#### ENTANGLEMENT ENTROPY OF COSMOLOGICAL PERTURBATIONS

WRITTEN BY

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### Abstract

This thesis summarizes our work on the entanglement entropy of cosmological perturbations. The purpose of this work is to connect and build upon progress in momentum space entanglement in quantum field theory, open quantum cosmological systems, the decoherence of primordial fluctuations in the early universe and the entropy of gravitational perturbations arising from a squeezed super-Hubble vacuum state. We discuss the origin of this entropy from gravitational nonlinearities and mode-couplings arising from quantum vacuum fluctuations. We demonstrate that the entropy of scalar cosmological perturbations can be viewed as momentum space entanglement entropy between sub- and super-Hubble modes. We calculate this entropy in a specific cosmological model, the inflationary universe. We find an upper bound on the duration of inflation to allow for a graceful exit consistent with the second law of thermodynamics.

### Abrégé

Cette thèse résume nos travaux sur l'entropie d'intrication quantique des perturbations cosmologiques. Le but de ce travail est de bâtir sur les récents progrès sur l'entropie d'intrication quantique et la théorie des champs pour les appliquer dans un context cosmologique, ou plus précisément sur les fluctuations cosmologique. Nous discutons de l'origine de cette entropie à partir des non-linéarités gravitationnelles et des couplages de modes résultant des fluctuations du vide quantique. Nous démontrons que l'entropie des perturbations cosmologiques scalaires peut être considérée comme une entropie d'intrication de l'espace cinétique entre les modes sous-et super-Hubble. Nous calculons cette entropie dans un modèle cosmologique spécifique, l'univers inflationnaire. Nous trouvons une limite supérieure sur la durée de l'inflation pour permettre une sortie gracieuse compatible avec la deuxième loi de la thermodynamique.

### Statement of contribution

This manuscript-based thesis introduces, contextualizes and builds up to a research paper, an original article currently under review. We state the contribution of the writer in the publication of the following.

S. Brahma, **O. Alaryani** and R. Brandenberger, "Entanglement entropy of cosmological perturbations," arXiv:2005.09688v2 [hep-th] (2020). Ref. [1] in the bibliography.

As co-author, my contributions include a survey of the literature, engaging in periodic discussions, reproducing and reviewing calculations that helped form the basis of the project.

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### Preface

This work expresses an initial curiosity in the intersection of quantum information theory and physical cosmology. We begin with an outline of the scope and structure of this thesis.

The first chapter reviews the fundamentals. We use a result from the general theory of relativity to introduce big bang cosmology, we explore the framework's predictions and shortcomings. Upon setting the stage for a paradigm shift connecting observations to the universe's quantum mechanical origin, we introduce inflationary cosmology. We briefly review the quantum-to-classical transition of fluctuations in the early universe, the theory of cosmological perturbations and the concept of entanglement entropy.

The second chapter connects topics we reviewed. We discuss reheating, a period of massive entropy generation, and the evolution of scales in the quantum theory of cosmological perturbations. We build-up a conceptual understanding of the *entanglement entropy of cosmological perturbations*.

The third chapter is our research paper. The article opens with motivation. We review that interactions suppress off-diagonal terms in the density matrix for our system, the super-Hubble modes. We calculate the entropy of cosmological perturbations due to the squeezing of the vacuum state of super-Hubble modes during inflation. We compute the entanglement entropy for super-Hubble modes and show that it is greater than the entropy for the squeezed vacuum. We require that the entanglement entropy is smaller than the thermal entropy after inflation. We conclude with a discussion of our findings.

The fourth chapter reviews this work and ends with closing remarks.

Figures include sketches from a variety of sources repurposed in a manner consistent in style and notation, omitting non-essential information. The Appendix includes all original figures and captions cited in this work.

### Chapter 1

### Background

Cosmology is the study of our universe at its grandest scales, in space and time. We begin our review of modern cosmology by introducing the foundation stone this field is built upon, the *cosmological principle*.

"There is nothing special, cosmologically, about the Earth; therefore our large-scale observations are the same as those which would be made by observers anywhere else in the universe." [2]

To set the stage for some physics, we introduce a system of coordinates.

"We consider the universe as a cosmic fluid whose atoms are galaxies. How can we get our bearings in such a fluid? Our time coordinate t is the proper time, measured by standard clocks falling freely with the fluid. These clocks lie at the intersection of the grid of spatial coordinate lines. Thus the coordinate grid is expanding with the galaxies, just as grid lines drawn on a rubber balloon expand as it is blown up. These coordinates which share in the expansion of the universe are described as comoving coordinates." [2]

Observations support the simplifying assumption that small-scale disparity in energy density are averaged out; the universe looks the same in every direction. A comoving observer sees the same at every point, in all-directions. We say that space exhibits translation and rotation invariance at cosmological scales. These symmetries allow us to study a universe that is *homogeneous* and *isotropic*.

#### 1.1 Standard "Big Bang" Cosmology

Spatial homogeneity, isotropy and expansion of a topologically flat space, allow us to write the metric of spacetime representing the simplest model of cosmology in comoving coordinates.

$$ds^2 = -dt^2 + a(t)^2 dx^2$$
(1.1)

This Friedmann-Lemaître-Robertson-Walker (FLRW) metric describes a uniformly growing separation of spatial coordinates, scaled by a function of time a(t), the scale factor. The flat FLRW metric describes our universe today at large distance scales. As the universe expands, the scale factor governs the growth of physical distance and correspondingly scales the comoving separat between any two points. We relate physical and comoving spatial separations as follows.

$$\Delta \boldsymbol{x}_{physical} = a(t)\Delta \boldsymbol{x} \tag{1.2}$$

We describe the dynamics of an evolving universe by studying this metric, as a solution to the Einstein equation. First, we approximate the matter in our universe as a perfect fluid, whose stress tensor will follow. The stress tensor relates the energy and pressure density with the four-velocity and the metric.

$$T_{\mu\nu} = (p+\rho)U_{\mu}U_{\nu} + pg_{\mu\nu}$$
  
$$\implies T^{\mu}_{\nu} = diag(-\rho, p, p, p)$$
(1.3)

Denoting a physical time derivative with an over-dot, we define the *Hubble parameter*.

$$H \equiv \frac{\dot{a}}{a} \tag{1.4}$$

To use the Einstein equation, one must compute the Einstein tensor, we state its relevant components to derive the *Friedmann equations*.

$$G_{tt} = 8\pi G T_{tt}$$

$$\implies H^2 = \frac{8\pi G}{3}\rho$$
(1.5)

The time component of the Einstein equation reveals the first Friedmann equation. The spatial component of the Einstein equation, combined with the first Friedmann equation

=

presents the second Friedmann equation.

$$G_{ii} = 8\pi G T_{ii}$$

$$\implies (\frac{\ddot{a}}{a}) = -\frac{4\pi G}{3}(3p+\rho)$$
(1.6)

The Friedmann equations are equations of motion of an expanding universe. They allow us to support insightful predictions punctuating the narrative of universal evolution.

Next, taking the time derivative of the first Friedmann equation and using the second Friedmann equation allows us to the evolution of energy density as a function of energy, pressure density and the Hubble parameter.

$$\dot{\rho} = -3H(\rho + p) \tag{1.7}$$

This is the *continuity equation* which limits the transfer of energy to a continuous flow governed by the evolution of the scale factor. We use the continuity equation to describe the evolution of an ideal gas with the following equation of state.

$$p = w\rho \tag{1.8}$$

Dust, defined as cold pressure-less matter, is described purely by an energy density  $\rho_m$ , where the equation of state parameter w = 0. The continuity equation produces an expression to describe the evolution of the energy density associated with dust,  $\rho_m \sim a^{-3}(t)$ . Similarly, we can determine the evolution of different forms of energy density, such as radiation with  $\rho_{rad} \sim a^{-4}(t)$  and dark energy, with  $\dot{\rho}_{DE}(t) = const$ . Studying the evolution of the energy density reveals distinct periods in the universe's evolution where the dominant form of energy density changes. These are summarized in the following figure. We denote the time of equal matter and radiation,  $t_{eq}$ .



Figure 1.1: The radiation-, matter- and dark energy-dominated epochs.

From Hubble's prediction of an expanding universe, to today's wealth of data from observations, evidence has established that the universe is growing. Evolving our model of the universe backwards in time reveals that physical separations were smaller in the past. Physical laws require the conservation of the mass-energy content of the universe. The energy density of the universe must have been compressed into a primordial soup of plasma. This is *standard "big bang" cosmology*. Standard cosmology did not stand up to scrutiny, we now demonstrate some of its shortcomings. A problem in the evolutionary history proposed by standard cosmology, is a discrepancy made clear with the observation of the *cosmic microwave background* (CMB). The following figure [3] compares a (blue) past light cone of current observations and a (red) forward light cone from the frame of the CMB, inferred from standard cosmology. The light cones fail to overlap. Standard cosmology fails to explain why causally disconnected patches demonstrate temperature fluctuations about the same mean. This is the *horizon problem*.



Figure 1.2: A spacetime diagram depicting the horizon problem.

Density fluctuations in the early universe can be viewed as energy *over-densities* and *under-densities*, relative to the mean. This picture implies the existence of a gravitational potential gradient, sustaining an accretion of matter. Density fluctuations and the action of gravity, build a hierarchy where the rich in energy density get richer, and the poor get poorer. Eventually, slight energy over-densities, by virtue of their initial condition, seed full-fledged galaxy clusters. This is the *theory of cosmological structure formation*.

At large scales, there exist non-random correlations between galaxies. Density perturbations produced before the time of equal matter and radiation, are unexplained by a causal mechanism in standard big bang cosmology. At the time of equal matter and radiation  $t_{eq}$ , marking a significant energy scale in theories of structure formation, we compare the comoving distance between two galaxies  $\Delta Gal$ . and the comoving light cone between them  $l_c(t_{eq})$ . The comoving light cone between the galaxies is the Hubble radius (the inverse of the Hubble parameter in natural units), at the time of equal matter and radiation. The dissonance is demonstrated in the following figure [4]. We note  $\Delta Gal. > l_c(t_{eq})$ . Therefore, the formation of structure is not sufficiently explained by standard cosmology. This is the structure formation problem.



Figure 1.3: A spacetime diagram depicting the structure formation problem.

Precise observations of the CMB demonstrate that the universe is close to flatness today. Standard cosmology claims this means it was much closer to flatness earlier in its history. Let us study why this is the case, and why a flat universe is at a repulsive fixed point in a radiation- or matter-dominated epoch. Using the first Friedmann equation, we describe the evolution of an expanding universe, regardless of its curvature, as follows.

$$H^2 + \epsilon T^2 = \frac{8\pi G}{3}\rho \tag{1.9}$$

Where  $\epsilon = \frac{k}{(aT)^2}$  and k describes the curvature of the topology. k = 0 represents a flat universe with a critical energy density  $\rho_c$ , defined as follows.

$$\rho_c = \frac{3H^2}{8\pi G} \tag{1.10}$$

In standard cosmology with conserved total entropy, the quantity  $\epsilon$  is constant. We observe the following.

$$\frac{\rho - \rho_c}{\rho_c} = \frac{3}{8\pi G} \frac{\epsilon T^2}{\rho_c} \sim \frac{1}{T^2} \tag{1.11}$$

As temperature increases, the curvature approaches flatness. We observe a small deviation from flatness today meaning the universe must have been extremely close to flat in the past. At high temperatures, say  $T = 10^{15} GeV$ , the energy density would have been extremely close to the critical density.

$$\frac{\rho - \rho_c}{\rho_c} \sim 10^{-50}$$
 (1.12)

Standard cosmology requires an unstable initial condition with very little curvature. This is the *flatness problem*.

The horizon, flatness and structure formation problems with standard cosmology motivated an altered retelling of the narrative, one that entails a period of accelerated expansion, the current paradigm of theoretical cosmology.

#### 1.2 Inflation

Inflation is a growth spurt, where the geometry of spacetime undergoes an all but immediate transition from the minute scales of quantum mechanics to the astronomical proportions governed by the general theory of relativity. Let's read this spacetime diagram [4] chrono-



Figure 1.4: A spacetime diagram depicting how inflation maintains causality.

logically, following the forward light cone,  $l_f(t)$ . In the beginning, space expands uniformly until standard cosmological evolution is modified, the expansion of space grows rapidly, this is the advent of inflation. This rush of growth is short-lived. The brakes are pulled and the original pace of universal expansion is restored. This transition entails the conversion of the field driving inflation into observable standard model fields, warming up the universe once again — this is called *reheating*. Next, charged particles are bound into electrically neutral atoms — this is called *recombination*. Hydrogen atoms, fresh from the oven, settle into stable energy states. At this point, matter is sparse enough for the free streaming of light toward us. That is to say, the mean free path of light is at least the size of the observable universe. Our act of looking back today, is depicted by the past light cone  $l_p(t)$ . Inflationary cosmology connects observations with a narrative of universal evolution from a primordial soup of plasma — saving the original big bang theory.

Inflation requires a special form of matter described by an equation of state parameter w = -1, This corresponds to a period where the universe becomes *vacuum-dominated*. This is captured by the *de Sitter solution* to the equations of general relativity. This is a space where the density of matter and radiation fall, as the universe expands. We further require that inflationary expansion last 60 *e-folds*, where the number of e-folds is  $N = \Delta \ln a$ . This constraint on the scale factor, solves the horizon problem [3].

Vacuum energy comes from the potential of a scalar field  $\phi$ , the *inflaton*. We write equation of motion of a scalar field, in a maximally-symmetric spacetime evolving in size as follows. Over-dots denote derivatives with respect to physical time t, the prime denotes a derivative with respect to  $\phi$  and V is the potential of the scalar field.

$$\ddot{\phi} + 3H\dot{\phi} + V'(\phi) = 0 \tag{1.13}$$

Our evolving universe exhibits accelerating expansion if the inflaton's potential energy exceeds its kinetic energy, and the second derivative of  $\phi$  is sufficiently small. To be precise, we require the following.

$$\dot{\phi}^2 \ll V(\phi) \tag{1.14}$$
$$|\ddot{\phi}| \ll |3H\dot{\phi}|, |V'|$$

These conditions are satisfied if we require that the following *slow-roll* parameters are sufficiently small. Here  $\bar{m}_p = (8\pi G)^{-1/2}$  is the reduced Planck mass.

$$\epsilon = \frac{\bar{m}_p^2}{2} \left(\frac{V'}{V}\right)^2$$

$$\eta = \bar{m}_p^2 \left(\frac{V''}{V}\right)$$
(1.15)

These conditions ensure the inflaton *slowly rolls down a potential*. Furthermore, we use the inflaton energy density to describe the evolution of the scale factor by rewriting the first Friedmann equation.

$$H^{2} = \frac{1}{3\bar{m}_{p}^{2}} (\frac{\dot{\phi}^{2}}{2} + V(\phi))$$
(1.16)

We visualize the evolution of the inflaton in the following figure.



Figure 1.5: The inflaton evolves like a ball rolling down a hill.

Next, we take a closer look at how quantum fluctuations transition into the domain of classical physics in inflationary cosmology.

### **1.3** Quantum-to-Classical Transition of Fluctuations in the Early Universe

"According to the inflationary scenario, all inhomogeneities in the universe are of genuine quantum origin" [5].

Today, we do not explicitly notice quantum mechanical properties imprinted in cosmological observations. We list two properties demonstrating the transition of fluctuations from the quantum to the classical.

- 1. The quantum state for metric perturbations produced in the early universe becomes highly squeezed, as the universe expands ( $\lambda_{perturbations} > H^{-1}(t)$ ). A squeezed quantum state exhibits less fluctuations of one variable (and a compensatory increase in fluctuations of its complement). A highly squeezed state is one where the uncertainty is minimized for one variable (and maximized for its complement), while maintaining Heisenberg's uncertainty principle [6].
- "Decoherence through the environment distinguishes the field amplitude basis as being the pointer basis". Therefore, perturbations are rendered indistinguishable from classical inhomogeneities.

We observe that quantum fluctuations of a scalar field and scalar fluctuations in the metric of spacetime grow into observable anisotropies in the cosmic microwave background. These points will be revisited in the coming sections, including our next discussion.

#### 1.4 Theory of Cosmological Perturbations

The theory of cosmological perturbations is a framework linking theoretical models of the early universe and state-of-the-art observations. The following figure depicts the evolution of energy scales.



Figure 1.6: Evolution of scales in inflationary cosmology.

The Hubble radius is fixed during inflation. A fixed comoving length scale (with wavenumber k) grows exponentially during inflation. Perturbations in the metric of spacetime come in three flavours: scalar, vector and tensor perturbations. We consider linearized scalar perturbations. We study their coupling with matter, for independent Fourier modes. In our work, we follow perturbations for a particular mode in two domains, *sub-Hubble* and *super-Hubble*. These are characterized in the following figure.

	sub-Hubble	Super-Hubble
<u>Definition</u>	$k/a \geq H(t), \ \lambda \leq H^{-1}(t)$	$k/a < H(t), \ \lambda > H^{-1}(t)$
<u>Origin</u>	Bunch-Davies Vacuum	Growth of sub-Hubble modes during inflation
<u>Analysis</u>	Quantum field theoretic	General Relatvistic

Figure 1.7: Metric perturbations as sub- and super-Hubble.

In our review of the quantum theory of cosmological perturbations, we follow a comoving mode in its transition between sub- and super-Hubble domains [7].

- 1. Sub-Hubble fluctuations originate, mode by mode, in their quantum vacuum state, at the advent of inflation.
- 2. As spatial separations grow exponentially, the length scale of fluctuations grows more rapidly than the fixed Hubble radius. When the Hubble radius matches the length scale of fluctuations, perturbations *freeze out*.
- 3. Fluctuations propagate on super-Hubble scales until *re-entering* the Hubble horizon at late cosmological times.
- 4. On larger scales, the amplitude  $v_k$  increases as the scale factor. This corresponds to the squeezing of the quantum state, at Hubble radius crossing. As the quantum vacuum state is squeezed, fluctuations manifest an observable, classical nature.

Let's elaborate. We begin with the equation of a free scalar matter field  $\varphi$  in in an unperturbed expanding background.

$$\ddot{\varphi} + 3H\dot{\varphi} - \frac{\nabla^2}{a^2}\varphi = 0 \tag{1.17}$$

The spatial gradient term dominates on sub-Hubble scales. The solution to the equation of motion describes oscillation of sub-Hubble fluctuations. Consider the Einstein-Hilbert action for gravity with our free scalar matter field, here g is the determinant of the metric of spacetime.

$$S = \int d^4x \sqrt{-g} \left[ -\frac{1}{16\pi G} R + \frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi - V(\varphi) \right]$$
(1.18)

In a fixed, longitudinal gauge, the metric and matter perturbations take the following form.

$$ds^{2} = a^{2}(\eta) \left[ (1 + 2\phi(\eta, \mathbf{x}))d\eta^{2} - (1 - 2\psi(t, \mathbf{x}))d\mathbf{x}^{2} \right]$$
  

$$\varphi(\eta, \mathbf{x}) = \varphi_{0}(\eta) + \delta\varphi(\eta, \mathbf{x})$$
(1.19)

In the hopes of reducing the degrees of freedom, the author of [7] notes that the free scalar matter field has no anisotropic stress at linear order, thus  $\psi = \varphi$ . Next, they determine a variable v in terms of which the action can be written in canonical form. We summarize their result.

$$S^{(2)} = \frac{1}{2} \int d^4x \left[ v'^2 - v_{,i}v_{,i} + \frac{z''}{z}v^2 \right]$$
(1.20)

Where the *Mukhanov variable*, v, is defined as follows.

$$v = a \left[ \delta \varphi + \frac{\varphi_0'}{\mathcal{H}} \phi \right] \tag{1.21}$$

Where  $\mathcal{H} = \frac{a'}{a}$  is the comoving Hubble parameter, implying that the prime denotes a derivative with respect to conformal time and  $z = \frac{a\varphi'_0}{\mathcal{H}}$ . Thus, they present the equation of motion following the action in canonical form in terms of the variable  $v_k$ , the  $k^{th}$  Fourier mode of v.

$$v_k'' + k^2 v_k - \frac{z''}{z} v_k = 0 (1.22)$$

The mass term in this equation of motion is given by the Hubble scale, as follows.

$$k_H^2 \equiv \frac{z''}{z} \simeq H^2 \tag{1.23}$$

The time-dependence of the mass leads to the propagation and growth of cosmological perturbations. For sub-Hubble perturbations,  $k > k_H$ , the solutions for  $v_k$  are constant amplitude oscillations. These oscillations freeze out at Hubble radius crossing,  $k = k_H$ . At super-Hubble scales,  $k \ll k_H$  the solutions for  $v_k$  increase as z.

We further develop this discussion in the second chapter. In the next section, we shift gears, pausing our discussion of cosmology.

#### 1.5 Entanglement Entropy

The axioms of quantum mechanics hold for a closed system, one that does not interact with its surroundings. When considering an interacting, open quantum system, they break down as follows.

"States are not rays in a Hilbert space. Measurements are not orthogonal projections. Evolution is not unitary." [8]

Consider a bipartite quantum system: a closed quantum mechanical system where two open sub-systems A and B interact. We decompose the closed system's Hilbert space into two corresponding spaces of states.

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \tag{1.24}$$

Given a state of the full system  $|\psi\rangle \in \mathcal{H}$ , we ask: What is the state of sub-system A? Can one use knowledge of the closed system to find the state of an open sub-system, i.e.  $|\psi^A\rangle \in \mathcal{H}_A$ ? [9]

The challenge in describing the state of sub-system A is that its state is correlated with that of its complement, sub-system B. The correlation, or mixing, of states between two open sub-systems is *quantum entanglement*.

We capture the states of a quantum system in its density matrix  $\rho$ , defined by the following outer product.

$$\rho = |\psi\rangle\langle\psi| \tag{1.25}$$

To fully describe the states of a sub-system, one accounts for an ensemble of orthogonal states  $|\psi_i^A\rangle$ , weighted by probabilities  $p_i$ . The density matrix of sub-system A,  $\rho_A$ , is defined as follows.

$$\rho_A = \sum_i p_i |\psi_i^A\rangle \langle \psi_i^A| \tag{1.26}$$

The density matrix of a bipartite system can reveal the states of one sub-system when it is *reduced*. The reduced density matrix of system A can be defined by *tracing over* the states of the other sub-system.

$$\rho_A \equiv T r_B \rho \tag{1.27}$$

Armed with the reduced density matrix, we define the entropy of a bipartite system. For a system, described by an ensemble of states, we consider the *Von Neumann entropy*.

$$S \equiv -\sum_{i} p_i \log p_i = -Tr(\rho_A \log \rho_A)$$
(1.28)

Now, we relate quantum entanglement and the Von Neumann entropy.

- 1. A system with one possible state occupies that state with unit probability. Knowing a system's state with certainty implies no ignorance, no entropy. A closed quantum system does not interact. It could exist in a pure state, without entanglement.
- 2. Quantum entanglement correlates the states of interacting quantum sub-systems. The entropy, as a measure of classical uncertainty, arises from the mixed nature of an interacting quantum sub-system.
- 3. Through interactions, open quantum sub-systems, become entangled. We identify an uncertainty in the state of a sub-system, upon its interaction with another. Thus the degree of uncertainty due to quantum entanglement is captured by the Von Neumann entropy. The entropy of the reduced density matrix of sub-system A, is also the entanglement entropy of A.

In our work, we consider entanglement in momentum-space between sub- and super-Hubble modes. We aim to describe the states of super-Hubble modes by tracing over the space of sub-Hubble modes. Next, we bring the elements of this review together.

### Chapter 2

### **Problem Setup**

In order to setup the problem, we further develop elements from the Background to explain what we mean by the entanglement entropy of cosmological perturbations. First, we resume our discussion of inflationary cosmology. The next phase of universal evolution is one of massive entropy production. Afterwards, we revisit our discussion of cosmological perturbations while framing the interactions between sub- and super-Hubble modes as quantum entanglement. Here we aim to bridge the basics with our research paper.

#### 2.1 Reheating

In inflationary cosmology, entropy is generated in a phase that restores heat after the universe's *super-cooled* expansion, this is *reheating*. Let's take a closer look at entropy during and after inflation.

1. Consider an inflating patch. As the patch grows exponentially, its temperature falls exponentially.

$$T \propto \exp\left(-Ht\right) \tag{2.1}$$

This is a period of super-cooling. If our inflating patch is a closed system, then our first guess is that the total entropy remains fixed.

2. The entropy per comoving volume, the *entropy density*, of our inflating patch falls as its temperature.

$$s \propto T^3,$$
 (2.2)

where the initial volume of the patch is  $H^{-3}$ .

3. After inflation, the inflaton decays into standard model fields, producing heat, and with it entropy.

$$s_f \propto T_{reheating}^3$$
 (2.3)

The entropy  $S_f$  after inflation in a fixed comoving volume is larger than the initial entropy at the onset of inflation by a factor of  $exp(3H\Delta t)$ , where  $\Delta t$  is the duration of inflationary expansion and we have assumed reheating is efficient, that temperature after inflation is only slightly smaller than temperature at the beginning of inflation.

Following similar reasoning, Kolb and Turner estimate that reheating raises the entropy of the universe by  $10^{130}$  [10]. Next, we demonstrate another estimate they present, the extent of the non-adiabatic nature of inflationary cosmology.

In the following figures, we characterize adiabatic growth by a constant product of temperature and the scale factor.



Figure 2.1: The evolution of the scale factor and the temperature in standard cosmology.



Figure 2.2: The evolution of the scale factor and the temperature in inflationary cosmology.

The great production of heat following inflation comes with a rise in entropy. The following figure demonstrates the evolution of entropy in inflation as a function of the scale factor.



Figure 2.3: The evolution of entropy in inflationary cosmology.

Next we look closely at a contribution of this total entropy due to quantum entanglement.

#### 2.2 Crossing the Horizon

Let's recall our discussion of momentum modes in the theory of cosmological perturbations. During inflation the Hubble radius, in physical coordinates, is constant but the comoving Hubble radius falls. Modes that are initially sub-Hubble become super-Hubble. Something interesting happens when the length of the comoving scale matches the Hubble radius, we call this *horizon crossing*. This is demonstrated in the following figure.



Figure 2.4: The physical length of a comoving scale relative to a growing horizon.

Before inflation, sub-Hubble fluctuations oscillate. When the length of a comoving scale matches the Hubble radius, we say that fluctuations *freeze out* [7], this means that oscillations stop. Beyond Hubble radius crossing, the quantum state describing a mode of fluctuation is a squeezed state. At the limit of large squeezing, quantum perturbations become indistinguishable from a classical stochastic process. Squeezing provides a necessary condition for classicalization. This explains our observation of anisotropies in the cosmic microwave background.

Sub- and super-Hubble Fourier modes evolve independently only at first order. At higher order there are cross terms mixing different modes. This is due to the nonlinear nature of Einstein's equations. The modes become entangled. We note that *the environment* (the sub-Hubble modes) *measures a system* (the super-Hubble modes), and this causes a decoherence in the quantum state of cosmological perturbations [11, 12].

Non-linear interactions, lead to a non-vanishing entropy of the density matrix describing the super-Hubble modes. In our work, we aim to compute the entanglement entropy in non-linear interactions between sub- and super-Hubble momentum modes, in an inflationary universe. This is what we mean by the *entanglement entropy of cosmological perturbations*.

### Chapter 3

# Entanglement Entropy of Cosmological Perturbations

#### Abstract

We show that the entropy of cosmological perturbations originating as quantum vacuum fluctuations in the very early universe, including the contribution of the leading nonlinear interactions, can be viewed as momentum space entanglement entropy between sub- and super-Hubble modes. The interactions between these modes causes decoherence of the super-Hubble fluctuations which, in turn, leads to a non-vanishing entropy of the reduced density matrix corresponding to the super-Hubble inhomogeneities. In particular, applying this to inflationary cosmology reveals that the entanglement entropy produced by leading order nonlinearities *dominates* over that coming from the squeezing of the vacuum state unless inflation lasts for a very short period. Furthermore, demanding that this entanglement entropy be smaller than the thermal entropy at the beginning of the radiation phase of standard cosmology leads to an upper bound on the duration of inflation which is similar to what is obtained from the Trans-Planckian Censorship Conjecture.

#### 3.1 Introduction

There has recently been a lot of interest in entanglement entropy in the context of quantum field theory and gravity (see e.g., [15] for reviews). In particular, the entanglement entropy of a conformal field theory is holographically related to properties of the bulk in the context of the AdS/CFT (anti-de-Sitter bulk/conformal field theory on the boundary [16]) correspondence (see e.g., [17]). In the same context, entanglement entropy can be related to properties of black holes in the AdS bulk [18]. The relationship between the bulk Einstein equations and properties of entanglement of the boundary CFT was explored in [19]. Entanglement entropy considerations have also been applied directly to black holes physics (see [20] for a review), and to de Sitter space in [21, 22]. There are also attempts to build up spacetime itself from quantum entanglement [23].

Most considerations of entanglement are based on a position space separation of the domain; for example, the separation between the inside of a black hole and the outside. However, in cosmology it is more natural to work in momentum space because it is the properties of the momentum modes of cosmological fluctuations which are generally probed (such as the power spectrum). Momentum space entanglement has been considered in [24] (see also [25]), and we will use methods from that work extensively.

Entanglement is a crucial, and rather essential, feature of quantum mechanical systems. In many early universe scenarios, the cosmological fluctuations which we measure today are postulated to emerge from quantum vacuum perturbations. This is the case not only in inflationary cosmology [26], but also in the *Ekpyrotic* scenario [27] and in the *matter bounce* scenario [28]. Cosmological perturbations (see *e.g.*, [7, 29] for reviews) are small amplitude fluctuations about the homogeneous and isotropic cosmological background. Because of their small amplitude, the inhomogeneities are generally described in Fourier space. To leading order, each Fourier mode evolves independently, and each mode obeys a harmonic oscillator equation with a time-dependent mass. The Hubble radius  $H^{-1}(t)$  (where *H* is the Hubble expansion rate) plays a key role in the dynamics of the modes: on sub-Hubble scales the canonical fluctuation variable oscillates, while it is squeezed on super-Hubble scales.

Successful early universe scenarios have the common feature that the fluctuation modes

which are probed today in cosmological observations were sub-Hubble in the early universe phase, thus allowing a causal generation mechanism. In the classes of models we consider here, the initial state for the fluctuations is taken to be the quantum vacuum state<sup>1</sup>. When the fluctuation modes exit the Hubble radius, their state becomes a squeezed vacuum state. The Hilbert space of states thus naturally divides into two parts - the super-Hubble mode space  $\mathcal{H}_A(t)$  and the sub-Hubble mode space  $\mathcal{H}_B(t)$ :

$$\mathcal{H}_{A}(t) = \prod \mathcal{H}_{k} |k| < H_{c}(t)$$
  
$$\mathcal{H}_{B}(t) = \prod \mathcal{H}_{k} |k| \ge H_{c}(t)$$
(3.1)

where  $\mathcal{H}_k$  is the harmonic oscillator Hilbert space of the k'th mode and  $H_c^{-1}(t)$  stands for the comoving Hubble radius. It is natural to consider the space of super-Hubble modes to be the system we consider, and the space of sub-Hubble modes to be the bath which we integrate over. Note that the comoving Hubble radius decreases as a function of time in the early universe phase of the models which we consider. This means that modes exit the Hubble radius. Hence, the boundary between the two Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$  depends on time: the dimension of the system Hilbert space is increasing. This is a specific feature of a system on a dynamically expanding background. Furthermore, although not explicitly stated above, we shall assume an ultraviolet (UV) cutoff ( $M_{\rm Pl}$ ) for the bath modes so that there is always a constant supply of modes which we integrate over. We assume that some underlying UV theory is able to provide the details of the dynamics of the modes lying in the range  $k > M_{\rm Pl}$  and shall not consider them in our work.

As mentioned above, in this paper, we consider the entropy of the space of super-Hubble modes which results from the entanglement with the bath of sub-Hubble modes. The question of entropy of cosmological perturbations has been considered previously. For example, in [31–33] the entropy of a classical field was studied, and the results were applied to compute the entropy of cosmological perturbations and gravitational waves in an inflationary universe. In [31–33], the source of entropy can be traced back to the loss of information about the phases of the fluctuations for super-Hubble modes, while a similar calculation for the coherent

<sup>&</sup>lt;sup>1</sup>String gas cosmology [30] does not fit into this class since there the initial fluctuations are taken to be thermal.

state basis was shown in [34]. In [35], the issue of entropy of cosmological perturbations was reconsidered, taking the loss of information which leads to entropy generation to be the loss of information due to the spreading of the wave function of the super-Hubble modes which results from squeezing. Entropy generation as a consequence of coupling to an environment was studied in [36]. In [37], entropy generation of cosmological fluctuations as a consequence of a truncation of the hierarchy of Green's functions was considered.

What was not considered in these previous works on entropy generation is the role of nonlinearities. Because of the nonlinear nature of the Einstein equations, there is always a mixing of modes for cosmological perturbations. In particular, there is a mixing between the sub- and super-Hubble modes. As discussed in [5, 11, 38, 39], this leads to decoherence of the reduced density matrix of super-Hubble modes<sup>2</sup>. This decoherence is crucial in order to explain why the cosmological perturbations become classical even though they have a quantum origin. The resulting density matrix of the super-Hubble modes is no longer that of a pure state, and hence leads to a non-vanishing entropy which we compute in this paper. We stress that, as shall become apparent later on, we calculate a lower bound on the amount of entanglement entropy of scalar density perturbations, produced in any model of inflation, due to the minimal gravitational nonlinearities which must always be present. Additional couplings or fields, or considering interactions between scalar and tensor modes, would lead to enhanced amounts of entropy production.

There are some similarities between our work and that of [44], where decoherence through neglecting observationally inaccessible correlators was considered, and that of [45] where decoherence via entropy field loops was studied (decoherence of fluctuations through entropy loops was considered earlier in [46]). There is also a connection with the work of [47] where super-Hubble entanglement through inflaton decay was considered.

Our notation is as follows: We use natural units in which the speed of light, Planck's constant and Boltzmann's constant are set to one. We consider a spatially flat background

<sup>&</sup>lt;sup>2</sup>See also [40] where the decoherence of super-Hubble modes as a consequence of the interaction with sub-Hubble modes was studied using different techniques, [41] where the decoherence through interaction with gravitational waves was considered, and [42, 43] where decoherence due to coupling to a more general environment was analyzed.

cosmology such that the metric can be written as

$$ds^{2} = -a^{2}(\eta) \left[ d\eta^{2} - d\mathbf{x}^{2} \right], \qquad (3.2)$$

where  $\eta$  is the conformal time which is related to the physical time t via  $dt = ad\eta$ , and **x** are the comoving spatial coordinates. The Hubble parameter is given in terms of the scale factor a(t) by

$$H(t) = \frac{\dot{a}}{a}, \qquad (3.3)$$

where the overdot represents the derivative with respect to t. We emphasize that the Hubble radius plays a crucial role in our analysis. Sub-Hubble modes of the canonical fluctuation variable oscillate while those on super-Hubble scales are squeezed [7, 29]. We denote the Planck mass by  $M_{\rm Pl}$ .

In the next section, we give a first pass at arriving at the entropy of cosmological perturbations due to the squeezing of super-Hubble modes during inflation. In Sec-3.3, we review the well-known argument that interaction between the perturbation modes, arising from minimal gravitational nonlinearities, leads to a suppression of the off-diagonal terms in the density matrix for the super-Hubble modes. This justifies an assumption used in Sec-3.2 for calculating the entropy due to the squeezed state. Finally, having set up our dominant interaction term in Sec-3.3, we go on to calculate the entanglement entropy density for our system (super-Hubble) modes in Sec-3.4. We estimate an order of magnitude for the upper bound of this quantity and show that it is greater than the entropy for the squeezed vacuum, as calculated in Sec-3.2. In Sec-3.5, interestingly we find an upper bound on the duration of inflation by requiring that this entanglement entropy remains smaller than the thermal entropy produced at the end of inflation<sup>3</sup>. We discuss our main findings in Sec-3.6.

<sup>&</sup>lt;sup>3</sup>This bound is similar to the bound obtained [48] by invoking the *Trans-Planckian Censorship Conjecture* (TCC) [49].
## 3.2 Reduced Density Matrix of Super-Hubble Modes

#### 3.2.1 The Squeezed Vacuum

We consider linear scalar cosmological perturbations about the background metric (3.2). Assuming that the matter source of the fluctuations has no anisotropic stress, the perturbations are described by a single field  $\zeta(x,t)$ , the curvature perturbation in comoving gauge. The metric including these fluctuations is

$$ds^{2} = -a^{2}(\eta) \left[ d\eta^{2} - (1+2\zeta) d\mathbf{x}^{2} \right].$$
(3.4)

The action for cosmological perturbations has a canonical kinetic term if we use the rescaled field (we are following the notation of [50])

$$\chi(x,\eta) \equiv z(\eta)\zeta(x,\eta) \tag{3.5}$$

with

$$z^{2}(\eta) \equiv 2 \epsilon_{H} a^{2} M_{pl}^{2} c_{s}^{-2}, \qquad (3.6)$$

where  $\epsilon_H$  is the first "slow-roll" parameter defined via

$$\epsilon_H \equiv -\frac{\dot{H}}{H^2}, \qquad (3.7)$$

and  $c_s^2$  is the speed of sound squared of the matter source. Although, later on, we shall only consider models of single-field inflation with no derivative self-couplings, we are keeping  $c_s \neq 1$  at this stage so that our expressions remain as general as possible<sup>4</sup>.

The linear cosmological perturbations about the classical background geometry can be canonically quantized [26]. We insert the ansatz for the fluctuating metric and matter into the total action (joint gravitational and matter action) and expand to quadratic order. Since at linear order each Fourier mode evolves independently, we can reduce the quantization to the standard quantization of a set of harmonic oscillators, the oscillators having a time dependent mass coming from the time dependence of the background. In terms of the

<sup>&</sup>lt;sup>4</sup>In the case  $c_s = 1$ , the action is  $\int d^4x \frac{1}{2} \left[ (\partial_\mu \chi)^2 - \frac{z''}{z} \chi^2 \right].$ 

usual ladder operators, the quadratic Hamiltonian  $H_2$  corresponding to scalar cosmological perturbations takes the form

$$H_{2} = \frac{1}{2} \int \frac{\mathrm{d}^{3}k}{(2\pi)^{3}} \left[ c_{s}k \left( c_{\mathbf{k}}c_{\mathbf{k}}^{\dagger} + c_{-\mathbf{k}}c_{-\mathbf{k}}^{\dagger} \right) \right] - \frac{1}{2} \int \frac{\mathrm{d}^{3}k}{(2\pi)^{3}} \left[ i \left( \frac{z'}{z} \right) \left( c_{\mathbf{k}}c_{-\mathbf{k}} - c_{\mathbf{k}}^{\dagger}c_{-\mathbf{k}}^{\dagger} \right) \right], \qquad (3.8)$$

where a prime denotes a derivative with respect to conformal time. As can be seen from (3.8), the squeezing term dominates in the limit  $aH \gg c_s k$ , for a given mode. In other words, the time-dependent squeezing interaction is dominant for super-Hubble modes.

This quadratic Hamiltonian generates the following equation of motion for the ladder operators

$$\frac{\mathrm{d}c_{\mathbf{k}}}{\mathrm{d}\eta} = \left(\frac{z'}{z}\right)c_{\mathbf{k}}^{\dagger} - ic_{s}kc_{\mathbf{k}}.$$
(3.9)

Given an initial condition at an instant of time,  $\eta_0$ , we can solve for this as

$$c_{\mathbf{k}}(\eta) = e^{i\theta_{k}(\eta)} \cosh\left[r_{k}(\eta)\right] c_{\mathbf{k}}(\eta_{0}) + e^{-i\theta_{k}(\eta)+2i\phi_{k}(\eta)} \sinh\left[r_{k}(\eta)\right] c_{\mathbf{-k}}^{\dagger}(\eta_{0}) .$$
(3.10)

In the above,  $r_k$  and  $\phi_k$  are the squeezing parameter and the squeezing angle, whereas  $\theta_k$  denotes the action of the rotation operator. The number of particles in a given mode k is proportional to the squeezing parameter  $n_k \sim \sinh^2 r_k$ . For inflation, the leading order time-dependence of these parameters is given by [51]

$$r_k(\eta) = -\sinh^{-1}\left(\frac{1}{2c_s k\eta}\right), \qquad (3.11)$$

$$\phi_k(\eta) = -\frac{\pi}{4} - \frac{1}{2} \tan^{-1} \left(\frac{1}{2c_s k\eta}\right),$$
(3.12)

$$\theta_k(\eta) = -k\eta - \tan^{-1}\left(\frac{1}{2c_s k\eta}\right).$$
(3.13)

Given the quadratic Hamiltonian, the evolution operator  $U_0(\eta)$  can be written as

$$U_{0}(\eta,\eta_{0})|0_{\mathbf{k}},0_{\mathbf{k}}\rangle = S_{k}(\eta)R_{k}(\eta)|0_{\mathbf{k}},0_{\mathbf{k}}\rangle , \qquad (3.14)$$

where  $S_k(r_k, \phi_k)$  and  $R_k(\theta_k)$  are the two-mode squeezing and rotation operators, respectively, which are defined as [51]

$$S_k := \exp\left[\frac{r_k}{2} \left(e^{-2i\phi_k} c_{-\mathbf{k}} c_{\mathbf{k}} - \text{h.c.}\right)\right], \qquad (3.15)$$

$$R_k := \exp\left[-i\theta_k \left(c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}} + c_{-\mathbf{k}}^{\dagger}c_{-\mathbf{k}} + 1\right)\right].$$
(3.16)

At the level of the quadratic Hamiltonian, the  $U_0(\eta)$  is unitary. However, once interaction terms are introduced, the evolution becomes necessarily non-unitary in the presence of bath modes [50]. The effect of the rotation operator is only to change the phase and would be of no consequence to us, and hence we drop it from hereon. The effect of the two-mode squeezing operator on the vacuum leads to the squeezed vacuum, which is defined as

$$|SQ(k,\eta)\rangle \equiv S_k(r_k,\phi_k) |0_{\mathbf{k}},0_{\mathbf{k}}\rangle$$

$$= \frac{1}{\cosh r_k} \sum_{n=0}^{\infty} e^{-2in\phi_k} \tanh^n r_k |n_{\mathbf{k}},n_{\mathbf{k}}\rangle ,$$
(3.17)

where

$$|n_{\mathbf{k}}, n_{\mathbf{-k}}\rangle \equiv \left[\frac{1}{n!} \left(c_{\mathbf{k}}^{\dagger} c_{\mathbf{-k}}^{\dagger}\right)^{n}\right] |0_{\mathbf{k}}, 0_{\mathbf{-k}}\rangle .$$
 (3.18)

For a given mode k, it is easy to see that this state is normalized, as follows:

$$\langle SQ(k,\eta) | SQ(k,\eta) \rangle$$

$$= \frac{1}{\cosh^2 r_k} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} e^{-2i(n-m)\phi_k} \tanh^{(m+n)} r_k \,\delta_{m,n}$$

$$= \frac{1}{\cosh^2 r_k} \sum_{n=0}^{\infty} \tanh^{2n} r_k = 1,$$
(3.19)

as required. The squeezed vacuum of all the modes can be obtained in a straightforward manner as the tensor product state

$$SQ(\eta)\rangle \equiv \prod_{k} |SQ(k,\eta)\rangle$$
 (3.20)

#### 3.2.2 The Reduced Density Matrix

The straightforward definition of the density matrix, corresponding to the squeezed state given in (3.20), is

$$\rho = |SQ(\eta)\rangle \langle SQ(\eta)| . \tag{3.21}$$

If we calculate the entropy corresponding to this state, naturally this is going to be zero since it is a pure state, given by the evolution of the vacuum under the quadratic Hamiltonian (3.8). More concretely, the density matrix expressed in terms of the two-mode occupation number basis reads

$$\rho = \prod_{k} \prod_{p} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{\cosh r_k \cosh r_p} e^{-2i\phi_k(n-m)} \tanh^n r_k \tanh^m r_p \left| n_{\mathbf{k}}, n_{\mathbf{-k}} \right\rangle \left\langle m_{\mathbf{p}}, m_{\mathbf{-p}} \right| , \quad (3.22)$$

which is still a pure density matrix.

Let us show this more explicitly, as follows. Our state can be written as a product state

$$|\psi\rangle = |\psi\rangle_A \otimes |\psi\rangle_B , \qquad (3.23)$$

where  $|\psi\rangle_A$  is the product state of all the super-Hubble modes, and  $|\psi\rangle_B$  over the sub-Hubble modes. Since we are focusing on the super-Hubble modes, our reduced density matrix is obtained by tracing over the sub-Hubble mode Hilbert space.

$$\rho_A \equiv \operatorname{Tr}_B \rho = \sum_j \langle j | \psi \rangle \langle \psi | j \rangle , \qquad (3.24)$$

where the sum is over the basis states of the Hilbert space of sub-Hubble modes. In the absence of entanglement between the sub- and super-Hubble modes, and given that the states of both subsystems are pure, the reduced density matrix  $\rho_A$  also corresponds to that of a pure state and hence has vanishing entropy.

So far, however, we have neglected any coarse graining or nonlinear effects. In particular, we have neglected entanglement effects between sub- and super-Hubble modes which are inevitably present because the equations of gravity are nonlinear. In the following we will take a first look at the entropy of cosmological perturbations after loss of some information about the state. In the following section we then show that this loss of information is an inevitable consequence of the entanglement between sub- and super-Hubble modes.

## 3.2.3 First View on Entanglement Entropy of Cosmological Pertubations

In order to get a non-vanishing von-Neumann entropy of the reduced density matrix  $\rho_A$ , we need to coarse-grain it in a suitable way to derive a mixed density matrix. In [31,32], it was

observed that the phase associated with the squeezing angle is sensitively dependent on the density perturbation whereas the amplitude is not. As a consequence, the coarse-grained entropy in [31, 32] was defined by averaging over the squeezing angle, which also leads to decoherence. In our setup, a similar "averaging" over the squeezing angles would lead to setting the off-diagonal elements to zero in the number basis, leading to a reduced density matrix of the form

$$\rho_{\rm sq} = \prod_{k} \sum_{n=0}^{\infty} \frac{1}{\cosh^2(r_k)} \tanh^{2n}(r_k) \left| n_{\mathbf{k}}, n_{-\mathbf{k}} \right\rangle \left\langle n_{\mathbf{k}}, n_{-\mathbf{k}} \right| \,.$$
(3.25)

A different perspective of arriving at the above form for the reduced density matrix would be to consider only the diagonal entries of (3.22), whereas assuming that the off-diagonal elements quickly fall-off to zero. The usefulness of this perspective lies in the fact that one does not have to refer to the phase in order to derive the reduced density matrix. However, now we need to justify our choice of ignoring the off-diagonal elements for the density matrix. One way to argue would be to consider that there are a lot of particles created for a given mode, with opposite momenta, with  $\phi_k$  being the phase of each of these particle pairs. But if we want to use the destructive interference, while group averaging these phases, as being responsible for suppressing the off-diagonal terms, then we are back to our previous argument. Instead, one might follow the arguments of [35,52] to justify the reduction of the density matrix as a result of assuming a distribution of coherent states as our initial state – instead of the usual vacuum – as a manifestation of our ignorance regarding initial conditions. If one assumes this as the starting point, it can be shown that the off-diagonal terms are naturally suppressed as long as one invokes equipartition of probabilities for the initial states in the ensemble [52]. We are neither advising this approach nor suggesting that it is better than considering the averaging procedure over random phases, but just pointing out that there have been different justifications for considering the above form of the reduced density matrix (3.25). In the next section, we will give an improved analysis and explain the decay of the off-diagonal elements as a consequence of decoherence resulting from entanglement between the modes.

The von-Neumann entropy associated with this reduced density matrix is given by

$$s_{sq}^{c} = -\operatorname{Tr}\left(\rho_{sq}\ln\rho_{sq}\right)$$

$$= -\prod_{k} \left[ \frac{1}{\cosh^{2}r_{k}}\ln\left(\prod_{p}\frac{1}{\cosh^{2}r_{p}}\right) - \frac{\tanh^{2}r_{k}}{\cosh^{2}r_{k}}\ln\left(\prod_{p}\frac{\tanh^{2}r_{p}}{\cosh^{2}r_{p}}\right) - \frac{\tanh^{4}r_{k}}{\cosh^{2}r_{p}}\ln\left(\prod_{p}\frac{\tanh^{4}r_{p}}{\cosh^{2}r_{p}}\right) - \dots \right]$$

$$= -\sum_{n=0}^{\infty} \left[ \prod_{k} \frac{\tanh^{2n}r_{k}}{\cosh^{2}r_{k}}\ln\left(\prod_{p}\frac{\tanh^{2n}r_{p}}{\cosh^{2}r_{p}}\right) \right]$$
(3.26)

First, we expand the product in the logarithm as a sum of logs, i.e.

$$\ln\left(\prod_{k} \frac{\tanh^{2n} r_k}{\cosh^2 r_k}\right) = \sum_{k} \ln\left(\frac{\tanh^{2n} r_k}{\cosh^2 r_k}\right).$$
(3.27)

Using this in (3.26), we can rewrite the entropy density (per comoving volume) as

$$s_{\rm sq}^c = -\left(\sum_{n=0}^{\infty} \prod_p \frac{\tanh^{2n} r_p}{\cosh^2 r_p}\right) \left(\sum_k \sum_{m=0}^{\infty} \frac{\tanh^{2n} r_k}{\cosh^2 r_k} \ln\left(\frac{\tanh^{2n} r_k}{\cosh^2 r_k}\right)\right).$$
(3.28)

Using the normalization (3.19), the term in the first parentheses is equal to 1. The entropy gets simplified to

$$s_{\rm sq}^{c} = \sum_{k} \sum_{n=0}^{\infty} \frac{\ln\left(\cosh^{2} r_{k} \left(\tanh r_{k}\right)^{-2n}\right)}{\cosh^{2} r_{k}} \tanh^{2n} r_{k}$$

$$= \sum_{k} \frac{\ln\left(\cosh^{2} r_{k}\right)}{\cosh^{2} r_{k}} \sum_{n=0}^{\infty} \tanh^{2n} r_{k} - \sum_{k} \frac{\ln\left(\tanh^{2} r_{k}\right)}{\cosh^{2} r_{k}} \sum_{n=0}^{\infty} \left[n \tanh^{2n} r_{k}\right]$$

$$= \sum_{k} \ln\left(1 + \sinh^{2} r_{k}\right) - \sum_{k} \sinh^{2} r_{k} \ln\left(\tanh^{2} r_{k}\right)$$

$$= \sum_{k} \left[\left(1 + \sinh^{2} r_{k}\right) \ln\left(1 + \sinh^{2} r_{k}\right) - \sinh^{2} r_{k} \ln\left(\sinh^{2} r_{k}\right)\right]. \quad (3.29)$$

In the large occupation number limit,  $n_k = \sinh^2 r_k \gg 1$ , we get back the same expression for the entropy density  $s \approx \sum_k \ln (\sinh^2 r_k)$ , as derived in [31,32]. However, we derived this result from the von-Neumann entropy formula for a quantum density matrix instead of using the Shannon entropy for a classical field. Note that one should expect that our expression matches that for the classical calculation, done earlier, only in the large squeezing limit. In this sense, one should view  $\sum_k \ln (\sinh^2 r_k)$  as the classical limit of the von-Neumann entropy calculated here within a quantum field theoretic approach, and it is thus compatible with previous results [31, 32] of considering the entropy of a classical field. Our result also matches with previous works as presented in [35].

In the case of slow-roll inflation with an approximately constant Hubble constant we can estimate the resulting entropy density by integrating over all super-Hubble modes and apply a infrared cutoff: we do not consider modes with wavelengths larger than the Hubble radius  $H^{-1}$  at the beginning of inflation. With the convention that the scale factor is set to one at the beginning of inflation, this implies that in (3.29) we need to integrate over all values of k with H < k < aH. At any time, this integral is dominated by the modes exiting the Hubble radius at that time, and we thus obtain<sup>5</sup>

$$s_{\rm sq}^c \sim a^3 H^3 \,. \tag{3.30}$$

To obtain the entropy density per physical volume element, we have to divide the above by  $a^3$ , and we hence get

$$s_{\rm sq} \sim H^3. \tag{3.31}$$

Before moving on, let us note that the entropy calculated in this section is not quite an entanglement entropy as it arises from the squeezing of the cosmological perturbations. The way we manage to get a nonzero result for a density matrix arising from a quadratic Hamiltonian (3.8) is by employing some yet-to-be-specified coarse-graining, due to which the pure density matrix in (3.22) is reduced to a mixed one (3.25), by ignoring the off-diagonal terms. In the next section, we shall give a rigorous argument as to how gravitational nonlinearities, responsible for decohering the quantum fluctuations into classical perturbations, necessarily render the density matrix diagonal. In this way, the entanglement between suband super-Hubble modes, due to mode-mixing arising from gravitational non-linearities, is also responsible for the entropy of cosmological perturbations calculated above<sup>6</sup>.

<sup>&</sup>lt;sup>5</sup>A more explicit calculation for this has been shown in Sec-3.4.

<sup>&</sup>lt;sup>6</sup>The key point is that this is in addition to the explicit entanglement entropy due to such interaction terms which we shall calculate later on.

## 3.3 Nonlinearities, Decoherence and Entropy Generation

Here we review the analysis of [39] which shows how the purely gravitational interactions which are inevitably present because of the nonlinearity of General Relativity lead to a decoherence of the reduced density matrix of the super-Hubble modes as a consequence of the interaction with the sub-Hubble fluctuations. For our purposes, we will focus on the case of inflation.

We shall now take into account the effects of the cubic Hamiltonian in addition to the quadratic Hamiltonian discussed in the previous section. This is the leading term which generates entanglement between the sub- and super-Hubble modes. We are considering the full cubic action for the density perturbations in the presence of a single matter field. If the matter is a canonically normalized scalar field, then the speed of sound  $c_s = 1$ . In more general models,  $c_s^2$  can be smaller than one, and this can significantly increase the size of the cubic interaction terms, resulting in a significant contribution to the equilateral-shape non-Gaussianity parameter  $f_{NL}$ . However, as a first pass, let us only consider vanilla matter models with  $c_s = 1$ , which should be sufficient to estimate a lower bound on the entanglement entropy for models of inflation.

We take the form of the cubic contribution to the Hamiltonian from [53], from now on setting  $c_s = 1$ , which is a generalization of the results from [54].

$$S_{3} = M_{\rm Pl}^{2} \int dt \, d^{3}x \left[ a^{3} \epsilon_{H}^{2} \zeta \dot{\zeta}^{2} + a \epsilon_{H}^{2} \zeta (\partial \zeta)^{2} - 2a \epsilon_{H} \dot{\zeta} \partial_{i} \zeta \partial_{i} \tilde{\chi} \right. \\ \left. + a^{3} \epsilon_{H} (\dot{\epsilon}_{H} - \dot{\eta}_{H}) \zeta^{2} \dot{\zeta} + \frac{\epsilon_{H}^{2}}{2} a \partial_{i} \zeta \partial_{i} \tilde{\chi} \right. \\ \left. - \frac{d}{dt} \left( a^{3} \epsilon_{H} (\epsilon_{H} - \eta_{H}) \zeta^{2} \dot{\zeta} \right) \right]$$
(3.32)

where  $\tilde{\chi} = a^2 \epsilon_H \partial^{-2} \dot{\zeta}$ . We have also introduced the second "slow-roll" parameter:

$$\eta_H = \frac{1}{H} \frac{\dot{\epsilon}_H}{\epsilon_H} \,. \tag{3.33}$$

We shall ignore the non-local terms that contain  $\tilde{\chi}$  since those are not the dominant terms in the action. Additionally, there are also terms which would get cancelled with each other (such as the  $\eta_H$  term in the second line would get cancelled by a similar term from the third line of (3.32)). Since, in the case of inflation, the dominant mode of  $\zeta$  has frozen out on super-Hubble scales, we will neglect interaction terms which contain  $\dot{\zeta}$ . Furthermore, we shall restrict our analyses only to the leading order terms in the slow-roll parameters, and would thus be left with the second term in the first line of (3.32) (the other terms being higher orders in  $\epsilon_H$  and  $\eta_H$ , or contain a  $\dot{\zeta}$ ). Hence, the dominant term in the interaction Hamiltonian is (after integration by parts, and recalling that  $H_{\rm int} = -\mathcal{L}_{\rm int}$ )

$$H_{\rm int} = \frac{M_{\rm Pl}^2}{2} \int d^3x \,\epsilon_H^2 \, a \,\zeta^2(\partial^2 \zeta) \,. \tag{3.34}$$

The  $H_{\text{int}}$  we are considering arises purely from gravitational non-linearities, originating from the cubic Lagrangian given in (3.32). As discussed above, in a model of single-field slow roll inflation without any derivative self-interaction, this would be the dominant term. However, for a nontrivial speed of sound model, there can a different term which significantly enhances the cubic interaction. This would lead to both a faster rate of decoherence as well as a greater amount of entanglement entropy. In this sense, our calculation should be understood to yield the minimum amount of entanglement entropy that *must* be produced in any inflationary model; multiple fields or more complicated interactions would only enhance our results.

Note here that there is an additional term, not shown above in the cubic Lagrangian, that is of the exact same form,  $\zeta^2(\partial^2 \zeta)$ , but with a pre-factor  $\epsilon_H \eta_H a$  [55]. This term is part of a large number of terms which are typically removed by a field redefinition [54] and do not affect the correlation functions for calculating the bispectrum. Strictly speaking, we should keep this term if we are interested in calculating the entropy corresponding to the  $\zeta$  field (and not for the redefined one). However, we drop it here to avoid additional clutter since it is straightforward to include its effects at the end by adding a factor of  $\epsilon_H \eta_H$ , in addition to the  $\epsilon_H^2$  in (3.34), to our results.

Having setup our interaction terms, we begin the evolution at the conformal time  $\eta_0$ , in a pure Gaussian product state of all of the modes, which has the wave function

$$\Psi[A, B](\eta_0) = \Psi_G[A](\eta_0)\Psi_G[B](\eta_0), \qquad (3.35)$$

where in this case we have indicated which variables the individual states depend on. As a

consequence of the interactions, the state evolves into

$$\Psi[A,B](\eta) = \Psi_G[A](\eta)\Psi_G[B](\eta)\Psi_I[A,B](\eta)$$
(3.36)

at a later time  $\eta$ , where the third factor is a consequence of the interaction Lagrangian.

The interaction contribution to the wave function is given by

$$\Psi_{I}[A,B](\eta) = \exp\left[\int_{k,k',q} \zeta_{k} \zeta_{k'} \zeta_{q} \mathcal{F}(k,k',q;\eta)\right], \qquad (3.37)$$

where k, k' stand for sub-Hubble modes, and q stands for a super-Hubble mode, and the kernel function  $\mathcal{F}(k, k', q; \eta)$  is given by an integration over time of the interaction Hamiltonian in momentum space (see [39] for details) with the property that its imaginary part blows up as  $\eta \to 0$ . In the above, the integration runs over all momenta with the property that k + k' + q = 0 (momentum conservation).

The reduced density matrix of the super-Hubble modes can be obtained by integrating over the sub-Hubble ones. In the field representation we have

$$\rho_A(\zeta,\bar{\zeta}) = \int \mathcal{D}_B \Psi[\zeta,B]) \Psi^*[\bar{\zeta},B], \qquad (3.38)$$

where  $\mathcal{D}_B$  stands for the integration over the sub-Hubble modes B. Eq. (3.38) yields

$$\rho_A(\zeta,\bar{\zeta}) = \Psi_G[\zeta]\psi_G[\bar{\zeta}] \int \mathcal{D}_B |\Psi_G[B]|^2 \exp\left[\int_{k,k',q} \zeta_k \zeta_{k'} \left(\zeta_q \mathcal{F}(k,k',q) + \bar{\zeta}_q \mathcal{F}^*(k,k',q)\right)\right] \\ \equiv \Psi_G[\zeta]\Psi_G[\bar{\zeta}]D[\zeta,\bar{\zeta}], \qquad (3.39)$$

where  $D[\zeta, \overline{\zeta}]$  is the decoherence factor. Focusing on a single super-Hubble mode q, the decoherence factor is

$$D[\zeta, \bar{\zeta}] \sim \exp\left[-\frac{4\pi (\Delta \zeta_q)^2}{q^3} \int_{k+k'=-q} P_G(k) P_G(k') (\mathrm{Im}\mathcal{F}(k, k', q))^2\right],$$
(3.40)

where the time dependence of the factors has been suppressed, where  $P_G$  is a property of the Gaussian wavefunction, and

$$\Delta \zeta_q = \zeta_q - \bar{\zeta}_q \,. \tag{3.41}$$

As is clear from (3.40), the decoherence factor decays in time on super-Hubble scales since the imaginary part of  $\mathcal{F}$  blows up. Note that the decoherence effect is dominated by the Hubble scale modes. There is no UV divergence in the loop diagram which produces the interaction. This is a consequence of the specific form of our interaction Lagrangian.

To conclude this section, we have reviewed how the interaction with the sub-Hubble modes leads to decoherence of the super-Hubble ones. For a particular mode, decoherence happens after Hubble radius crossing. The important thing for us is the fact that decoherence leads to the damping of the off-diagonal terms such that the reduced density matrix of the super-Hubble modes become diagonal very quickly. In the previous section, we had calculated the entropy corresponding to the squeezing of the super-Hubble modes, *assuming* that their density matrix turns diagonal which we have given a concrete justification for in this section. As promised, we show that even for the entropy of the cosmological perturbations which solely arises from the quadratic Hamiltonian, nonlinearities play a crucial role by making the density matrix diagonal. In the following section, we will compute the entanglement entropy which the non-Gaussianities directly generate.

## 3.4 Enhanced Entanglement Entropy due to Nonlinearities

#### 3.4.1 Setup

Having set up our interaction terms, let us discuss how one can calculate the entanglement entropy of the cosmological perturbations due to the effects of these coupling terms. To calculate the entanglement entropy, we shall follow the prescription of [24], and generalize their results for flat spacetime to inflationary backgrounds.

Given our breakup of the Hilbert space (3.1)  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$  into system and environment modes, our Hamiltonian can be expressed as

$$H = H_A \otimes \mathbb{I} + \mathbb{I} \otimes H_B + \lambda H_{\text{int}}, \qquad (3.42)$$

where  $H_{A,B}$  denote the free part of the Hamiltonian and  $\lambda$  is a time-dependent constant. The ground state of the free theory, *neglecting the interactions*, is denoted by  $|0,0\rangle = |0\rangle \otimes |0\rangle$ ,

and one can write the interacting vacuum of the entangled system as

$$|\Omega\rangle = |0,0\rangle + \sum_{n\neq 0} A_n |n,0\rangle + \sum_{n\neq 0} B_N |0,N\rangle + \sum_{n,N\neq 0} C_{n,N} |n,N\rangle, \qquad (3.43)$$

where  $|n\rangle$  denotes an n-particle state of the system (in fact, a product state over all super-Hubble k modes), and  $|N\rangle$  is the corresponding state for the bath.

Following the analyses of [24], one finds that the leading order contribution to the entanglement entropy for such a system can be written as

$$S_{\text{ent}} = -\lambda^2 \log \left(\lambda^2\right) \sum_{n,N \neq 0} \frac{|C_{n,N}|^2}{(E_0 + \tilde{E}_0 - E_n - \tilde{E}_N)^2},$$
(3.44)

where we can express the matrix element  $C_{n,N}$  in terms of standard perturbation theory as

$$C_{n,N} = \langle n, N | H_{\text{int}} | 0, 0 \rangle.$$
(3.45)

Note that our definition of  $C_{n,N}$  differs slightly from that of [24] for later convenience. Before going on to calculate this matrix element, and the corresponding entanglement entropy for our cosmological system, let us review the flat space calculation first through an explicit example.

#### **3.4.2** Calculation for flat space

Considering a cubic interaction term, one can write the action for a massive scalar field as

$$S = \int d^4x \left( -\frac{1}{2} \left( \partial_\mu \varphi \right)^2 - \frac{1}{2} m^2 \varphi^2 - \frac{\lambda}{3!} \varphi^3 \right) \,. \tag{3.46}$$

For a flat (3 + 1)-dimensional spacetime, the field can be decomposed in terms of the usual ladder operators as

$$\varphi(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3 \sqrt{2\omega_k}} \left( a_{\mathbf{k}} e^{-i \,\mathbf{k}.\mathbf{x}} + a_{\mathbf{k}}^{\dagger} e^{i \,\mathbf{k}.\mathbf{x}} \right) \,, \tag{3.47}$$

where  $\omega_k = \sqrt{m^2 + k^2}$ . Here, instead of putting the fields in a box as in [24], we choose to work with continuous field variables, as would be more appropriate for cosmological perturbations later on. However, we still have a scale  $\mu$  which separates our system from the environment, using the same convention as in [24]. In other words, we are interested in calculating the entanglement entropy between the modes with momenta k above and below  $\mu$ . In this case, the only nontrivial contribution to the matrix element would be from an excited state of a 3-particle one which can be written as

$$|p_1 p_2 p_3\rangle = a_{\mathbf{p}_1}^{\dagger} a_{\mathbf{p}_2}^{\dagger} a_{\mathbf{p}_3}^{\dagger} |0\rangle . \qquad (3.48)$$

Recalling that the interaction Hamiltonian is  $(\lambda/3!) \varphi^3$ ,  $\lambda$  having dimension of mass, the required matrix element (3.45) can be written as

$$C_{n,N}^{\text{flat}} = \int d^3x \langle p_1 p_2 p_3 | \left[ \int \frac{d^3k}{(2\pi)^3 \sqrt{2\omega_k}} \left( a_{\mathbf{k}} e^{-i \,\mathbf{k}.\mathbf{x}} + a_{\mathbf{k}}^{\dagger} e^{i \,\mathbf{k}.\mathbf{x}} \right) \right]^3 | 0 \rangle$$

$$= \int d^3x \langle p_1 p_2 p_3 |$$

$$\left[ \int d^3k_1 \int d^3k_2 \int d^3k_3 \,\frac{1}{(2\pi)^9 \sqrt{\omega_{k_1} \omega_{k_2} \omega_{k_3}}} \left( a_{\mathbf{k}_1}^{\dagger} e^{i \,\mathbf{k}_1.\mathbf{x}} \right) \left( a_{\mathbf{k}_2}^{\dagger} e^{i \,\mathbf{k}_2.\mathbf{x}} \right) \left( a_{\mathbf{k}_3}^{\dagger} e^{i \,\mathbf{k}_3.\mathbf{x}} \right) \right] | 0 \rangle$$

$$= \frac{1}{2^{3/2}} \int d^3x \left[ \frac{1}{\sqrt{\omega_{p_1} \omega_{p_2} \omega_{p_3}}} e^{i \,(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3).\mathbf{x}} \right]$$

$$= \frac{1}{2^{3/2}} \frac{(2\pi)^3}{\sqrt{\omega_{p_1} \omega_{p_2} \omega_{p_3}}} \delta^3 \left( \mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3 \right) . \qquad (3.49)$$

In the second line above, we only keep the creation operators as required, whereas in the third line we have used the orthonormality property of the inner product to eliminate the integrals over  $(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ . In the final step, we used the integration over the spatial coordinate, and the remaining delta function implies that at least one of the spatial momenta must be above, and at least one below, the scale demarcating the system and the environment.

The entanglement entropy for this system can be then evaluated by plugging in the above expression into (3.44)

$$s_{\text{ent}}^{\text{flat}} = -\lambda^2 \log \left(\lambda^2\right) \frac{1}{2^3 (2\pi)^6} \times \qquad (3.50)$$
$$\int_{\{p\}_{\mu}} \prod d^3 p_i \frac{\delta_{\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3}}{\omega_{p_1} \omega_{p_2} \omega_{p_3} \left(\omega_{p_1} + \omega_{p_2} + \omega_{p_3}\right)^2}$$

where the integrals are over a set of momenta such that there can only be two configurations of interest – either one of  $(p_1, p_2, p_3)$  is greater than  $\mu$  while the rest are below  $\mu$ , or two of them are above while one is below  $\mu$ . We have also divided the total entanglement entropy by the (infinite) volume to express it as an entanglement entropy density ( $\equiv S_{ent}^{flat}/Vol$ ).

#### 3.4.3 Vacuum & Interaction Hamiltonian

Let us first outline the differences we anticipate between the flat space calculation above and our case for cosmological perturbations. Firstly, the interaction parameter  $\lambda = \lambda(\eta)$  will now be time-dependent. Secondly, the vacuum for the system modes is now given by the squeezed vacuum, and the mode functions corresponding to the vacuum in curved spacetime will have a different form of their momentum dependence. Since the vacuum of the super-Hubble modes will now be the squeezed vacuum, there now are contributions of terms with both creation and annihilation operators in our case. Finally, a major conceptual difference arises from the fact that the scale separating our system from the bath is given by the (comoving) Hubble scale which is time-dependent since we are working with comoving coordinates (and, in addition, by itself has a weak time-dependence of its physical value during inflation), and is not some arbitrary, tunable parameter  $\mu$  as in the flat space case. With this in mind, let us begin by factoring the Hamiltonian for the overall system as

$$H = H_{\rm sys} + H_{\rm bath} + H_{\rm int} \,, \tag{3.51}$$

where the  $H_{\text{sys}}$  and  $H_{\text{bath}}$  is the quadratic Hamiltonian, for the super and sub-Hubble modes respectively, as given in (3.8). Next, we write down the vacuum modes for the unperturbed systems, ignoring nonlinearities, as

$$|0,0\rangle = |0\rangle_{k>aH} \otimes |SQ(\eta)\rangle_{k
(3.52)$$

The  $|0,0\rangle$  is the vacuum state for both the system as well as the bath modes. For the super-Hubble modes, the vacuum is given by the squeezed state as given in (3.20). On the other hand, we have the usual Minkowski vacuum for the sub-Hubble modes, denoted by  $|0\rangle$ .

The explicit form of the interaction Hamiltonian naturally depends on the choice of the interaction term we choose between the perturbation modes. As mentioned earlier, for this paper, we shall restrict ourselves to only cubic perturbation terms which arise naturally from gravitational nonlinearities in any model of inflation, as captured by our interaction Lagrangian given in (3.32). We emphasize once again that considering more complicated interactions or more fields can lead in a different term dominating  $H_{\text{int}}$ , which would end up producing enhanced amounts of entanglement entropy. In this precise sense, we give a lower bound on the amount of entropy production coming from scalar modes during inflation.

For our dominant interaction term of the form

$$M_{\rm Pl}^2 \int dt \, d^3x \, a \, \epsilon_H^2 \, \zeta \, (\partial \zeta)^2 \,, \qquad (3.53)$$

we can write down the interaction Hamiltonian by converting the  $\zeta$  field to our canonical field  $\chi$ , and then expanding in terms of the creation and annihilation operators in momentum space. We find the following expression [56]:

$$\lambda(\eta)H_{\text{int}} = \lambda(\eta) \int_{\Delta} \left[ \sqrt{\frac{k_2 k_3}{k_1}} \left( c^{\dagger}_{-\mathbf{k}_1} c^{\dagger}_{-\mathbf{k}_2} c^{\dagger}_{-\mathbf{k}_3} + c_{\mathbf{k}_1} c^{\dagger}_{-\mathbf{k}_2} c^{\dagger}_{-\mathbf{k}_3} + \dots \right) + \sqrt{\frac{k_2 k_1}{k_3}} \left( c^{\dagger}_{-\mathbf{k}_1} c^{\dagger}_{-\mathbf{k}_2} c^{\dagger}_{-\mathbf{k}_3} + \dots \right) + \sqrt{\frac{k_1 k_3}{k_2}} \left( c^{\dagger}_{-\mathbf{k}_1} c^{\dagger}_{-\mathbf{k}_2} c^{\dagger}_{-\mathbf{k}_3} + \dots \right) \right] .$$

$$(3.54)$$

where all the terms in the parentheses (...) are the same and include all possible (momentumconserving) combinations of the ladder operators. We have also defined

 $\int_{\Delta} := \int \frac{\mathrm{d}^3 k_1}{(2\pi)^3} \frac{\mathrm{d}^3 k_2}{(2\pi)^3} \frac{\mathrm{d}^3 k_3}{(2\pi)^3} (2\pi)^3 \delta^3(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3).$  The difference in the momenta dependence of our choice of  $H_{\rm int}$  from, say, one with time-derivatives such as  $\mathcal{L}_3 \sim \zeta(\zeta')^2$ , would be that some of the terms in the expression above would come with a minus sign since, in that case, the interaction term couples the field with its conjugate momentum [50]. The prefactor is given by (keeping in mind that we go from cosmic time to conformal time)

$$\lambda(\eta) = \frac{\sqrt{\epsilon_H}}{2\sqrt{2} \, a M_{\rm Pl}} \,, \tag{3.55}$$

where, as anticipated, we get a time-dependent interaction parameter. We now have all the ingredients – the vacuum state and the interaction Hamiltonian – to calculate the matrix element given in (3.45).

#### 3.4.4 Matrix element

Let us revisit our calculation of the matrix element for the cubic Lagrangian in Minkowski space. The crucial difference between that calculation and the one for inflation would be that instead of only keeping the term which solely involves creation operators from the interacting Hamiltonian, we shall also have to consider terms of the form  $c_{\mathbf{k}_1}c^{\dagger}_{-\mathbf{k}_2}c^{\dagger}_{-\mathbf{k}_3}$  and  $c_{\mathbf{k}_1}c_{\mathbf{k}_2}c^{\dagger}_{-\mathbf{k}_3}$ . This is easy to understand since for the case of flat spacetime, the only nonzero contribution for the matrix element between the Minkowski vacuum and an excited state (with, say, three

particles for a cubic interaction) can come if we sandwich a term consisting of three creation operators in between. If there exists any annihilation operator, it would simply annihilate the vacuum, resulting in zero. On the other hand, for inflation, we have a tensor product of the Minkowski vacuum for the sub-Hubble modes and the squeezed vacuum for thr super-Hubble ones (3.52). In this case, the ladder operator(s) corresponding to the sub-Hubble modes must be creation ones  $c^{\dagger}_{-\mathbf{k}}$  whereas the one(s) corresponding to the super-Hubble modes can be either  $c^{\dagger}_{-\mathbf{k}}$  or  $c_{\mathbf{k}}$ . This is so because an annihilation operator  $c_{\mathbf{k}}$  does *not* annihilate the squeezed vacuum  $|SQ(k,\eta)\rangle$ . One can see this explicitly from the form of the two-mode squeezed vacuum, as given in (3.17).

Having said this, let us list all the possible choices of interaction terms which can appear in the matrix elements:

- Terms of the form  $c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$ : There can be either two system (super-Hubble) modes and one bath (sub-Hubble) mode or vice-versa.
- Terms of the form  $c_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$ : There can be either two system modes and one bath mode or vice-versa. However, the annihilation operator must always correspond to the super-Hubble mode.
- Terms of the form  $c_{\mathbf{k}}c_{\mathbf{k}}c_{-\mathbf{k}}^{\dagger}$ : There must be two system modes, corresponding to the two annihilation operators, and can, therefore, only be one bath mode.
- The terms proportional to  $c_{\mathbf{k}}c_{\mathbf{k}}c_{\mathbf{k}}$  necessarily yield zero for the matrix element since the annihilation operator corresponding to any of the bath modes annihilates the Minkowski vacuum.

Let us consider the first case in detail in the following calculation while we leave the details of the other terms for the Appendix. Therefore, the term of interest for us from the  $H_{\rm int}$  (3.54), for calculating (3.45), is the following:

$$\left(\sqrt{\frac{k_2k_3}{k_1}} + \sqrt{\frac{k_1k_3}{k_2}} + \sqrt{\frac{k_1k_2}{k_3}}\right) c_{-\mathbf{k}_1}^{\dagger} c_{-\mathbf{k}_2}^{\dagger} c_{-\mathbf{k}_3}^{\dagger} \subset H_{\text{int}}$$

Next, we need to find the explicit action of a creation operator on the squeezed vacuum. Using the definition of the two-mode squeezed state from (3.17), we can formally express the

action of a creation operator on it as

$$c_{-\mathbf{p}}^{\dagger} \left| SQ\left(k,\eta\right) \right\rangle \,. \tag{3.56}$$

Schematically, it implies that we are considering an excited state with a particle of energy p over our squeezed vacuum. A similar iteration would create higher order excited states over the squeezed vacuum. However, recall that for a cubic interaction term, the only non-zero contribution to the matrix element comes from having the first excited state over both the squeezed and the Minkowski vacuum. Also, since we are only considering cubic interactions, there can be only two choices — either one of the modes is in the system and two are in the bath or two of them are in the system while one is in the bath. However, it will be clear from the following that the dominant contribution to the entanglement entropy comes from having two of the modes in the bath and one in the system. This is not at all surprising keeping in mind that the decoherence rate is also dominated by having two short-wavelength modes and one long-wavelength one.

Let us consider the former option first, *i.e.*  $p_1, p_2 > aH$  while  $p_3 < aH$ . The appropriate excited state to consider is of the form

$$|n,N\rangle = \left|1_{\mathbf{p}_{1}} 1_{\mathbf{p}_{2}}\right\rangle \otimes c^{\dagger}_{-\mathbf{p}_{3}} \left|SQ\left(k,\eta\right)\right\rangle \,. \tag{3.57}$$

The only other novelty for our calculation is the effect of the squeezed vacuum on the inner product. Recall the standard result

$$\langle SQ(k,\eta) | c_{\mathbf{p}} c_{-\mathbf{q}}^{\dagger} | SQ(k,\eta) \rangle = [\langle SQ(k,\eta) | | S(k,\eta)Q \rangle + \langle SQ(k,\eta) | N_{\mathbf{p}} | SQ(k,\eta) \rangle] \delta^{3}(\mathbf{p}+\mathbf{q})$$

$$= (1 + \sinh^{2} r_{p}) \delta^{3}(\mathbf{p}+\mathbf{q}),$$

$$(3.58)$$

where we have written things schematically to avoid clutter. To explicitly see how this result comes about, one should write down the unitary transformation of the creation and annihilation operator under the squeezing operator, *i.e.*  $S^{\dagger}cS$  and  $S^{\dagger}c^{\dagger}S$  as linear combinations of  $c, c^{\dagger}$ , dropping all momenta indices. Also, note that  $S^{\dagger} = S^{-1}$ . See the Appendix for more details. The rest of the calculation follows exactly that of flat space, and it is easy to evaluate the matrix element as

$${}^{(c^{\dagger}c^{\dagger}c^{\dagger})}C_{n,N}^{\rm sq} = (2\pi)^3 \left(1 + \sinh^2 r_{p_3}\right) \left(\sqrt{\frac{p_2 p_3}{p_1}} + \sqrt{\frac{p_1 p_3}{p_2}} + \sqrt{\frac{p_1 p_2}{p_3}}\right) \,\delta^3(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3) \,. (3.59)$$

It is clear that for our choice of  $p_1, p_2 \in$  bath while  $p_3 \in$  system, the dominant term in the above comes from the third term  $\left(C_{n,N} \propto \sqrt{\frac{p_1 p_2}{p_3}}\right)$ . It is also evident from the above calculation that if we had two modes in the system and one in the bath, then the dominant term in the matrix element would have the form

where we have chosen  $p_1 > aH$  and  $p_2, p_3 < aH$ . Already at this stage we can see that the entanglement entropy for cosmological perturbations, during inflation, peaks in the "squeezed" limit  $p_3 \ll p_1 \approx p_2$ , given the momentum structure of the matrix element, for  $(c^{\dagger}c^{\dagger}c^{\dagger})C_{n,N}^{\text{sq}}$ whereas it gets its maximum contribution in the "folded" limit  $p_3 + p_2 \approx p_1$  for the other case  $(c^{\dagger}c^{\dagger}c^{\dagger})C_{n,N}^{\text{fold}}$ .

#### 3.4.5 Entanglement entropy

Let us recall the formula for the leading order term in the entanglement entropy

$$S_{\text{ent}} = -\lambda^2 \ln(\lambda^2) \sum_{n,N \neq 0} \frac{|C_{n,N}|^2}{\left(E_0 + \tilde{E}_0 - E_n - \tilde{E}_N\right)^2},$$
(3.61)

where a sum is implied on both types of  $C_{n,N}$  calculated in (3.59) and (3.60). Note our slight difference in convention of defining the matrix element  $C_{n,N}$  as in (3.45), with that of [24]. In order to calculate the entanglement entropy, we need to reinstate factors of the coupling parameter  $\lambda(\eta) = \sqrt{\epsilon_H} / (2\sqrt{2} a(\eta) M_{\rm Pl})$  as well as the energy corresponding to the ground and excited states, both for the Minkowski and the squeezed vacuum, considered above. However, what we really need in the above formula is the energy difference between the first excited state and the ground state, for both the Minkowski and the squeezed vacua. This is the same for both the system and the bath modes and is given by  $\omega_k := k$  for (nearly) massless scalar excitations.

Note that the sum over (n, N) translates into integrals over all the momentum modes in the formula (3.44). Recall that there was a similar integral over all momentum modes also in the expression of the entropy arising from the squeezing part of the quadratic Hamiltonian, as shown in (3.29). However, unlike in that case, we would have the integrals over all momentum conserving configurations involving  $(\mathbf{p_1}, \mathbf{p_2}, \mathbf{p_3})$  and not over individual modes as is expected for an entanglement entropy coming from cubic interactions. Keeping this is mind, the entanglement entropy (per unit comoving volume) is given by

where we have only kept the dominant terms from the matrix elements (3.59) and (3.60). It is important to discuss the limits of the above integral first: We have introduced  $M_{\rm Pl}$  as the natural *physical* UV cutoff and the comoving wavenumber at the beginning of inflation as the infrared cutoff. We set  $a_i = 1$  for the scale factor at the beginning of inflation (and therefore, in our convention, a is always > 1). We also assume that the Hubble parameter, H, remains constant during inflation. Furthermore, the UV cutoff for the comoving momenta is given by  $aM_{\rm Pl}$  which signifies the fact that the integration of the environment is over a fixed number of bath modes, even though we are considering an accelerating background. This is so because although the environment is continuously depleted by modes getting redshifted into the system, there is also a constant supply of modes from the UV into the bath<sup>7</sup>. However, the system has an increasing phase space of modes as more and more modes become super-Hubble as time goes on, and given our infrared cutoff which states that there were no comoving modes which were super-Hubble before inflation started. Naturally, we have to assume that inflation starts at a finite time in the past which reinforces the need of having an UV cutoff for the perturbation modes.

Let us now estimate the integrals  $I_1$  and  $I_2$  given in (3.62). For  $I_1$ , when we have two

<sup>&</sup>lt;sup>7</sup>This mode creation is a source of non-unitarity which is one of the arguments for the TCC [48, 49].

bath modes and one system mode, the integrand would naturally have its largest contribution coming from the squeezed limit, as shown below:

$$I_{1} = -(2\pi)^{3}\lambda^{2}\ln(\lambda^{2}) \int_{H}^{aH} \frac{d^{3}p_{3}}{(2\pi)^{3}} \int_{aH}^{aM_{\mathrm{Pl}}} \frac{d^{3}p_{2}}{(2\pi)^{3}} \int_{aH}^{aM_{\mathrm{Pl}}} \frac{d^{3}p_{1}}{(2\pi)^{3}} \delta^{3}(\mathbf{p}_{1} + \mathbf{p}_{2} + \mathbf{p}_{3}) \times \\ \left(\frac{p_{1}p_{2}}{p_{3}}\right) \frac{(1 + \sinh^{2}r_{p_{3}})^{2}}{(p_{1} + p_{2} + p_{3})^{2}} \\ = -\lambda^{2}\ln(\lambda^{2}) \int_{H}^{aH} \frac{d^{3}p_{3}}{(2\pi)^{3}} \int_{aH}^{aM_{\mathrm{Pl}}} \frac{d^{3}p_{2}}{(2\pi)^{3}} \left(\frac{p_{2}\sqrt{p_{2}^{2} + p_{3}^{2} + 2p_{2}p_{3}\cos\Theta}}{p_{3}}\right) \times \\ \frac{(1 + \sinh^{2}r_{p_{3}})^{2}}{\left(\sqrt{p_{2}^{2} + p_{3}^{2} + 2p_{2}p_{3}\cos\Theta} + p_{2} + p_{3}\right)^{2}} \\ \approx -\lambda^{2}\ln(\lambda^{2}) \int_{aH}^{aM_{\mathrm{Pl}}} \frac{d^{3}p_{2}}{(2\pi)^{3}} \int_{H}^{aH} \frac{d^{3}p_{3}}{(2\pi)^{3}} \frac{(aH)^{4}}{2^{4}p_{3}^{5}} \\ \sim \frac{\epsilon_{H}}{3(2\pi)^{4}2^{6}a^{2}M_{\mathrm{Pl}}^{2}} \left(aH)^{4} \left[(aM_{\mathrm{Pl}})^{3} - (aH)^{3}\right] \times \\ \left[\frac{1}{H^{2}} - \frac{1}{(aH)^{2}}\right] \times \ln(\lambda^{2}) \lesssim \epsilon_{H} H^{2} M_{\mathrm{Pl}} a^{5} \ln(\lambda^{2}) .$$
(3.63)

In the second line, we have killed the  $p_1$  integral using the delta function, introducing the angle  $\Theta$  between  $\mathbf{p}_2$  and  $p_3$ . In the next line, we introduce the crucial approximation that the integrand peaks in the limit  $\Theta \to \pi/2$  and  $p_2 \gg p_3$ , *i.e.* the squeezed limit. This would help us in getting an upper bound on the entanglement entropy corresponding to the  $I_1$  term. We have also used the expression for the squeezing parameter from (3.11) and used the approximation that  $1 + \sinh r_k \approx \sinh r_k$ , for large squeezing, in this step. It is then easy to see that the integration over the bath modes is dominated by the upper limit (the UV cutoff scale), while the integral over the system mode  $p_3$  is dominated by the lowest value of  $p_3$ , i.e. by the infrared (IR) cutoff scale. We have only kept the leading terms in the integrals in the same spirit to arrive at our lower estimate for the entropy density, ignoring numerical factors. We note that a factor of  $a^3$  should be divided from the final result in order to account for the entanglement entropy density (total entropy per unit *physical* volume). We are then left with a factor of  $(a/a_i)^2$  (recall, we have set  $a_i = 1$ ) and this reflects the fact that the phase space of the system modes is growing, and the contribution to the  $p_3$  integral is dominated by the IR cutoff. Collecting everything, the estimate<sup>8</sup> of the entanglement

 $<sup>^{8}</sup>$ To remind the readers, this is a lower bound on the amount of entanglement entropy produced in any

entropy per unit physical volume coming from  $I_1$  is given by

$$s_{\text{ent}}^{I_1} \lesssim \epsilon_H \ H^2 \ M_{\text{Pl}} \ a^2 \ \ln(\lambda^2) \,, \tag{3.64}$$

where a > 1 is such that the number of *e*-foldings of inflation is given by  $N := \ln a$  in our convention.

Let us now first show that the contribution coming from  $I_2$  to the entanglement entropy density would be subdominant to the above result. In this case of having two system and one bath mode, the largest contribution to the integrand would come from the folded limit  $p_1 \approx p_2 + p_3$ . Following the calculation as in the previous case, we can arrive at an upper bound for the estimate of this term in a similar way. However, note that once we eliminate the integral over the bath mode  $p_1$  using the delta function, none of the system mode integrals which are left have any dependence on  $M_{\rm Pl}$ . The other difference lies in the additional squeezing terms leading to an extra factor of the IR cutoff in the final result, namely,

$$s_{\rm ent}^{I_2} \lesssim \epsilon_H \ H^5 \ \frac{1}{M_{\rm Pl}^2} \ a^3 \ \ln(\lambda^2) \,.$$
 (3.65)

Once again, we have expressed this final result in terms of the entanglement entropy per unit physical volume and have only given a rough estimate of the upper bound. Thus, we find

$$f := \frac{s_{\text{ent}}^{I_1}}{s_{\text{ent}}^{I_2}} = \frac{1}{a} \left(\frac{M_{\text{Pl}}}{H}\right)^3, \qquad (3.66)$$

which means that  $s_{\text{ent}}^{I_2}$  shall always remain subdominant to  $s_{\text{ent}}^{I_1}$ , provided  $f > 1 \Rightarrow N < 3 \ln(M_{\text{Pl}}/H)$ . In the next section, we shall show that combining the observed scalar power spectrum with the fact that the entanglement entropy of cosmological perturbations during inflation remain smaller than the thermal entropy produced during (p)reheating leads to this condition being always satisfied. Therefore, we can always ignore the entanglement entropy corresponding to having two system and one bath mode when compared to that of having two sub- and one super-Hubble mode.

Note that the above estimates were calculated using the approximations of squeezed and folded shapes, in which the integrands reach their peak values. The full integrals do not lend model of inflation since we are only considering cubic interactions of density perturbations alone, which come from minimally coupling a scalar field to GR. There are necessarily other sources such as those due to non-Gaussian terms for tensor perturbations.

themselves to having simple analytic forms and we have thus avoided writing them down explicitly. The effect of removing these approximations would result in some small numerical factors appearing in front of our estimates, as in (3.64). However, recall that we have only shown here the result of the calculation of the entanglement entropy coming from the terms of the form  $c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$ , arising from the interaction Hamiltonian in (3.54). As mentioned earlier, there are other terms, proportional to  $c_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$  and  $c_{\mathbf{k}}c_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$ , which also contribute to the entanglement entropy. As shown in the Appendix, in the limit of large squeezing,  $r_k \gg 1$ , the contribution of all of these terms are either proportional to  $s^{I_1}_{\text{ent}}$  or to  $s^{I_2}_{\text{ent}}$ . Naturally, we neglect the terms proportional to  $s^{I_2}_{\text{ent}}$  since they are sub-dominant. And the terms which are proportional to  $s^{I_1}_{\text{ent}}$  shall add to our estimate for the entanglement entropy density (3.64). All of this is to say that in our order of magnitude estimate for the entanglement entropy density of cosmological perturbations during inflation, there should be some  $\mathcal{O}(1)$  numerical factor appearing, namely

$$s_{\text{ent}} \sim \mathcal{O}(1) \ln(\lambda^2) \epsilon_H H^2 M_{\text{Pl}} a^2.$$
 (3.67)

There are two sources which contribute to this  $\mathcal{O}(1)$  number – one from the additional terms, as shown in the Appendix, and the other coming from the fact that we are estimating the integral by its upper bound. From now on, we shall drop this number as well as the logarithmic factor in our upcoming discussions.

Now that we have an estimate for the entanglement entropy due to the gravitational nonlinearities, let us compare this with the contribution coming from the squeezing part of the quadratic Hamiltonian, as in (3.29). As mentioned earlier, for large  $r_k \gg 1$ , the entropy density (per physical volume), coming from (3.29), is given by (3.31)

$$s_{\rm sq} = \frac{1}{a^3} \int_H^{aH} d^3k \ln\left(\sinh^2 r_k\right) \sim H^3,$$
 (3.68)

where we have, once again, ignored some small numerical factors.

Although  $s_{ent}$  corresponding to cubic interactions arising from gravitational nonlinearities is suppressed by a factor of  $\epsilon_H$  (as it should be), it is still greater than  $s_{sq}$ . One way to easily see this is to approximate the value of the observed scalar power spectrum as

$$P_{\zeta} \sim \frac{1}{\epsilon_H} \left(\frac{H}{M_{\rm Pl}}\right)^2 \sim 10^{-9} \,, \tag{3.69}$$

such that  $\epsilon_H \sim 10^9 (H/M_{\rm Pl})^2$ . Let us define the ratio

$$t := \frac{s_{\text{ent}}}{s_{\text{sq}}} \sim \epsilon_H \left(\frac{M_{\text{Pl}}}{H}\right) a^2 \sim 10^9 \left(\frac{H}{M_{\text{Pl}}}\right) e^{2N}.$$
(3.70)

As we shall see from the bounds on N that we will derive in the next section, this quantity t > 1 and thus the entanglement entropy from non-Gaussianities would be larger than that corresponding to the squeezed vacuum, provided inflation lasts a reasonable amount of time and is not fine-tuned to be extremely small. This is quite a remarkable result since this implies that the entanglement entropy due to (cubic) gravitational nonlinearities are larger than that due to the (squeezing part of the) quadratic action!

## **3.5** Upper bound on the duration of inflation

We have seen that the entanglement entropy density of cosmological perturbations produced by nonlinearities builds up during a period of inflation as

$$\frac{a}{a_i} = e^N, (3.71)$$

where N is the number of e-foldings of inflation, and  $a_i$  is the value of the scale factor at the beginning of inflation (which we had set equal to 1 in the last section, for simplicity). In order to allow a graceful exit from inflation consistent with the second law of thermodynamics, it is important to make sure that the entropy due to these interactions remain subdominant to the entropy in the thermal radiation state after inflation. This thermal entropy density is given by

$$s_{\rm th} = \frac{4\pi^2}{45} g^* T_R^3 \,, \tag{3.72}$$

where  $T_R$  is the initial temperature of the radiation bath, and  $g^*$  is the number of spin degrees of freedom in the radiation bath. Assuming rapid thermalization after inflation, and nearly constant Hubble parameter during inflation, this yields

$$s_{\rm th} \simeq \frac{4\pi^2}{45} g^* H^{3/2} M_{\rm Pl}^{3/2} \,.$$
 (3.73)

Making use of the result (3.67), the requirement

$$s_{\rm th} > s_{\rm ent} \tag{3.74}$$

yields the condition

$$N < \frac{1}{4} \ln\left(\frac{M_{\rm Pl}}{H}\right) + \frac{1}{2} \ln \epsilon_H^{-1} \tag{3.75}$$

(modulo numerical factors). The value of  $\epsilon_H$  is given in terms of H and  $M_{\rm Pl}$  via the equation (3.69), invoking the observed value of the amplitude of the power spectrum of cosmological perturbations. Inserting the resulting relation for  $\epsilon_H$  yields

$$N < \frac{5}{4} \ln\left(\frac{M_{\rm Pl}}{H}\right) - \frac{9}{2} \ln 10,$$
 (3.76)

which is very close the bound [48]

$$N < \ln\left(\frac{M_{\rm Pl}}{H}\right) \tag{3.77}$$

which results from the TCC [49]. Note that this bound on the duration of the inflationary phase is the same as derived in [57], where it was argued that beyond that time the de Sitter phase cannot be given a well-defined classical background interpretation due to the buildup of entanglement<sup>9</sup>.

We are thus led to speculate the the TCC may have a derivation based on entropy considerations and the second law of thermodynamics. It is already known that entropy considerations have also proven useful [60] to derive the de Sitter swampland conjecture [61,62], one of the various constraints on effective field theories to be consistent with string theory (see e.g. [63,64] for reviews).

Note that we have derived a lower bound on the entanglement entropy due to the minimal gravitational nonlinearities (ignoring those due to tensor perturbations). We might speculate that if we were to do a more detailed calculation, our entropy bound on N might turn out to be in even closer agreement with the bound from the TCC. Note that the bound (3.76) can be relaxed if we consider H to be decreasing substantially during inflation, or if the thermal history of the universe after inflation is non-standard. However, as shown in [65, 66], in these cases the TCC bound is also relaxed. Note, also, that if we take into account entanglement

<sup>&</sup>lt;sup>9</sup>In a later paper [58], another (and much larger) time scale was introduced as the time scale beyond which the actual de Sitter background breaks down. It was then argued [59] that low energy effective field theory remains valid up to that time.

entropy due to modes which were already super-Hubble at the beginning of inflation, the bound can be strengthened, in the same way that the TCC bound is strengthened if we consider pre-inflation evolution [66, 67]. Finally, it has also been pointed out that deriving the TCC from different quantum gravity arguments can, by itself, lead to a refinement of it [68] and can bring it closer to our bound.

Returning to the discussion at the end of the previous section concerning the ratio of the entropies produced by nonlinear entanglement effects on one hand, and by pure decoherence of the linear modes on the other, we see that if the duration of inflation saturates the above bound (3.76), then the entanglement entropy dominates by a factor of  $(M_{\rm Pl}/H)^{3/2}$ , the result we promised to derive earlier. In other words, unless inflation lasts for a very short period of time,  $s_{\rm ent}$  would always dominate over  $s_{\rm sq}$ .

Note that a related bound on the duration of inflation based on entanglement considerations was given in [69], where it was argued that, interpreting the current horizon entropy of the Universe as entanglement entropy, there is a number of e-foldings of inflation before which there is no entropy and we cannot talk about a de Sitter background.

## **3.6** Conclusions and Discussion

In this work, we have derived the entanglement entropy of inflationary scalar perturbations, corresponding to nonlinearities arising from gravity. Although entropy of cosmological perturbations is a rich subject by itself, what is novel to our work is that we calculate the *entanglement* entropy to the leading order of cubic interactions, going beyond the calculation of entropy corresponding to the squeezing of the super-Hubble vacuum state. Remarkably, we show that this cubic (and higher order) interactions are essential even to calculate the entropy corresponding to the quadratic Hamiltonian. This is so because decoherence arising from these terms is what is responsible for reducing the pure density matrix to a mixed one, by suppressing the off-diagonal terms. These higher order interaction Hamiltonians themselves lead to mode-couplings such that there is an entanglement between the superand sub-Hubble modes which is a direct manifestation of the quantum origin of these vacuum fluctuations<sup>10</sup>. The entanglement entropy corresponding to these interactions is what we have calculated for the first time by treating the super-Hubble modes as our system and the sub-Hubble ones as a bath.

Our result shows that the entanglement entropy density scales as  $H^2 M_{\rm Pl} (a/a_i)^2$ , where  $a_i$  is the scale factor at the beginning of inflation. In order to allow for a graceful exit from inflation consistent with the second law of thermodynamics, this entropy must be smaller than the thermal entropy after inflation. This leads to an upper bound on the duration of inflation which is very close to the bound obtained from the TCC. Interestingly, the non-linearities produce the dominant contribution to the entropy of cosmological perturbations, surpassing the one for the squeezed vacuum, provided  $\epsilon > (H/M_{\rm Pl}) (a_i/a)^2$  and is not fine-tuned to be extremely small. Using the upper bound derived on the duration of inflation, this translates into the statement that the entanglement entropy due to cubic interactions dominate over the one due to the (quadratic) squeezing term, provided inflation does not last for a very short period of time.

As we have shown, the calculation of the entanglement entropy of cosmological perturbations simplifies when done in momentum space. It is easy to appreciate this properly if one compares our result with that for determining the full non-unitary evolution of the density matrix of the system modes as has been done, for instance, in [50] (see [56] for the case of tensor modes). The time evolution of the reduced density matrix involves non-Hamiltonian terms, and might even contain non-Markovian terms, which depend on the so-called Lindblad operator. If one were to try and calculate the solution of the time-dependent reduced density matrix and then evaluate the von Neumann entropy associated with it, the calculation would become much harder and rather intractable. In this paper, we give a complementary way of calculating the entanglement entropy without having to deal with the full dynamics since, as emphasized earlier, we only require to calculate certain matrix elements for our purposes. The fact that these two seemingly different methods yield the same result for the

<sup>&</sup>lt;sup>10</sup>This property of the entanglement entropy corresponding to the interactions alone is something unique for models of the early-universe which explain macroscopic perturbations as originating from quantum vacuum fluctuations, unlike the entropy corresponding to the squeezing of the modes which can also be interpreted as some type of classical Shannon entropy.

entanglement entropy has been shown in [70] for any quantum field theory. In addition, going to momentum space makes it easy to impose a UV cutoff for the bath modes, as has been done in this case.

The natural next step for us would be to calculate the entanglement entropy corresponding to primordial gravitational waves. Once again, assuming the simplest model of inflation, nonlinearities would arise from gravitational interactions which would lead to decoherence and entropy production. Therefore, this calculation would also give an improved lower bound on the amount of entropy which must be produced in any model of inflation. Furthermore, the leading interactions between the tensor perturbations are *not* slow-roll suppressed which typically lead them to decohere faster than their scalar counterpart [56]. Anticipating along similar lines, we expect that the entanglement entropy of tensor modes would be somewhat enhanced, and this will be studied in future work. The cubic interactions coupling tensor and scalar modes also need to be taken into account which will result in enhancing both the entanglement entropy density of the scalar as well as the tensor perturbations.

Finally, we note that our analysis has been done in the context of inflationary cosmology, but the methods also apply to other early universe scenarios in which the primordial fluctuations are quantum in origin, in particular to the *matter bounce* and to the *Ekpyrotic* scenarios.

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### Appendix: Full Entanglement entropy

In the main body of the paper, we have shown in detail the derivation of the entanglement entropy due to the  $c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$  terms coming from the interaction Hamiltonian in (3.54). However, as mentioned earlier, there are other terms which also contribute to the entropy. Let us first consider the terms of the form  $c_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$  appearing in (3.54):

$$\left[c_{\mathbf{p}_{1}}c_{-\mathbf{p}_{2}}^{\dagger}c_{-\mathbf{p}_{3}}^{\dagger} + c_{\mathbf{p}_{2}}c_{-\mathbf{p}_{3}}^{\dagger} + c_{\mathbf{p}_{3}}c_{-\mathbf{p}_{2}}^{\dagger}c_{-\mathbf{p}_{3}}^{\dagger}\right]\left(\sqrt{\frac{p_{1}p_{2}}{p_{3}}} + \sqrt{\frac{p_{1}p_{3}}{p_{2}}} + \sqrt{\frac{p_{2}p_{3}}{p_{1}}}\right).$$
 (3.78)

For terms such as these, we can have two possibilities as before – two sub-Hubble modes and one super-Hubble mode or the other way around. Let us take the former case first. In this case, if  $p_1, p_1 > aH$  and  $p_3 < aH$ , then the first term proportional to  $\sqrt{\frac{p_1p_2}{p_3}}$  would naturally be the dominant one. For this case, the only term which contributes would be the last one, proportional to  $c_{\mathbf{p}_3}$ . This is a crucial argument, so let us emphasize it again – the matrix element can be nonzero if there is no annihilation operator present in the inner product corresponding to sub-Hubble modes. The reason for this is the same as why there were no annihilation elements present in the inner product for the flat space calculation.

In this case, we need to calculate an inner product of the form

$$\langle SQ(k,\eta) | c_{\mathbf{p}}c_{\mathbf{q}} | SQ(k,\eta) \rangle = \langle 0_{\mathbf{k}}, 0_{-\mathbf{k}} | S_{k}^{\dagger}(r_{k},\phi_{k}) c_{\mathbf{p}}c_{\mathbf{q}}S_{k}(r_{k},\phi_{k}) | 0_{\mathbf{k}}, 0_{-\mathbf{k}} \rangle$$

$$= -e^{i\phi_{p}} \cosh r_{p} \sinh r_{p} \delta^{3}(\mathbf{p}+\mathbf{q}).$$

$$(3.79)$$

In deriving this, we have used the transformation of the annihilation operator under the unitary action of the squeezing operator, namely [71]

$$S^{-1}aS = a\cosh r + a^{\dagger}e^{i\phi}\sinh r, \qquad (3.80)$$

where we have dropped the momentum indices for simplicity. We have also used the fact that  $S^{\dagger} = S^{-1}$ .

The matrix element corresponding to this term would be given by

$$(cc^{\dagger}c^{\dagger})C_{n,N}^{\mathrm{sq}} \sim -(2\pi)^3 \left(e^{i\phi_{p_3}}\cosh r_{p_3}\sinh r_{p_3}\right) \sqrt{\frac{p_1p_2}{p_3}} \,\delta^3\left(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3\right) \,.$$
 (3.81)

Now let us recall that what enters in the formula of the entanglement entropy is not  $(cc^{\dagger}c^{\dagger})C_{n,N}^{sq}$  but rather its amplitude squared, *i.e.*  $\left|\binom{(cc^{\dagger}c^{\dagger})}{n,N}C_{n,N}^{sq}\right|^{2}$ . In the limit of large squeezing,

 $\sinh r_{p_3} \approx \cosh r_{p_3} \gg 1$ , and it is easy to see that the entanglement entropy corresponding to this term would be the same as that coming from  $s_{\text{ent}}^{I_1}$ , as in (3.64).

Let us now return to our other possibility of having two super-Hubble modes  $p_2, p_3 < aH$ and one sub-Hubble mode  $p_1 > aH$ . In this case, once again, the only nonzero contribution comes from the term proportional to  $c_{\mathbf{p}_3}$  in (3.78). Of course now one of the creation operators,  $c_{\mathbf{p}_2}^{\dagger}$ , corresponds to a super-Hubble mode and thus we have an inner product of the form  $\langle SQ(k,\eta) | c_{\mathbf{p}}c_{-\mathbf{q}}^{\dagger} | SQ(k,\eta) \rangle$  in addition to the one appearing in (3.79). Collecting these terms, the matrix element can easily be calculated to give

$$(cc^{\dagger}c^{\dagger})C_{n,N}^{\text{fold}} \sim -(2\pi)^3 \left(e^{i\phi_{p_3}} \cosh r_{p_3} \sinh r_{p_3}\right) \left(1 + \sinh^2 r_{p_2}\right) \left(\sqrt{\frac{p_1p_3}{p_2}} + \sqrt{\frac{p_1p_2}{p_3}}\right) \delta^3 \left(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3\right) (3.82)$$

Once again, it is easy to see that in the limit  $r_{p_3} \gg 1$ , the contribution of this term to the entanglement entropy would be exactly the same as that of  $s_{\text{ent}}^{I_2}$ . Thus, the contribution of this term would be subdominant, for the same reason as that of  $s_{\text{ent}}^{I_2}$ .

Finally there remains one last type of terms which arise from the interaction Hamiltonian (3.54), which are proportional to  $c_{\mathbf{k}}c_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}}$ . These are the terms which go as

$$\left[c_{\mathbf{p}_{1}}c_{\mathbf{p}_{2}}c_{-\mathbf{p}_{3}}^{\dagger} + c_{\mathbf{p}_{2}}c_{-\mathbf{p}_{3}}^{\dagger} + c_{\mathbf{p}_{3}}c_{\mathbf{p}_{2}}c_{-\mathbf{p}_{3}}^{\dagger}\right]\left(\sqrt{\frac{p_{1}p_{2}}{p_{3}}} + \sqrt{\frac{p_{1}p_{3}}{p_{2}}} + \sqrt{\frac{p_{2}p_{3}}{p_{1}}}\right).$$
(3.83)

For such terms, the only nonzero contribution appears when there are two super-Hubble and one sub-Hubble mode. In this case, there shall appear two factors of the inner product  $\langle SQ(k,\eta)| c_{\mathbf{p}}c_{\mathbf{q}} | SQ(k,\eta) \rangle$  in the matrix element  $(ccc^{\dagger})C_{n,N}^{\text{fold}}$ . It should be clear from the calculations above that the entanglement entropy corresponding to this term shall be the same as  $s_{\text{ent}}^{I_2}$  and shall, therefore, be sub-dominant. Once again, we have assumed the large squeezing limit to arrive at this conclusion.

## Chapter 4

# Conclusion

This thesis presents an overview of our work in determining the entanglement entropy of cosmological perturbations.

First, we reviewed the fundamentals of cosmology, assuming an understanding of Einstein's theory of general relativity. Next, we discussed the quantum theory of cosmological perturbations. Moreover, we discussed bipartite quantum systems in order to define the entanglement entropy. In a discussion of reheating and squeezed vacuum states, we identified links connecting elements of our review. This developed intuition for what we call the entanglement entropy of cosmological perturbations.

In our research paper, we presented the momentum-space entanglement entropy density of scalar perturbations in the metric of an inflationary spacetime, due to the non-linear nature of Einstein's equations. We saw that quantum decoherence leads to the tracing out of non-diagonal density matrix elements, producing a reduced density matrix describing the quantum states of super-Hubble modes. We compared this to the total thermal entropy in reheating, yielding an upper bound on the duration of inflation in line with the second law of thermodynamics and ensuring a graceful exit from accelerated expansion. We closed our paper with next steps and anticipate an application of our methodology to different models of cosmology.

This thesis was simply a glimpse into the author's learning experience in the past year. We hope readers enjoyed being a part of this journey.

# Appendix

The following figure is adopted from [13].



The following figure is adopted from [3].



**FIGURE 8.7** Past light cones in a universe expanding from a Big Bang singularity, illustrating particle horizons in cosmology. Points at recombination, observed today as parts of the cosmic microwave background on opposite sides of the sky, have nonoverlapping past light cones (in conventional cosmology); no causal signal could have influenced them to have the same temperature.

The following figures are adopted from [4].



Figure 2. A sketch (conformal separation vs. time) of the formation of structure problem: the comoving separation  $d_c$  between two clusters is larger than the forward light cone at time  $t_{eq}$ .



Figure 4. Sketch (physical coordinates vs. time) of the solution of the homogeneity problem. During inflation, the forward light cone  $l_f(t)$  is expanded exponentially when measured in physical coordinates. Hence, it does not require many e-foldings of inflation in order that  $l_f(t)$  becomes larger than the past light cone at the time of last scattering. The dashed line is the forward light cone without inflation.



The following figure is adopted from [14].

The following figure is adopted from [7].



Fig. 1. Space-time diagram (sketch) showing the evolution of scales in inflationary cosmology. The vertical axis is time, and the period of inflation lasts between  $t_i$  and  $t_R$ , and is followed by the radiation-dominated phase of standard big bang cosmology. During exponential inflation, the Hubble radius  $H^{-1}$  is constant in physical spatial coordinates (the horizontal axis), whereas it increases linearly in time after  $t_R$ . The physical length corresponding to a fixed comoving length scale labelled by its wavenumber k increases exponentially during inflation but increases less fast than the Hubble radius (namely as  $t^{1/2}$ ), after inflation.
The following figures, adopted from [10], denote the scale factor R(t).



Fig. 8.2: Comparison of the evolution of R and T in the standard and inflationary cosmologies. Note the enormous jump in entropy  $(S \propto R^3 T^3)$  at the end of inflation.



Fig. 8.3: Summary of the evolution of  $\rho_{\phi}$ ,  $\rho_R$ , and S during reheating.



Fig. 8.4: The evolution of the physical size of the comoving scale,  $\lambda$ , and of the Hubble radius,  $H^{-1}$ , in the standard and the inflationary cosmologies. In the standard cosmology (i.e., no inflation) a given scale crosses the horizon but once; while in the inflationary cosmology all scales begin sub-horizon sized, cross outside the horizon ("good bye") during inflation, and re-enter again ("hello again") during the post-inflationary epoch. Note that the largest scales cross outside the horizon first and re-enter last. The growth in the scale factor  $[N = \ln(R_{\rm RH}/R)]$  between the time a scale crosses outside the horizon during inflation and the end of inflation is also indicated. For a galaxy,  $N_{\rm GAL} = \ln(R_{\rm RH}/R_1) \sim 45$ , and for the present horizon scale,  $N_{\rm HOR} = \ln(R_{\rm RH}/R_2) \sim 53$ . Causal microphysics operates only on scales less than  $H^{-1}$  (indicated by arrows). During inflation  $H^{-1} \equiv H_I^{-1} = \text{const}$ , and in the post-inflation era,  $H^{-1} \sim t \propto R^{1/n}$  (n = 1/2—radiation dominated, n = 2/3—matter dominated).

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