat model of Chapter 3, de Sitter space expands eternally, lacking the flat *in* and *out* regions that allow for an unambiguous particle interpretation. This makes it an ideal testing ground for the adiabatic regularization scheme developed above. In this chapter, we investigate particle creation for a massive, conformally coupled scalar field propagating in four-dimensional de Sitter space. After reviewing the geometry and selecting the Bunch-Davies vacuum as our initial state, we compute the regularized Bogoliubov coefficients and extract the mean particle number per mode. From these, we obtain the diagonal entropy and effective temperature spectra for two representative masses: the critical mass $m = H/2$ and a heavy mass $m = H$.

5.1.1 Global Coordinates and Coordinate Patches

The geometric structure of de Sitter space is more easily described as the hyperboloid

$$-\alpha^2 = v^2 - w^2 - x^2 - y^2 - z^2 \tag{5.1}$$

embedded in a flat five dimensional space $\mathbb{R}^5$ with Lorentzian metric

$$\mathrm{d}s^2 = \mathrm{d}v^2 - \mathrm{d}w^2 - \mathrm{d}x^2 - \mathrm{d}y^2 - \mathrm{d}z^2. \tag{5.2}$$

One can introduce a coordinate system on the hyperboloid that is described by the following relations:

$$\begin{aligned} v &= \alpha \sinh \frac{\zeta}{\alpha}, & w &= \alpha \cosh \frac{\zeta}{\alpha} \cos \chi \\ x &= \alpha \cosh \frac{\zeta}{\alpha} \sin \chi \cos \theta, & y &= \alpha \cosh \frac{\zeta}{\alpha} \sin \chi \sin \theta \cos \phi \\ z &= \alpha \cosh \frac{\zeta}{\alpha} \sin \chi \sin \theta \sin \phi. \end{aligned} \tag{5.3}$$

The metric (5.2), in these coordinates, may be written as

$$\mathrm{d}s^2 = \mathrm{d}\zeta^2 - \alpha^2 \cosh^2 \frac{\zeta}{\alpha} \{\mathrm{d}\chi^2 + \sin^2 \chi (\mathrm{d}\theta^2 + \sin^2 \theta \mathrm{d}\phi^2)\}. \tag{5.4}$$

There are apparent singularities in this metric, but these are artifacts of the spherical-like coordinates used for the spatial part. At $\chi = 0$ and $\chi = \pi$, we have $\sin^2 \chi = 0$; similarly, at $\theta = 0$ and $\theta = \pi$, we have $\sin^2 \theta = 0$. These are simply the singularities that occur with polar coordinates. Apart from these, there are no physical singularities, and the chart covers the whole hyperboloid. The spatial sections are $\mathbb{S}^3$ spheres that have constant positive curvature. Their geodesic normals are lines that contract to a minimum spatial separation and then expand again to infinity.

Another common set of coordinates that can be introduced is the so-called **static patch** of de Sitter space. This coordinate system maps the flat five-dimensional embedding coordinates (v, w, x, y, z) to a set of static coordinates (t, r, θ, ϕ). Such a map is given by

$$\begin{aligned} v &= \sqrt{\alpha^2 - r^2} \sinh \frac{t}{\alpha} \\ w &= \sqrt{\alpha^2 - r^2} \cosh \frac{t}{\alpha} \\ x &= r \cos \theta \\ y &= r \sin \theta \cos \phi \\ z &= r \sin \theta \sin \phi. \end{aligned} \tag{5.5}$$

Here, t acts as the static time coordinate, and r is the radial coordinate, restricted to $0 \leq r < \alpha$. With this, (5.2) becomes

$$\mathrm{d}s^2 = \left(1 - \frac{r^2}{\alpha^2}\right) \mathrm{d}t^2 - \left(1 - \frac{r^2}{\alpha^2}\right)^{-1} \mathrm{d}r^2 - r^2 (\mathrm{d}\theta^2 + \sin^2 \theta \mathrm{d}\phi^2). \tag{5.6}$$

There are singularities in this metric. Specifically, when $r \to \alpha$, we have $g_{tt} \to 0$ and $g_{rr} \to \infty$; but again, these are artifacts of the coordinate system and not true

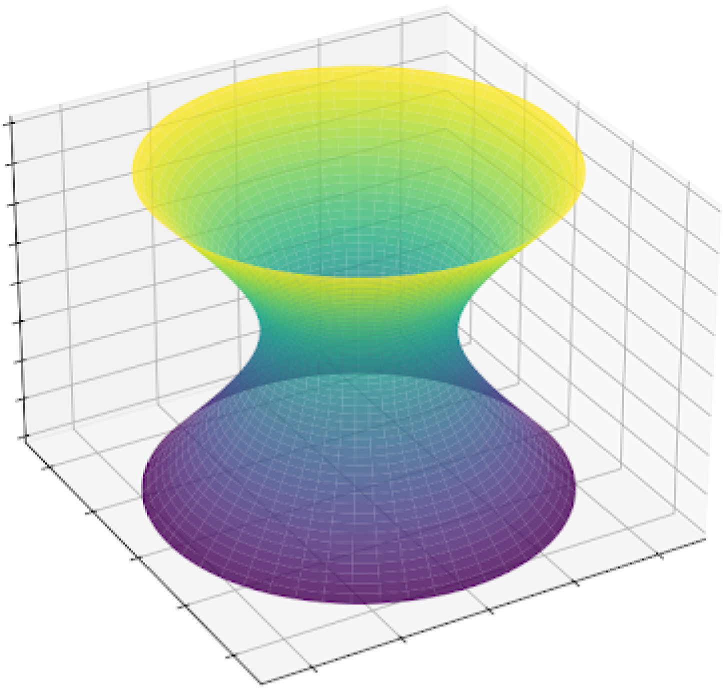

FIGURE 5.1: De Sitter space represented by a hyperboloid embedded into a 5d Minkowski spacetime. Two dimensions are suppressed.

physical singularities.

Finally, another coordinate system that is of particular importance in cosmological models is a map of the embedding coordinates to the set (t, x, y, z), known as the **Poincaré patch** of de Sitter space:

$$t = \alpha \ln \frac{w+v}{\alpha}, \qquad x^i = \frac{\alpha x^i}{w+v}, \tag{5.7}$$

where the usual spatial coordinates are represented by $x^i \in (x, y, z)$. This chart covers only half of the hyperboloid since the time coordinate t is not defined when $w + v \leq 0$.

The metric that describes the Poincaré patch of de Sitter space corresponds to the spatially flat ($k = 0$) FLRW model with an exponential scale factor:

$$ds^2 = dt^2 - e^{2Ht}(dx^2 + dy^2 + dz^2) \tag{5.8}$$

where H is a constant known as the Hubble parameter and is related to α by $H = \alpha^{-1}$. The Hubble parameter is also related to the scale factor $a(t)$ by $H = \dot{a}/a$. One may perform a conformal transformation and rewrite the metric (5.8) in terms of the conformal time η:

$$ds^2 = \frac{1}{H^2\eta^2}(d\eta^2 - dx^2 - dy^2 - dz^2). \tag{5.9}$$

The scale factor in terms of the conformal time is $a(\eta) = -(H\eta)^{-1}$, with $\eta \in (-\infty, 0)$.

The relevant Christoffel symbols are

$$\begin{aligned}\Gamma^i_{0j} &= \Gamma^i_{j0} = H\delta^i_j \\ \Gamma^0_{ij} &= He^{2Ht}\delta_{ij}.\end{aligned} \tag{5.10}$$

The components of the Ricci tensor, which are calculated from the Christoffel symbols, yields

$$\begin{aligned}R_{00} &= -3H^2 \\ R_{ij} &= 3H^2 g_{ij},\end{aligned} \tag{5.11}$$

and the Ricci scalar is

$$R = 12H^2. \tag{5.12}$$

5.2 Scalar Field Dynamics in de Sitter

5.2.1 The Massive Conformally Coupled Scalar Field Equation

For a real scalar field propagating in a spacetime with the metric given by (5.9), the action is

$$S[\phi] = \frac{1}{2}\int d^4x\sqrt{-g}[g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - (m^2 + \xi R)\phi^2]. \tag{5.13}$$

The equation of motion for the field is the covariant Klein-Gordon equation, and due to spatial homogeneity, the mode solutions are separable (c.f., (3.13)):

$$u_{\vec{k}}(\vec{x}, \eta) \propto e^{i\vec{k}\cdot\vec{x}}\phi_k(\eta). \tag{5.14}$$

In this setting, $\sqrt{-g} = a^4(\eta)$, so the covariant d'Alembertian becomes

$$\Box_g = a^{-2}\partial_\eta^2 + 2a'a^{-3}\partial_\eta - a^{-2}\nabla^2, \tag{5.15}$$

where ∇^2 denotes the usual Laplacian operator.

The modes (5.14) will obey the covariant Klein-Gordon equation if the temporal mode ϕ_k obeys

$$\phi_k'' + 2\frac{a'}{a}\phi_k' + (k^2 + a^2m^2 + a^2\xi R)\phi_k = 0. \tag{5.16}$$

To eliminate the first-derivative term and bring the equation into the form of a harmonic oscillator, we introduce an auxiliary field $\chi_k(\eta)$ scaled by the expansion factor:

$$\phi_k(\eta) = \frac{\chi_k(\eta)}{a(\eta)}. \tag{5.17}$$

Taking the derivatives, we obtain

$$\begin{aligned} \phi_k' &= \frac{\chi_k'}{a} - \chi_k\frac{a'}{a^2} \\ \phi'' &= \frac{\chi_k''}{a} - 2\frac{a'}{a^2}\chi_k' - \frac{a''}{a^2}\chi_k - 2\frac{a'^2}{a^3}\chi_k. \end{aligned} \tag{5.18}$$

Substituting into equation (5.16), and multiplying everything by $a(\eta)$, we obtain the equation for $\chi_k(\eta)$:

$$\chi_k'' + \left(k^2 + a^2m^2 + a^2\xi R - \frac{a''}{a}\right)\chi_k = 0. \tag{5.19}$$

The Ricci scalar R was already calculated in the previous section, and it is given in terms of the Hubble parameter $R = 12H^2$ and, since we are interested in the conformally coupled setting, we set $\xi = \frac{1}{6}$. Now, we need to evaluate the geometric terms, namely the derivatives of $a(\eta)$. In the Poincaré patch, $a(\eta) = 1/H\eta$, so:

$$\begin{aligned} a' &= \frac{1}{H\eta^2} \\ a'' &= -\frac{2}{H\eta^3}, \end{aligned} \tag{5.20}$$

and also

$$\frac{a''}{a} = \frac{2}{\eta^2}. \tag{5.21}$$

With this at hand, we see that the term $a^2\xi R$ in equation (5.19) cancels with the a''/a term, and we finally obtain:[1]

$$\chi_k'' + \left(k^2 + \frac{m^2}{H^2\eta^2}\right)\chi_k = 0. \tag{5.22}$$

[1]The term $1/m^2H^2$ is the conformal factor $C(\eta)$, but we switched to using the scale factor in terms of η.

This is a Bessel differential equation, and its general solution [59] is given by

$$\chi_k(\eta) = \sqrt{-k\eta}\left[A_k H_\nu^{(1)}(-k\eta) + B_k H_\nu^{(2)}(-k\eta)\right]. \tag{5.23}$$

$H_\nu^{(1)}(-k\eta)$ and $H_\nu^{(2)}(-k\eta)$ are the Hankel functions of the first and second kinds, respectively, and are defined as linear combinations of the more common Bessel functions of the first and second kinds:

$$\begin{aligned} H_\nu^{(1)}(-k\eta) &= J_\nu(-k\eta) + iY_\nu(-k\eta) \\ H_\nu^{(1)}(-k\eta) &= J_\nu(-k\eta) - iY_\nu(-k\eta) \end{aligned} \tag{5.24}$$

where the index ν depends on the mass of the field,

$$\nu = \sqrt{\frac{1}{4} - \frac{m^2}{H^2}}. \tag{5.25}$$

The A_k and B_k are complex coefficients that will be determined through boundary conditions in the next section.

Regarding the mass of the field, there are four different cases that characterize the behavior of the index ν, dictating whether the mode functions freeze or oscillate at late times:

1. **Massless Limit**:
   If $m \to 0$, the index evaluates to $\nu = 1/2$. Bessel functions of half-integer order become spherical Bessel functions, which are just sines and cosines. In this limit, the mode equation is $\chi_k'' + k^2\chi_k = 0$, identically replicating a massless field equation of motion in Minkowski spacetime. The field experiences no particle production because its conformal symmetry is unbroken[40, 41].

2. **Light Fields** $(0 < m < H/2)$:
   For masses strictly less than half the Hubble parameter, the expression under the square root is positive, making the index ν real $(0 < \nu < 1/2)$. These fields are known to map to the complementary series representations of the de Sitter group $SO(1,4)$ [60]. Physically, when these modes cross the Hubble horizon ($-k\eta \sim 1$), they exhibit a power-law decay ($\chi_k \sim (-\eta)^{1/2-\nu}$), becoming non-oscillatory and effectively freezing in amplitude.

3. **Critical Fields** $(m = H/2)$:
   For $m = H/2$ (what we are calling the *critical mass*), the index of the mode function vanishes ($\nu = 0$). The modes are then governed by the zeroth-order Hankel function of the first kind, $H_0^{(1)}(-k\eta)$. Unlike the light fields, which

settle into a stable power-law decay in the super-horizon regime, the small-argument expansion of the zeroth-order Hankel function introduces a logarithmic dependence. When these modes cross the Hubble horizon ($-k\eta \sim 1$), the mode function evolves asymptotically as $\chi_k \sim (-\eta)^{1/2} \ln(-k\eta)$. What ends up happening is that this term prevents the field amplitude from fully freezing out.

4. **Heavy Fields** ($m > H/2$):
When m exceeds the critical threshold $H/2$, the term $(1/4 - m^2/H^2)$ becomes negative. Consequently, the index ν becomes purely imaginary. It is standard to define a real parameter $\mu = \sqrt{m^2/H^2 - 1/4}$, such that $\nu = i\mu$. These massive fields belong to the principal series representations of $SO(1,4)$ [61–63]. Just like the critical field, principal series fields never completely freeze out; the modes continue to oscillate rapidly even well outside the Hubble horizon.

5.2.2 The Bunch-Davies Vacuum

A requirement for a consistent definition of particle production is that we need to clearly and unambiguously identify both the *in* and *out* vacuum states. In Chapter 3, both the early- and late-time regions were taken to be asymptotically flat in order to provide such a framework. In light of the fact that we are now working in a spacetime that has no such regions, the question is: how does one choose a preferred vacuum state that can meaningfully characterize the state of the field throughout its entire evolution?

In the case of a massless, conformally coupled scalar field propagating in a conformally flat geometry, the vacuum is uniquely determined by conformal symmetry and is commonly referred to as the conformal vacuum. For massive fields or fields with non-conformal coupling in de Sitter spacetime, the natural criterion is invariance under the $SO(1,4)$ group.

Imposing de Sitter invariance does not, by itself, single out a unique state. Rather, there is a whole family of quantum states that presents such invariance, referred to as the α-vacua. These states share the same symmetry properties but differ in their short-distance structure. Among them, the **Bunch-Davies vacuum** is the unique member of the α-family whose short-distance behavior matches that of the Minkowski vacuum. [60, 61, 64–67].

Let us examine how the modes behave in the remote past. As $\eta \to -\infty$, the physical wavelength of any comoving mode $\lambda_{phys} = 2\pi a(\eta)/k$ is infinitesimally small. Because the scale factor $a(\eta) = -1/H\eta$ approaches zero in this region, every mode, regardless of its momentum, was deeply sub-horizon,[2] meaning that $k_{phys} = k/a \gg H$. The mode equation then reduces to that of a free scalar field in Minkowski spacetime.

The Bunch–Davies vacuum is selected by requiring that, in this sub-horizon early-time regime, the rescaled de Sitter modes reproduce the standard positive-frequency behavior of flat spacetime. Explicitly, one imposes $\chi_k \sim \exp\{-ik\eta\}$ as $\eta \to -\infty$, fixing the short-distance structure of the state.[3] This asymptotic Minkowski condition distinguishes the Bunch–Davies vacuum from the other α-vacua.

Now, the coefficients A_k and B_k, must be found to satisfy all the above conditions. The large-argument asymptotic expansions [50] for the Hankel functions of the first and second kind are given by

$$H_\nu^{(1)}(-k\eta) \sim \sqrt{-\frac{2}{k\eta\pi}} \exp\left\{-i\left(k\eta + \frac{\nu\pi}{2} + \frac{\pi}{4}\right)\right\}, \quad k\eta \to -\infty \tag{5.26}$$

$$H_\nu^{(2)}(-k\eta) \sim \sqrt{-\frac{2}{k\eta\pi}} \exp\left\{i\left(k\eta + \frac{\nu\pi}{2} + \frac{\pi}{4}\right)\right\}, \quad k\eta \to -\infty. \tag{5.27}$$

Substituting these asymptotic forms back into equation (5.23), we obtain

$$\chi_k \sim \sqrt{\frac{2}{\pi}} \left[A_k \exp\left\{-i\left(k\eta + \frac{\nu\pi}{2} + \frac{\pi}{4}\right)\right\} + B_k \exp\left\{i\left(k\eta + \frac{\nu\pi}{2} + \frac{\pi}{4}\right)\right\}\right], \tag{5.28}$$

and from that, it is clear that in order to recover the Minkowski positive-frequency behavior, all the B_k need to vanish:

$$B_k = 0 \quad \forall k. \tag{5.29}$$

To find A_k, it is simply a matter of equating its term with the Minkowski positive frequency plane wave:

$$\sqrt{\frac{2}{\pi}} A_k \exp\left\{-i\left(k\eta + \frac{\nu\pi}{2} + \frac{\pi}{4}\right)\right\} = \frac{1}{\sqrt{2k}} \exp\{-ik\eta\}, \tag{5.30}$$

which leads us to

$$A_k = \frac{1}{2}\sqrt{\frac{\pi}{k}} \exp\left\{\frac{i\pi}{2}\left(\nu + \frac{1}{2}\right)\right\}. \tag{5.31}$$

[2] To maintain consistency with the previous section, we can also describe the sub-horizon regime as $-k\eta \gg 1$.

[3] (Here, we are using $\exp\{-ik\eta\}$ instead of $\exp\{-i\omega_k\eta\}$ since, in the sub-horizon regime, all modes are strongly ultraviolet, so that in the limit, $\omega_k = \sqrt{k^2 + m^2} \to k$)

Now that A_k and B_k have been properly chosen, we may write the solution of equation (5.22) as

$$\chi_k^{(BD)}(\eta) = \frac{\sqrt{-\pi\eta}}{2} e^{i\frac{\pi}{2}\left(\nu+\frac{1}{2}\right)} H_\nu^{(1)}(-k\eta). \tag{5.32}$$

The modes given by equation (5.32) define the Bunch-Davies vacuum $\left|0^{(BD)}\right\rangle$. Throughout the next sections, this will be the "true state" of the system within the Heisenberg picture, against which the reference vacuum state will be projected against.

5.3 Application of Adiabatic Regularization

5.3.1 Defining the Adiabatic Vacuum and Extracting β_k

To define the reference state against which particles will be defined, and that will be used to extract the mean number of particles per mode created during the expansion, we need to compute the second order WKB approximation. First, making use of the expression given by equation (4.25), with $\omega_k(\eta) = \sqrt{k^2 + \frac{m^2}{H^2\eta^2}}$, we obtain for $W_k \approx W_k^{(0)} + W_k^{(2)}$:

$$W_k \approx \frac{H^2 m^2 \left(\frac{3}{2}H^2\eta^2 k^2 + \frac{1}{4}m^2\right) - 2\left(H^2\eta^2 k^2 + m^2\right)^3}{2H\left(H^2\eta^2k^2 + m^2\right)^{\frac{5}{2}}\eta}, \tag{5.33}$$

so that the second-order adiabatic mode is given by substituting the above equation into

$$\chi_k^{(2)}(\eta) = \frac{1}{\sqrt{2W_k}} \exp\left[-i\int^\eta W_k(\eta')d\eta'\right]. \tag{5.34}$$

As it is, we have an extraordinary problem at hand. It is, of course, completely possible to find a closed form for $\chi_k^{(2)}(\eta)$, but it is totally impractical to use it directly to find $\beta_k^{(2)}(\eta)$ by applying the Wronskian condition (4.13). But we can use a trick to simplify the calculations and obtain its spectrum computationally.

In terms of the Bunch-Davies modes and the second-order adiabatic modes, the Wronskian condition reads

$$\beta_k^{(2)} = -i\left(\chi_k^{(A)}\partial_\eta\chi_k^{(BD)} - \partial_\eta\chi_k^{(A)}\chi_k^{(BD)}\right). \tag{5.35}$$

If we take the time derivative of equation (5.34), we obtain

$$\partial_\eta\chi_k^{(2)} = \left(-\frac{\partial_\eta W_k}{2W_k} - iW_k\right)\chi_k^{(2)}. \tag{5.36}$$

Substituting this back into equation (5.35) and taking the absolute square, the exponential cancels out, leaving a purely algebraic expression evaluated at a specific time η:

$$|\beta_k|^2 = \frac{1}{2W_k}\left|\partial_\eta \chi_k^{(BD)} + \left(\frac{\partial_\eta W_k}{2W_k} + iW_k\right)\chi_k^{(BD)}\right|^2 . \tag{5.37}$$

Additionally, the derivative of the Bunch-Davies mode can be evaluated as

$$\partial_\eta \chi_k^{(BD)} = \chi_k^{(BD)}\left(\frac{1}{2\eta} - k\frac{H_\nu^{(1)\prime}(-k\eta)}{H_\nu^{(1)}(-k\eta)}\right). \tag{5.38}$$

Now, we can analyze $|\beta_k^{(2)}|^2$ across various stages of the universe's expansion. A Python routine was implemented to evaluate the complex Hankel functions and compute an array of values for $y = |\beta_k^{(2)}|^2$ across the required range of $x = -k\eta$ (which contemplates the sub-horizon, horizon crossing, and super-horizon regions), and generate the particle production spectra shown in figure 5.2. We had set $H = 1$ and used a logarithmic grid of 500 points, from $x_{\min} = 10^{-2}$ to $x_{\max} = 10^{2.5}$. The code loops over the k values, computes W_k, $\partial_\eta W_k$, $\chi_k^{(BD)}$, its derivative, and finally $|\beta_k^{(2)}|^2$.

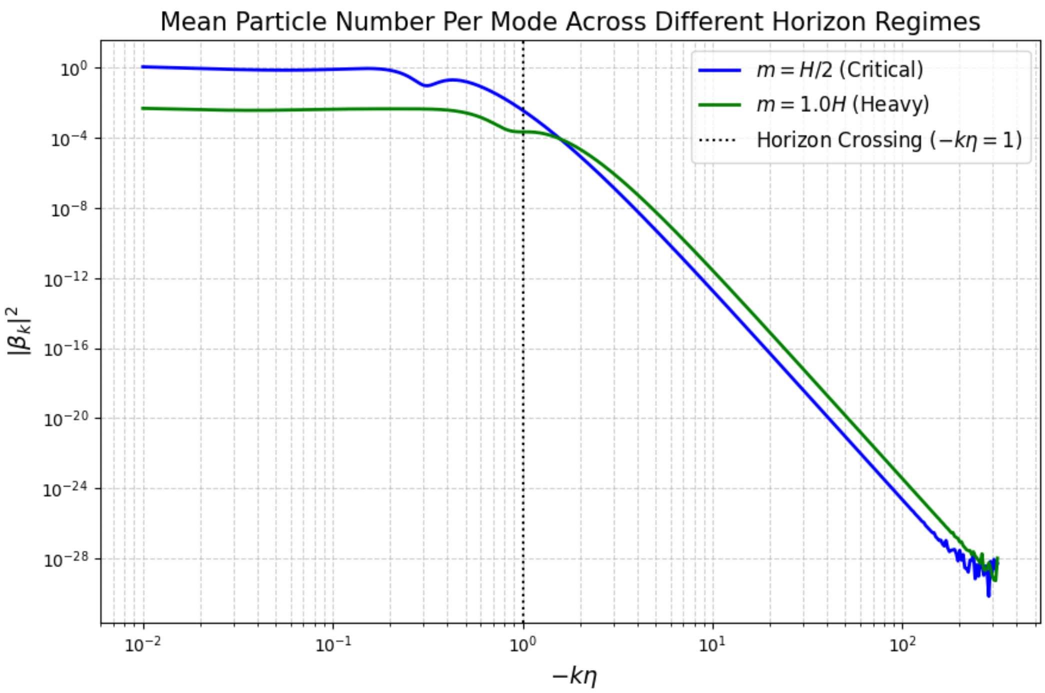

FIGURE 5.2: The spectrum of the mean particle number per mode, for two different masses.

Both curves correspond to two different choices of masses explored in Section

5.2.1. As one would expect, in the deep sub-horizon regime, all three curves demonstrate negligible particle production, with values of $|\beta_k|^2$ suppressed to low magnitudes. At these early times, the physical wavelength of the mode is significantly smaller than the Hubble radius, meaning that the spacetime curvature effects are minimal. Here, the mode functions adiabatically follow the Bunch-Davies vacuum, and the WKB approximation upon which the regularization is based becomes exact. As the universe expands, modes are "stretched" beyond the Hubble horizon.

Now that we have obtained the spectra of $|\beta_k^{(2)}|^2$, we are ready to calculate the regularized density $n^{\mathrm{reg}}(\eta)$:

$$\begin{aligned} n^{\mathrm{reg}}(\eta) &= \frac{1}{[2\pi a(\eta)]^3} \int d^3k \left|\beta_k^{(2)}(\eta)\right|^2 \\ &= \frac{1}{2\pi^2 a(\eta)^3} \int_0^\infty dk\, k^2 \left|\beta_k^{(2)}(\eta)\right|^2 . \end{aligned} \tag{5.39}$$

At first glance, equation (5.39) seems to have a time dependence. However, the particle number density is, in fact, constant. We encourage the reader to refer to Appendix B.1 to see why that must be the case. This integral is computed numerically using Simpson's rule.

For a field with critical mass $m = \frac{1}{2}H$, we have obtained

$$\begin{aligned} n^{\mathrm{reg}}_{\mathrm{crit}}(\eta) &= n_{\mathrm{crit}} \\ &= 9.876 \times 10^{-4}, \end{aligned} \tag{5.40}$$

while for a heavy field of mass $m = H$, the particle number density is [4]

$$\begin{aligned} n^{\mathrm{reg}}_{\mathrm{heavy}}(\eta) &= n_{\mathrm{heavy}} \\ &= 2.958 \times 10^{-5}. \end{aligned} \tag{5.41}$$

As expected, the density of produced particles of a heavy field is much smaller than that of a field of critical mass.

[4]This density represents the number of particles per unit physical volume in units of H^3, but we had set $H = 1$.

5.4 Diagonal Entropy in de Sitter space

5.4.1 Entropy Production, Effective Temperature and Mass Dependent Thermalization

Finally, we are ready to calculate the spectrum of the diagonal entropy for the scalar field in de Sitter space. Because the Bogoliubov transformation relating the Bunch-Davies vacuum and the reference state (the adiabatic vacuum) is diagonal in momentum space, due to the spatial homogeneity of our model, the considerations made in Chapter 3 to relate both states are still valid. That is, the Bunch-Davies vacuum can be written as a squeezed state:

$$\left|0^{(BD)}\right\rangle = \sqrt{1-|\lambda_k|^2}\sum \lambda_k^n \left|n_k^{\text{reg}}, n_{-k}^{\text{reg}}\right\rangle^{(2)} \tag{5.42}$$

where $\lambda_k = |\beta_k^{(2)}(\eta)/\alpha_k^{(2)}(\eta)|^2$.

The diagonal elements of the density matrix per mode are

$$\rho_{nn}^{(k)} = (1-\lambda_k)\lambda_k^n, \tag{5.43}$$

and the diagonal entropy per mode is

$$S_d^{(k)} = (1+n_k^{\text{reg}})\ln(1+n_k^{\text{reg}}) - n_k^{\text{reg}}\ln(n_k^{\text{reg}}), \tag{5.44}$$

where $n_k^{\text{reg}} \equiv |\beta_k^{(2)}|^2$ [5]. With the same numerical array of values for n_k^{reg} used to plot figure 5.2, we can plot the spectra of $S_d^{(k)}$. Figure 5.3 illustrates this spectrum for the critical and heavy masses. We used the same parameters for the grid, $x_{\text{min/max}}$ etc., that were used for the plot 5.2.

It is not surprising that the plots 5.2 and 5.3 are almost identical. For the entirety of the sub-horizon regime and the vast majority of the super-horizon regime for $m \geq H/2$, the regularized particle number is $n_k^{\text{reg}} \ll 1$. In this limit, $\ln(1+n_k^{\text{reg}}) \approx 0$, so the diagonal entropy per mode can be approximated by $S_d^{(k)} \approx -n_k^{\text{reg}}\ln(n_k^{\text{reg}})$. While the particle number n_k^{reg} changes very quickly across the spectrum, $\ln(n_k^{\text{reg}})$ behaves almost like a constant, which is why both figures have the same shape.

The total entropy density is given by evaluating the integral

$$s_d(\eta) = \frac{1}{2\pi^2 a(\eta)^3}\int_0^\infty dk\, k^2 S_d^k(\eta). \tag{5.45}$$

[5] From now on, we will use n_k^{reg} instead of $|\beta_k^{(2)}|^2$

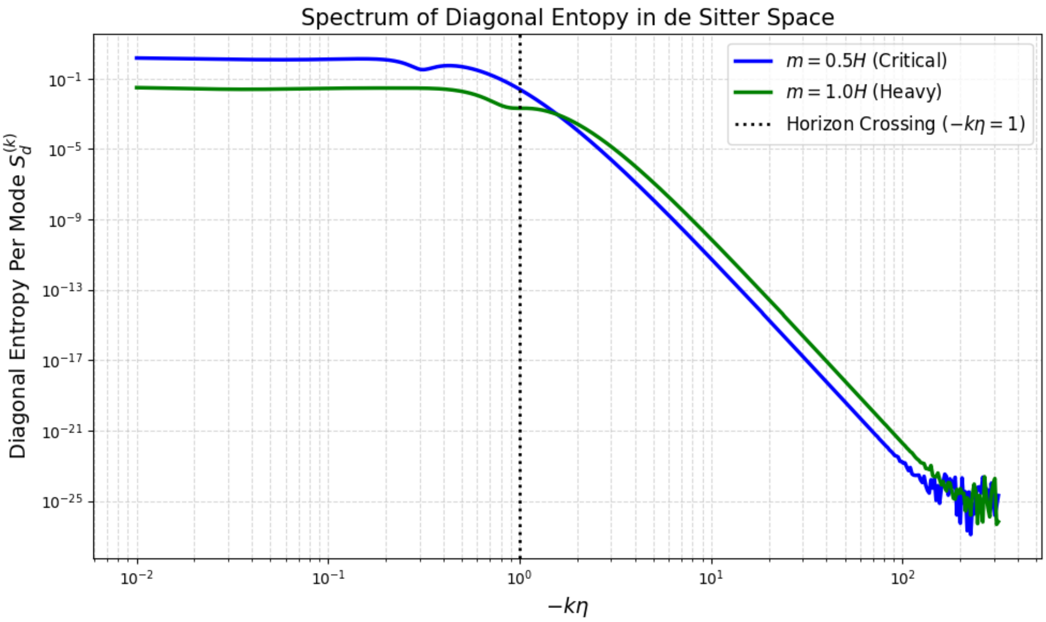

FIGURE 5.3: Spectra of the diagonal entropy per mode for the critical mass and heavy mass.

In the same way as the particle number density, this quantity appears to have a time dependence, but it is constant (see Appendix B.2). To evaluate it numerically, we employ Simpson's rule.

For the critical mass, we obtain

$$s_d^{\text{crit}} = 3.296 \times 10^{-3}, \tag{5.46}$$

and for the heavy mass,

$$s_d^{\text{heavy}} = 2.582 \times 10^{-4}. \tag{5.47}$$

Finally, we can write an effective temperature for each mode, just as we did in Chapter 3. The general formula is

$$T_{\text{eff}}^{(k)} = \frac{\omega_{\text{phys}}}{\ln\left(1 + \frac{1}{n_k^{\text{reg}}}\right)}. \tag{5.48}$$

The comoving momentum k is related to the physical momentum as k_{phys} by $k_{\text{phys}} = k/a(\eta)$. Since $a(\eta) = -1/(H\eta)$, the physical momentum is $k_{\text{phys}} = -k\eta H$. Therefore, the dispersion ω_{phys} is

$$\omega_{\text{phys}} = H\sqrt{k^2\eta^2 + \left(\frac{m}{H}\right)^2} \tag{5.49}$$

With the same array of the n_k previously computed, we evaluate (5.48). Figure

5.4 shows the resulting effective temperature spectra for $m = \frac{1}{2}H$ and $m = H$. For the critical mass, the effective temperature diverges for super-horizon modes, while for $m = H$, the effective temperature for the same modes approaches a constant value. Remarkably, this constant is numerically close to the de Sitter horizon temperature [25] $T_{\text{dS}} = H/(2\pi) \approx 0.159$ for $H = 1$. This indicates that for $m = H$, super-horizon modes effectively thermalize at the Gibbons-Hawking temperature.

Another interesting behavior that is worth pointing out is that, in the deep sub-horizon regime, the effective temperature exhibits infinite growth; however, this does not mean that we have particle production. In fact, as shown in Figure 5.2, particle production is heavily suppressed in the UV regime. So, what is happening here? Remember that temperature is an intensive quantity. A single mode with a very high frequency can have a large effective temperature even if its occupation number is very small. Consider an analogy: a single photon with frequency ω in an otherwise empty cavity can be assigned an effective temperature $T = \omega/\ln(2)$ if we ask what temperature would give a mean occupation number of $1/2$. The fact that T is high does not mean the cavity contains many photons. T being high simply reflects the high energy scale of the mode.

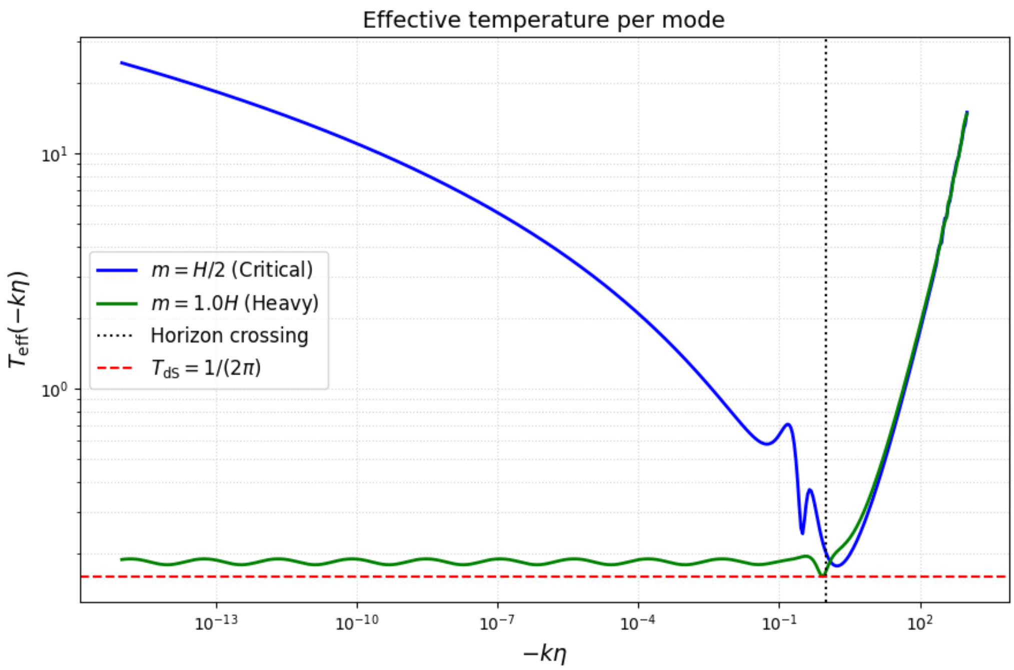

FIGURE 5.4: Effective temperature per mode for the critical mass and heavy mass. The Gibbons-Hawking temperature is represented by the red dotted line.

The fact that, for $m = H$, the super-horizon effective temperature approaches T_{dS} is not so trivial. The Gibbons–Hawking temperature is usually associated with the temperature measured by a static observer in de Sitter space, that is, one who remains at fixed spatial coordinates in the static patch and experiences a **cosmological horizon** [6]. Such an observer detects a thermal bath of particles at temperature T_{dS} as a consequence of horizon thermodynamics. Our result for $m = H$ indicates that, despite the different observer perspectives and the different physical interpretations of temperature, the statistical distribution of created particles in the Bunch-Davies vacuum has the same thermal scale $H/2\pi$.

On the other hand, the critical mass exhibits an enormous rise in T_{eff} when $-k\eta \to 0$. This divergence is a direct consequence of the special value $\nu = 0$ for this mass. The Hankel function of order zero contains a logarithmic term for small arguments, which propagates into $|\beta_k^{(2)}|^2$ and causes it to grow without bound in the infrared. Consequently, $n_k \to \infty$, and the denominator in (5.48) grows only as $\ln[-\ln(-k\eta)]$, while the numerator remains finite ($\omega \to m = H/2$), yielding an effective temperature that grows infinitely.

[6]Until now, we have been talking about the behavior of certain quantities in the sub- and super-horizon regimes, but notice that what we are referring to is **not** a cosmological horizon. In our coordinates within the Poincaré patch, the horizon refers to the dynamical Hubble radius ($R_H = 1/H$), and "horizon crossing" refers to the scale at which the physical wavelength of a quantum fluctuation exceeds the causal boundary of the expansion and freezes out. While a freely falling comoving observer does not encounter a localized event horizon radiating thermal energy, our analysis demonstrates the infrared sector of the spectrum for $m = H$ approaches a nearly constant value, numerically close to $T_{\text{dS}} = H/(2\pi)$. This indicates that the statistical distribution of super-horizon modes in the Bunch–Davies vacuum seems to have the same thermal scale that characterizes the static patch description, despite the distinct observer constructions involved. See reference [68] for a complete discussion about horizons.

Chapter 6

Conclusions and Discussions

In this work, we have investigated the thermodynamic aspects of particle creation in expanding universes, with a particular focus on the emergence of entropy and effective temperature from a unitary quantum evolution. The concept of diagonal entropy, originally introduced in the context of non-equilibrium quantum thermodynamics, was used as a measure of irreversibility that naturally arises when one discards the unobservable phase information that appears in the off-diagonal elements of the density matrix in the instantaneous energy eigenbasis.

In Chapter 2, we provided the formalism of quantum scalar fields propagating in a curved spacetime, highlighting the inherent ambiguity in defining a unique vacuum state and the necessity of Bogoliubov transformations to relate different mode decompositions. This formalism was applied in Chapter 3 to a simple toy model: a $1+1$-dimensional asymptotically flat FLRW universe. By choosing the specific conformal factor $C(\eta) = A+B\tanh(\rho\eta)$, we obtained exact mode functions in terms of hypergeometric functions and derived the Bogoliubov coefficients connecting the *in* and *out* vacua. The resulting state was shown to be a two-mode squeezed vacuum, with correlations between modes of opposite momenta. The diagonal entropy per mode took the form $S_d^{(k)} = (1+n_k)\ln(1+n_k) - n_k \ln n_k$, where $n_k = |\beta_k|^2$ is the mean occupation number. This result already hinted at a thermodynamic interpretation: despite the global purity of the state, the loss of phase coherence leads to an effective entropy that behaves as if the modes were populated according to a thermal distribution with an effective temperature $T_{\text{eff}}^{(k)} = \omega_k / \ln(1+1/n_k)$.

Chapter 4 was utilized to introduce the techniques required to study particle production in more a realistic situation. A naive definition of particles utilizing the instantaneous Minkowski vacuum (the zeroth-order WKB approximation) leads to ultraviolet divergences that render quantities such as the particle number density and the energy density meaningless. To overcome this problem, we introduced the method of adiabatic regularization, constructing an adiabatic vacuum order by order via the WKB approximation. The basic idea is to use this adiabatic vacuum of Ath order as a reference state. The Bogoliubov coefficient $\beta_k^{(A)}$ obtained from the

Wronskian between the exact mode solutions and the adiabatic modes is then free of ultraviolet divergences.

Chapter 5 is the core of this dissertation. We applied the adiabatic regularization scheme to a massive, conformally coupled scalar field in four-dimensional de Sitter spacetime. After reviewing the geometry of de Sitter and the properties of the Bunch–Davies vacuum, we computed numerically the regularized particle number per mode for several masses. The spectra (Figure 5.3) exhibit the expected ultraviolet decay. For the critical mass $m = H/2$, we observed a logarithmic infrared divergence, while for the heavy mass $m = H$, the occupation number saturates to a finite constant.

The most notable result arose from the effective temperature analysis. For $m = H$, the super-horizon value of T_{eff} numerically approaches a constant that is identified with the de Sitter horizon temperature $T_{\text{dS}} = H/(2\pi) \approx 0.159$, where $H = 1$. This indicates that for this specific mass, the occupation numbers obtained from the adiabatic regulariation scheme match those of a thermal Bose–Einstein distribution at the Gibbons–Hawking temperature. In contrast, for the critical mass $m = H/2$, the effective temperature diverges logarithmically as $-k\eta \to 0$.

6.1 Limitations and Future Directions

Several limitations of the present work should be pointed out, each leading to possible directions for future research.

1. **Backreaction**:
   Throughout this dissertation, we have neglected the backreaction of the created particles on the spacetime geometry. In principle, the energy density $\langle T_{00} \rangle$ computed from regularized modes (of fourth-adiabatic order) could be used as a source in the semiclassical Einstein equations, modifying the expansion history. This would be particularly relevant in modern cosmological models, during the later stages of inflation or during reheating.

2. **Interacting Fields**:
   We have considered only a free scalar field. Interactions introduce additional channels for particle production [69] and could modify the diagonal entropy through collisional processes. A systematic study of interacting fields in de Sitter would be a natural next step.

3. **Fluctuation theorems**:
   The diagonal entropy satisfies a number of properties expected from a thermodynamic entropy, but it would be desirable to connect it directly with non-equilibrium fluctuation theorems. For instance, one could investigate whether the probability distribution of the work done by the expansion satisfies a Crooks relation [70] or a Jarzynski equality [71], with the diagonal entropy playing the role of the entropy production. In this direction, reference [72] provides a formulation of work distributions for scalar fields, contemplating static curved spacetimes.

Appendix A

Fundaments of General Relativity

A.1 Tensor Densities

In general relativity, physical quantities must be expressed in a form that remains invariant under arbitrary coordinate transformations. For integrals over spacetime, this requires identifying an appropriate volume element that transforms in such a way that the entire integral behaves as a scalar.

A **tensor density** of weight w is an object that, under a coordinate transformation $x^\mu \to x^{\mu'}$, transforms as:

$$T^{\mu'\nu'\dots}{}_{\alpha'\beta'\dots} = \left|\frac{\partial x'}{\partial x}\right|^w \frac{\partial x^{\mu'}}{\partial x^\mu}\frac{\partial x^{\nu'}}{\partial x^\nu}\dots\frac{\partial x^\alpha}{\partial x^{\alpha'}}\frac{\partial x^\beta}{\partial x^{\beta'}}\dots T^{\mu\nu\dots}{}_{\alpha\beta\dots}, \tag{A.1}$$

where $|\partial x'/\partial x|$ is the determinant of the Jacobain of the transformation. Ordinary tensors corresponds to the weight $w = 0$, while tensor densities carry an additional factor that compensates for the Jacobian determinant.

We give special attention to the metric tensor. Its determinant $g = \det\{g_{\mu\nu}\}$ transforms, under coordinate transformations as

$$g' = \left|\frac{\partial x}{\partial x'}\right|^2 g, \tag{A.2}$$

so that $\sqrt{-g}$ behaves as a scalar density of $w = +1$:

$$\sqrt{-g'} = \left|\frac{\partial x}{\partial x'}\right|\sqrt{-g}. \tag{A.3}$$

This property makes the quantity $d^4x\sqrt{-g}$ invariant under coordinate transformations:

$$d^4x'\sqrt{-g'} = d^4x\sqrt{-g}. \tag{A.4}$$

Therefore, when integrating scalar quantities over curved spacetime, the invariant measures must include $\sqrt{-g}$:

$$\int d^4x\sqrt{-g}f(x). \tag{A.5}$$

This combination ensures that the integral defines a scalar independent of the coordinate system.

A.2 Maximally Symmetric Spaces

It is assumed that the universe is homogeneous and isotropic on large scales in *space*. This, in turn, leads to the statement that it is possible to foliate the universe into spacelike three-dimensional hypersurfaces, where each of these hypersurfaces exhibits maximal symmetry. Before describing the FLRW metrics in the next appendix, we will first review the main features of these maximally symmetric spaces.

A maximally symmetric space is a space that possesses the largest possible number of independent isometries, that is, symmetries under coordinate transformations that leave the metric invariant. In n dimensions, the maximal number of linearly independent Killing vectors is

$$N_{max} = \frac{n(n+1)}{2}. \tag{A.6}$$

This corresponds to the number of parameters that characterize the group of rigid motions (translations and rotations) in flat space. A space that achieves this upper bound is called maximally symmetric.

These spaces are also characterized by constant curvature: their Riemann tensor takes the specific form

$$R_{\mu\nu\rho\sigma} = \frac{R}{n(n-1)}(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho}), \tag{A.7}$$

where R is the scalar curvature. It follows that the Ricci tensor and scalar curvature satisfies:

$$R_{\mu\nu} = \frac{R}{n}g_{\mu\nu}, \tag{A.8}$$

$$R = \text{constant}. \tag{A.9}$$

Hence, the geometry of a maximally symmetric space is determined by a unique parameter, that is, the curvature scalar R, or equivalently, by a curvature length L, defined by $R = \pm n(n-1)/L^2$.

The three possible cases corresponds to:

- **Positive curvature** ($R > 0$): corresponds to a spherical geometry;
- **Zero curvature** ($R = 0$): corresponds to a flat geometry;
- **Negative curvature** ($R < 0$): corresponds to a hyperbolic geometry.

A.3 Conformal Transformation

A conformal transformation is a rescaling of the metric tensor by a positive and smooth function of spacetime coordinates. Given a metric $g_{\mu\nu}(x)$, the transformed metric is

$$\tilde{g}_{\mu\nu}(x) = \Omega^2(x) g_{\mu\nu}(x), \tag{A.10}$$

is said to be *conformally related* to the original metric $g_{\mu\nu}$. The scalar function Ω is called the **conformal factor**.

Conformal transformations preserve the structure of angles of the spacetime defined by $g_{\mu\nu}$. This property makes conformal transformations very useful in cosmology and in quantum field theory in curved spacetime, where the physical effects of spacetime expansion can often be separated from purely geometric scaling factors.

In practice, many metrics of interest, including the FLRW metrics, can be written in a conformally flat form, i.e.

$$ds^2 = \Omega^2 \eta_{\mu\nu} dx^\mu dx^\nu, \tag{A.11}$$

where $\eta_{\mu\nu}$ is the Minkowski metric.

This representation makes it easier to study field propagation, because conformally flat invariant field equations take the same form as in flat spacetime, up to the scaling by the conformal factor.

When the conformal factor depends only on time, we can introduce a new time coordinate, the **conformal time** η, defined such that the metric appears explicitly conformally flat. For instance, the line element of an spatially flat FLRW universe, when conformal time is introduced, is written as

$$ds^2 = a^2(\eta)(-d\eta^2 + dx^2 + dy^2 + dz^2). \tag{A.12}$$

Appendix B

Some Mathematical Derivations

B.1 Time Independence of the Particle Number Density in de Sitter Space

In the Poincaré patch of de Sitter space, the scale factor in terms of conformal time is given by $a(\eta) = -1/(H\eta)$, where $\eta \in (-\infty, 0)$. The fundamental quantum operator defining the particle number expectation value is the Bogoliubov coefficient $|\beta_k(\eta)|^2$.

To evaluate the time dependence of the physical observables, we must first establish the functional dependencies of $|\beta_k(\eta)|^2$. The exact mode solution for the Bunch-Davies vacuum is governed by the Hankel function $H_\nu^{(1)}(-k\eta)$. Similarly, the n-th order adiabatic frequency $W_k^{(n)}$ and its temporal derivatives are constructed from the zeroth-order frequency ω_k:

$$\omega_k = \sqrt{k^2 + \frac{m^2}{H^2\eta^2}} = \frac{1}{|\eta|}\sqrt{(-k\eta)^2 + \frac{m^2}{H^2}}. \tag{B.1}$$

By defining the dimensionless physical momentum $x = -k\eta$, we observe that ω_k factors into an overall amplitude $1/|\eta|$ and a pure function of x and the mass-to-Hubble ratio m/H. When substituting these exact modes and the adiabatic reference states into the absolute square of the Wronskian condition, the explicit $1/|\eta|$ and $\sqrt{-\eta}$ amplitude scalings divide out completely. Consequently, the Bogoliubov coefficient does not depend on k and η independently, but is strictly scale-invariant:

$$|\beta_k(\eta)|^2 = F(-k\eta) = F(x) \tag{B.2}$$

The regularized physical particle number density is defined by integrating the momentum distribution over all comoving modes and dividing by the physical volume:

$$n(\eta) = \frac{1}{2\pi^2 a(\eta)^3}\int_0^\infty dk k^2 |\beta_k(\eta)|^2. \tag{B.3}$$

To evaluate the time evolution of this density, we perform a change of variables from the comoving wavenumber k to the dimensionless physical momentum $x = -k\eta$. Since η is strictly negative in the expanding patch, we have $k = x/|\eta|$ and $dk = dx/|\eta|$. The integration limits remain $[0, \infty)$.

Substituting this transformation and the scale factor $a(\eta) = 1/(H|\eta|)$ into the density integral yields

$$n(\eta) = \frac{1}{2\pi^2 \left(\frac{1}{H^3|\eta|^3}\right)} \int_0^\infty \left(\frac{dx}{|\eta|}\right) \left(\frac{x}{|\eta|}\right)^2 F(x), \tag{B.4}$$

which can be simplified to

$$n(\eta) = \frac{H^3}{2\pi^2} \int_0^\infty dx x^2 F(x), \tag{B.5}$$

proving that the physical density is in equilibrium; the constant curvature of de Sitter space (defined by the Ricci scalar $R = 12H$) excites the quantum field, creating particles at the exact rate necessary to "counter" the exponential volumetric expansion.

B.2 Time independence of the Entropy Density in de Sitter Space

While the particle density $n(\eta)$ is a constant of motion, the macroscopic thermodynamic irreversibility of the system is governed by the total diagonal entropy. The physical diagonal entropy density $s_d(\eta)$ is obtained by integrating the entropy per mode $S_d^{(k)}$ over the phase space, as follows:

$$s_d(\eta) = \frac{1}{2\pi^2 a(\eta)^3} \int_0^\infty dk k^2 S_d^{(k)}(\eta). \tag{B.6}$$

Because the entropy per mode $S_d^{(k)}$ is constructed exclusively from the scale-invariant Bogoliubov coefficient $|\beta_k|^2$, it is also strictly a function of x. Applying the identical change of variables $x = -k\eta$ yields the exact same cancellation of $|\eta|^3$:

$$s_d(\eta) = \frac{H^3}{2\pi^2} \int_0^\infty dx x^2 S_d(x) = \text{constant}. \tag{B.7}$$

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