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Inflationary Universe

Power Spectra in Single-Field Inflation and Adiabatic Regularization



Alinea, Allan Lambit

Dissertation in Physics
Osaka University

Inflationary Universe

Power Spectra in Single-Field Inflation and Adiabatic Regularization



Alinea, Allan Lambit

under the supervision of
Prof. TAKAHIRO KUBOTA

a dissertation submitted in partial fulfillment
of the requirements for the degree of
Doctor of Science in Physics (March, 2017)

Department of Physics,
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Osaka University, Japan

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B5-paper version

This manuscript was typset using LaTeX installed on the free operating system Ubuntu. Some figures were drawn using LibreOffice, Inkscape, or Gimp or a combination of these softwares. Long calculations were done or verified through Maxima with the WXMaxima front end, Maple™, or Mathematica™. Allan L. Alinea acknowledges the open-source community and makers of the mentioned proprietary softwares for making things possible.

The cover page is a photo of chili peppers situated on top of an inverted elongated deep plate. The chili peppers are arranged to resemble the symbol infinity. This symbol dwells deeply into the core of the subject of this study—adiabatic regularization.

Osaka, Japan 2017

The night, tho' clear, shall frown–
And the stars shall look not down
From their high thrones in the heaven,
With light like Hope to mortals given–
But their red orbs, without beam,
To thy weariness shall seem
As a burning and a fever
Which would cling to thee for ever.
(Spirits of the Dead by Edgar Allan Poe)

When in Rome live like a Roman.
But do not be an unreasonable Roman.
Along the way, normality of nature
guarantees that you will find just people.

There are two types of questions namely,
those that ask something and
those that tell something.
The second type could be evil for it could mean
insult, expression of vanity, humiliation, ...

Publications

Cosmology and Particle Physics

N. Misumi, T. Kubota, and A. L. Alinea, *The double-soft limit in cosmological correlation functions and graviton exchange effects*, JCAP **1701**, no. 01, 013 (2017) [arXiv:1610.02467 [hep-th]]

A. L. Alinea, *Adiabatic regularization of power spectra in nonminimally coupled chaotic inflation*, JCAP **1610**, no. 10, 027 (2016) [arXiv:1607.05328 [gr-qc]].

A. L. Alinea, T. Kubota, and W. Naylor, *Logarithmic divergences in the k-inflationary power spectra computed through the uniform approximation*, JCAP **1602**, no. 02, 028 (2016) [arXiv:1506.08344[gr-qc]].

A. L. Alinea, Y. Nakanishi, T. Kubota, and W. Naylor, *Adiabatic regularisation of power spectra in k-inflation*, JCAP **1506**, no. 06, 019 (2015) [arXiv:1503.08073 [gr-qc]].

Physics Education

AL Alinea and W Naylor, *Polarization of physics on global courses*, 2015 Physics Education **50** 210 [arXiv: 1405.0095]

AL Alinea and W Naylor, *Gender gap and polarization of physics on global courses*, [arXiv:1605.03302]. (submitted for publication)

The above list includes the research articles published (or submitted for publication) during the period AY 2014-2017 corresponding to the duration of the author's doctoral study. It is divided into two main categories namely, Cosmology and Particle Physics, and Physics Education. The latter includes side publications corresponding to the research interest of the author in softer side of physics related to learning experience and its psychology. The former corresponds to the main track of this work. It includes the three main research articles (see the boxed publications above) the subjects of which form the backbone of this manuscript.

Nomenclature

- Unless otherwise specified, the metric signature is $(-,+,+,+)$.
- For the most part, we use natural units where the Planck's constant, the speed of light in vacuum, and Boltzmann constant are all set to unity ($\hbar = c = k_B = 1$).
- The reduced Planck mass $M_{\rm pl} = (\hbar c/8\pi G)^{1/2} = 2.4 \times 10^{18}\,{\rm GeV/c^2}$ is usually set to unity except in **Chapter 8** where it is made explicit to better appreciate the range of field values being compared with $M_{\rm Pl}$.
- The lowercase Greek tensor indices $\alpha, \beta, \ldots$ take on values 0, 1, 2, 3 with 0 being the temporal index and the remaining three numbers being the spatial indices. Lowercase Roman indices on the other hand, take on values 1, 2, and 3 (spatial indices).
- We follow the summation convention: the occurrence of repeated indices unless otherwise specified, indicates summation.
- Derivative with respect to the coordinate time t if not written-out explicitly, is usually denoted by an overdot e.g., $\mathrm{d}x(t)/\mathrm{d}t = \dot{x}(t)$.
- We use the symbol prime as a shorthand for derivative with respect to the conformal time when the argument of a given function is not specified; otherwise, the prime indicates differentiation with respect to the argument of a given function (e.g., $f'(x) = \mathrm{d}f/\mathrm{d}x$).
- Depending on the context, the symbol prime is also used to denote a new quantity (e.g., in the transformation $t \to t' = t + \alpha$), or to distinguish one variable to another when using the same symbol proves economical (e.g., $\mathbf{k}$ and $\mathbf{k}'$ as integration variables).

- Ordinary and partial derivatives are denoted by the usual symbols, e.g., $\partial_i v$, $v_{,i}$, $\mathrm{d}v/\mathrm{d}\tau$, $v_{,\tau}$.

- Covariant derivative is denoted by ∇ or semicolon followed by the index of the variable of differentiation, e.g., $\nabla_\mu A^\alpha$, $A^\alpha_{;\mu}$. When no confusion may arise, we also use ∇_i for spatial covariant derivative in place of the other notation D_i.

- An overbar indicates a given quantity is a background quantity (e.g., $\bar{\phi}$) as opposed to those quantities that include fluctuations about the background (e.g., $\phi(x) = \bar{\phi}(t) + \delta\phi(x)$). It is also used to distinguish the slow-roll parameters in minimally and nonminimally coupled model of inflation (e.g., $\bar{\epsilon}$ vs ϵ.)

- When there is a need to distinguish a classical field from a field operator, we place a hat over an operator.

- A wide hat over a variable means the variable is defined in the Einstein frame as opposed to that in the Jordan frame (e.g., $\widehat{R}$ vs R.)

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Abstract

The power spectrum of primordial cosmological perturbations is one of the most important physical quantities in inflationary cosmology. From a mathematical and field-theoretic perspective, self-consistency requires that two-point function of these perturbations and the power spectrum are divergence-free. In this work, we characterize the divergences present in one implementation of a promising semi-analytical method for calculating the ("bare") power spectrum, namely, uniform approximation. Our analysis indicates that all divergences in the calculation in minimally coupled general single-field inflation, are logarithmic in nature, and that the power spectrum is only finite up to second order in the slow-roll parameters. In addition to this, we perform adiabatic regularization of the power spectrum in two generalizations of the canonical inflation model covering minimally and nonminimally coupled cases. In both of these cases, we find that the physical power spectrum converges to the "bare" power spectrum. This justifies the use of the "bare" power spectrum in standard calculations in inflationary cosmology.

Introduction

It may be said that the biggest thing that a sentient being pasted on the surface of a (spherical) planet can see, is the sky. Humans have been looking up at the sky since time immemorial. Back then when modern humans emerged about 200 000 years ago, this act could be an empty observation without wonder. If it is true that our neural pathways "corrected" themselves to enable deep thinking starting only about 50 000 years ago as what some relics of the past seem to suggest, then we could be staring at the sky, on and off, for about 150 000 years aimlessly. Yet, we were looking up at the sky and it did not matter whether it was aimless or not. The development of intelligence might be slow, but as the largest part of our view was the sky, when we learned how to do science, it was astronomy that we found.

Today, although humans spend significant amount of time looking down on other humans, we still find some time to look up at the sky. Astronomy, the oldest of the natural sciences, emerged as a systematic field of knowledge rooted to observation and logical thinking, from its initial marriage to a less rigorous and highly opinionated field of astrology reflecting our personal but somewhat misguided connection to the heavenly bodies. Through time, astronomy had reached the moon, stars, and galaxies, to the point that we had to construct another science dealing with an even bigger thing—the Universe. Cosmology is the study of the Universe, its history and future, and its large-scale structure. Together with astronomy, cosmology is a fruit of hundreds of thousand years of staring at the sky, a tool to understand the whole sky including us, and a fulfillment of our insatiable curiosity about the sky.

* * * *

Broadly speaking, this work is about the origin of the Universe—the whole sky plus us. Long time ago, way even beyond the formation of our planet, that is, about 14 billion years ago, the Universe was just a speck. Some conditions might have been met for this speck to undergo a rapid exponential expansion—a process called inflation—leading to an increase in size of about a factor of e^{60}. Although it might be good to imagine this as a sort of explosion, the former should be differentiated in that explosion corresponds to a rapid expansion *in* space while inflation is a rapid exponential expansion *of* space. Inflation stretched the ever present quantum fluctuations and amplified them. When inflation finally stopped, the stretched and amplified fluctuations seeded the structure formation that eventually resulted in what we nowadays call galaxies and clusters of galaxies.

Since these large-scale structures originated from quantum fluctuations—the primordial cosmological perturbations—their distribution must be related to the distribution of their origin. It follows that one way to probe into the past, and study the origin of the Universe, is to perform measurements of distribution of the over-densities and under-densities about some mean, attributable to small- and large-scale *matter* fluctuations. Another way is to perform measurements of distribution of the over-densities and under-densities about some mean, attributable to small- and large-scale *radiation* fluctuations. If the Universe were small in the past, then matter and radiation could be entangled in some sort of hot matter-radiation soup, so we may think. The expansion could have disentangled them with the matter fluctuations turning into clusters of galaxies and the radiation left alone by the uninterested matter particles, started traveling freely in space. Since the photons constituting radiation were once coupled with matter back then when the Universe was young, it should carry the imprint of the past in the same way that today's clusters of galaxies do.

Our current understanding of the Universe indicates that it is homogeneous and isotropic on large scales; this is the cosmological principle. This principle is supported by galaxy surveys and measurements of the cosmic microwave background (CMB) radiation—the radiation composed of freely traveling photons we have just described above. Focusing on the latter, the homogeneity and isotropy correspond to a nearly Gaussian distribution of CMB temperature fluctuations. This means that the primordial cosmological perturbations that gave rise to them must have been also nearly Gaussian. If this is so,

from a field-theoretic perspective, the two-point function of the primordial cosmological perturbations, or more particularly, the power spectrum, should be (nearly) sufficient to describe the distribution of the primordial cosmological perturbations and the CMB radiation.

This brings us to the more specific subject of this work within the broader area of inquiry about the origin of the Universe, namely, the power spectrum. Since this is a work in theoretical physics, our focus is on the more abstract aspect of this quantity in relation to quantum fluctuations that gave rise to or affected the formation of the Universe or a part thereof (eg., the CMB). To be clear, we deal with two kinds of fluctuations namely, the scalar and tensor perturbations. From an experimental point of view, the scalar perturbation is directly linked to the CMB temperature fluctuation and the distribution of matter in the Universe while the tensor perturbations are reflected in the polarization of the CMB radiation. From a theoretical point of view, we are interested (a) in the computation of the power spectrum and (b) in questions about the self consistency of such computation. In this work, without ignoring the aim to fulfill the corresponding objective for the former, namely, to compute the power spectrum, the trajectory that we follow is more geared for the latter.

It is hard to fully explain the idea of self-consistency in the calculation of the power spectrum that we wish to convey in the above paragraph, without actually going through a long explanation and mathematical details that may not be suitably covered in this introduction; the main body of this manuscript serves that purpose. Nonetheless, it is imperative that we at least leave some words here to properly introduce the more technical aspect of this work hopefully, in a slightly less technical but understandable way. The question we are interested in, of self-consistency with regards to the calculation of the power spectrum, stems from the divergence of the equal-time two-point functions of scalar and tensor perturbations evaluated at the same point in space—coincidence limit—in the short-wavelength limit.

Mathematically, considering the scalar perturbation ζ (for illustrative purposes), the two-point function $\langle\zeta(\mathbf{x},t)\zeta(\mathbf{y},t)\rangle$ is related to the power spectrum $\Delta_s^2(k,t)$, by the equation

$$\langle\zeta(\mathbf{x},t)\zeta(\mathbf{y},t)\rangle = \int \frac{\mathrm{d}k}{k}\frac{\sin k|\mathbf{x}-\mathbf{y}|}{k|\mathbf{x}-\mathbf{y}|}\Delta_s^2(k,t),$$

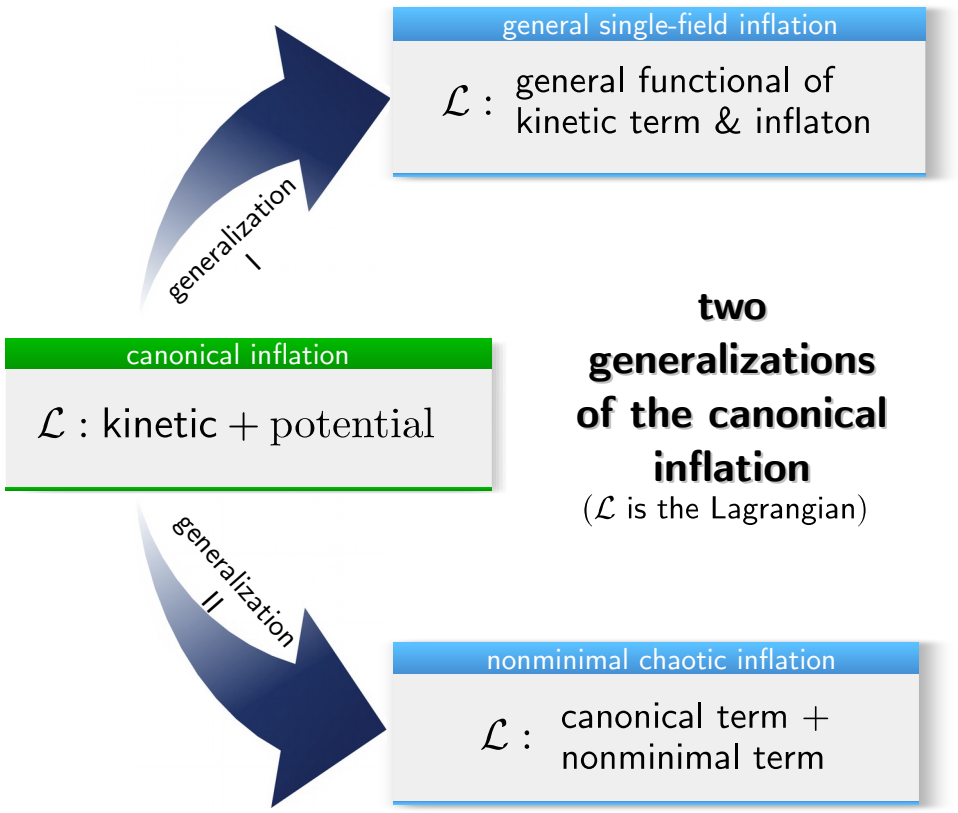
where k is the wavenumber, t is time, and $\mathbf{x}$ indicates position. In the coincidence limit, the cardinal sine function tends to unity and in the short-wavelength limit, the power spectrum tends to $\sim k^2$; thus, the two-point function diverges quadratically in k. One way out of this, and this is what we follow in this work, is to remove the divergences through adiabatic regularization. Put simply, adiabatic regularization decomposes the quantity ζ_k (where the subscript k means it is expressed in Fourier space,) contained in $\Delta_s^2(k,t)$, isolates the divergent-yielding parts, and subtracts the divergent-yielding parts of the integrand above; hence, yielding a finite result.

Consistency-wise, such a regularization of the two-point function is correspondingly reflected in the power spectrum. A similar analysis leads one to consider the same for the case of tensor perturbations. Mathematically, one considers the power spectrum in the equation above as the "bare" power spectrum, $\Delta^{2(b)}$. Then the divergent-yielding parts of the perturbations are used to construct a subtraction term, $\Delta^{2(s)}$. The resulting difference of these two terms is the regularized or physical power spectrum, $\Delta^{2(r)}$; that is,

$$\Delta^{2(r)} = \Delta^{2(b)} - \Delta^{2(s)}.$$

This brings us to the very essence of point (b) above namely, the adiabatic regularization of the power spectrum. To spell it out clearly, *this study aims to perform adiabatic regularization of scalar and tensor power spectra in inflationary cosmology.*

It is worth noting that this research is not the first in line. Some other people have already dealt with the case of canonical inflation (see **Chapter 7**); that is, "basic" single-field inflation described by the standard Lagrangian kinetic-plus-potential term, within the framework of general relativity (and quantum field theory in curved background). In this work, we consider two general cases encompassing the canonical case (see the figure below). The first one involves the generalization of the Lagrangian in the canonical case to that one involving a general functional of the kinetic term and the scalar field that drives inflation—the inflaton. The second one involves the standard kinetic-plus-potential term and an additional term called the nonminimal coupling term, explicitly coupling the inflaton and gravity. The first one does not involve this nonminimal coupling term and is said to be minimally coupled; the second one is said to be nonminimally coupled.



As for the result, in the canonical case, the regularized power spectrum turns out to be simply the "bare" power spectrum. For the power spectrum of observational and theoretical interest in inflationary cosmology, one considers the limit where the perturbations are significantly "stretched" by the inflationary expansion of the Universe; they are termed as superhorizon modes (see **Chapter 5**). In this limit, the "bare" power spectrum is constant while the subtraction term decays with the expansion of the Universe. As it turns out, for the two generalizations we considered in this work, the regularized power spectrum is effectively the same as the "bare" power spectrum both for scalar and tensor perturbations; the result in the canonical case extends to our generalizations.

Such a result might seem surprising and at the same time the calculation looks trivial. It might seem surprising because the subtraction term does not

have a significant effect on the physical power spectrum of observational and theoretical interest. And it might seem trivial because after all the ruckus about regularization, we effectively end up with nothing but the original "bare" power spectrum; the effort might appear useless. However, this mix of two somewhat extreme descriptions, is what makes this study interesting. How $\Delta^{2(s)}$ becomes simply $\Delta^{2(b)}$ is explained in this manuscript with the help of other studies dealing with a similar topic. Such an explanation, and calculations based on sound physics ideas, are necessary to reach the end and to justify the end, even assuming that the end is trivial which we believe it is not.

So far we have elaborated about point (b) above to which as we have mentioned above, this work is geared. Although point (a) takes a minor part, it is necessary that we mention something about it to complete the overall picture that we wish to paint in this introduction. As stated above, point (a) is about the calculation of the power spectrum. In a sense, the adiabatic regularization of power spectrum is a calculation of the power spectrum itself (that is, the regularized one,) but we have positioned it under the domain of inquiry about consistency; a consistent power spectrum corresponds to a finite (not sullied by divergences) two-point function of perturbations that it describes. To be clear, point (a) pertains to the precise calculation of the "bare" power spectrum. It boils down to this because as far as the domain of this study is concerned, the subtraction term can be calculated to any precision we want while this does not hold for the former. In possible future cases that we might discover, wherein the subtraction term might not have a trivial effect, the "bare" power spectrum is the limiter to the precision of the regularized power spectrum. The idea is, if we can calculate it precisely then we will have a good result to be compared with experimental results. This idea is timely due to the ever increasing precision of measurements of the CMB.

Setting aside the complexities associated with quantization, the "bare" power spectrum is essentially derived from a differential equation called the Mukhanov-Sasaki equation. In general, this equation has no analytic solution so theorists often rely on semi-analytical approximations. In the course of this study, while dealing with the adiabatic regularization of power spectrum in minimally coupled general single-field inflation, we stumbled upon a promising semi-analytical method for solving the Mukhanov-Sasaki equation called the uniform approximation; the calculation involved is laborious but the basic idea is simple and unlike some other semi-analytical approximation schemes, the

precision can be extended arbitrarily through analytically computable correction terms. Unfortunately, when we applied it to calculate the power spectrum using an existing expansion scheme for inflationary parameters found in the literature, the method yielded divergent results. Repetition of the laborious calculation from different angles did not eliminate this problem and so we were compelled to instead, examine the problem itself. While not necessarily ignoring the need for the solution of this problem, a rigorous scrutiny of the problem itself, we believe, will the pave the way for a solution that can be crucial to our future studies.

Part of this work then is the examination of the divergences associated with a specific application of the uniform approximation to the calculation of the power spectrum in minimally coupled general single-field inflation. Specifically, we characterize the form of the divergence, and identify where in the list of corrections to some base result for the power spectrum the divergences start to appear. The sections on uniform approximation are lumped in a single chapter together with a discussion involving a less powerful semi-analytical approximation scheme often used in the literature, based on the Hankel function approximation. Owing to the divergence problem associated with the application of the uniform approximation, we opted to use the Hankel-function approximation for the computation of the "bare" power spectra in minimally coupled and nonminimally coupled single-field inflation, to be used in adiabatic regularization.

Scope and Limitation

This study is about the calculation of the regularized power spectra in minimally coupled general single-field inflation and nonminimally coupled single-field (chaotic) inflation, and examination of the divergences in the application of the uniform approximation in the calculation of the ("bare") power spectrum. While we have essentially laid down the coverage of this work above, it is good to mention what this study does not cover in order to have a clearer view of its scope and limitation.

- This study is restricted to single-field inflation, both minimally and nonminimally coupled. Needless to say, we do not cover multi-field inflation. In covering single-field inflation, the scope is limited to slow-roll inflation.

- The power spectrum in this work corresponds to the free-part of the inflationary action. No attempt is made to incorporate the interaction terms. As such, we do not deal with loop corrections and the interesting topic of non-Gaussianity, much less the question of renormalizability.

- This is not a research on the experimental side of inflationary cosmology. Readers will not find here extensive tables of recent experimental results, designs of the latest instruments to probe the CMB or far away galaxies, and recent advances on data analysis. We simply quote some data from the literature as needed, to have a feel about the magnitudes of some physical quantities in inflationary cosmology in our discussions.

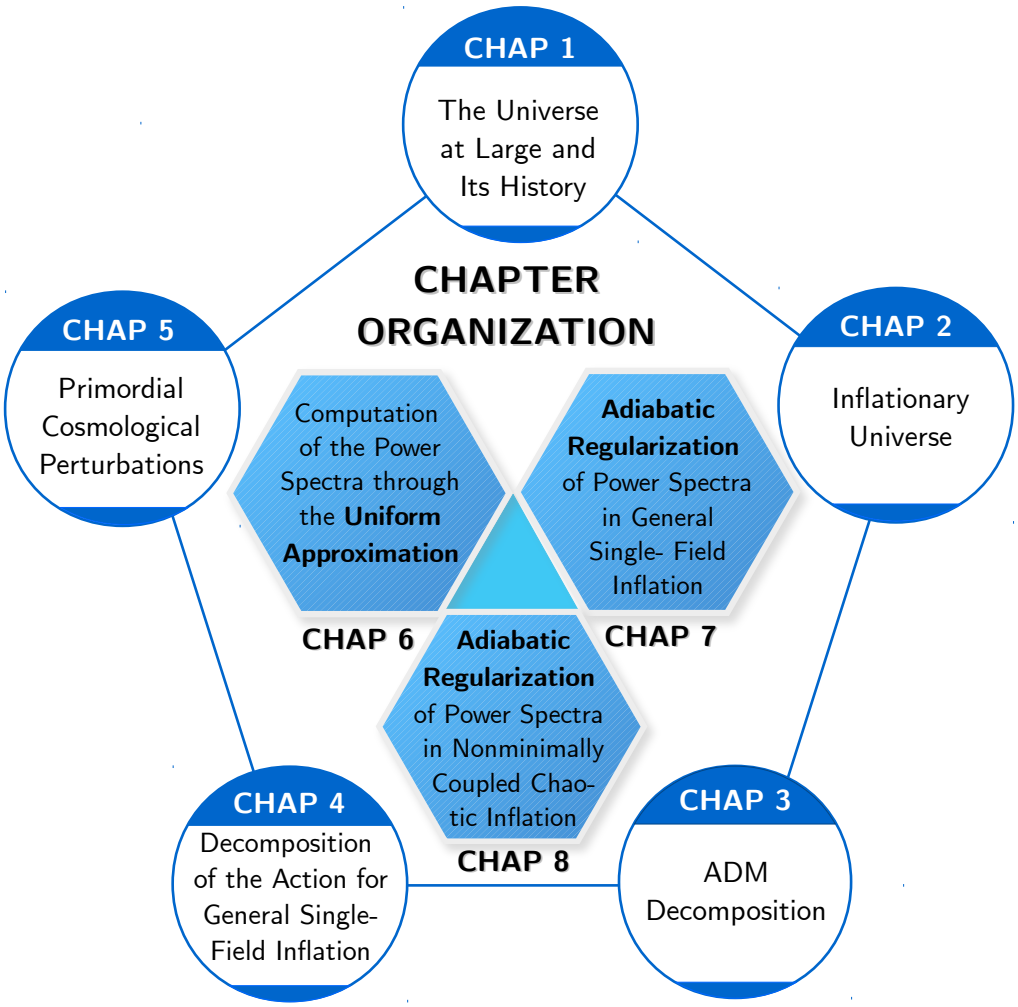
- The discussion on nonminimally coupled chaotic inflation includes a calculation involving frame transformation; from Jordan frame to Einstein frame and vice versa. The adiabatic subtraction in the process of adiabatic regularization we perform in this case, is done only in the Jordan frame. As the analysis could take up significant space so as to require a manuscript of its own, we do not deeply examine here the frame invariance of adiabatic regularization.

- The use of the uniform approximation in the calculation of power spectra is restricted to the leading order. We do not include in our calculation the error correction terms associated with this semi-analytical approximation scheme. These correction terms are not necessary in the analysis of the divergences resulting from the specific application of this method we cover in this work.

Organization

This manuscript consists mainly of eight chapters that can be divided into two main divisions (see the figure below). The first division includes the first five chapters covering the ideas needed to understand the conceptual underpinnings of cosmic inflation, and mathematical and field-theoretic tools crucial in dealing with the more rigorous aspect of this topic in relation to adiabatic regularization and uniform approximation of the power spectrum. **Chapter 1** is about the homogeneous and isotropic universe (on large scales) that we have. It covers a short history of the Universe and the background equations termed

as the Friedmann equations describing the Universe. In **Chapter 2**, we pose the



question why the Universe is effectively homogeneous (and isotropic) and discuss inflation as a good theory to answer this question. This chapter basically introduces the notion of inflation from a conceptual and field-theoretic point of view. **Chapter 3** contains the mathematical instrument in the name of ADM decomposition helpful in decomposing the action describing single-field inflation with respect to the primordial cosmological perturbations. In **Chapter 4** we use this decomposition scheme to calculate the second-order action necessary

to calculate the power spectrum. It is also in this chapter, that we formally introduce and mathematically define the gauge-invariant primordial cosmological perturbations. The following chapter—**Chapter 5**—covers the derivation of the Mukhanov-Sasaki equation and a rigorous description and analysis of the behavior of primordial cosmological perturbations. In preparation for the calculation of the power spectrum in the next chapter, we derive the basic working equation for the power spectrum in terms of the perturbations, in this chapter.

The second division forms the bulk of the original research in this work. Readers with sufficient familiarity with the fundamental ideas laid down in the first division (e.g., researchers in the field of inflationary cosmology) may directly jump to the second division for a fast reading of this manuscript. It includes three chapters covering uniform approximation and adiabatic regularization. In **Chapter 6**, we introduce the method of uniform approximation, its promising features, and possible practical defects in its implementation as a tool to calculate the ("bare") power spectrum. Together with this method, we also included a relatively short but sufficient discussion of another approximation scheme based on using the Hankel function. Whereas our treatment of uniform approximation is mainly restricted to some technical problems associated with its use, the Hankel approximation is the one we mainly use for the actual calculation of the ("bare") power spectrum. In the last two chapters—**Chapters 7** and **8**—we deal with the adiabatic regularization of power spectrum, with **Chapter 7** containing the bulk of the discussion about the basics of this regularization scheme. The second to the last chapter involves minimally coupled general single-field inflation while the last chapter deals with the nonminimally coupled single-field (chaotic) inflation. Note that although the preparatory ideas covered in the first division is laid down with a minimally-coupled inflation in mind, as the nonminimally coupled case is only covered in **Chapter 8**, their utility extends up to the last chapter. The additional supporting ideas needed to comprehend nonminimally coupled inflation are provided in last chapter.

The Way this Manuscript is Written

When a researcher dives deeper into his or her own field of study, there usually comes a point when some concepts and relationships become self-evident truths that he or she may not be able to explain them to an uninitiated person.

In some respect, this may be seen as one of the ways by which the brain conserves its resources; when a certain relationship is established, its utility in succeeding investigation may elevate it to an ensemble of self-explanatory primitive constructs that serve as ground to probe more complicated questions. However, because these constructs are in fact, only pseudo-primitive as they are based on more fundamental ideas, there might come a point when we might lose grip of them and someday ask why they hold in the first place. Furthermore, to a curious newcomer, ideas and relationships which are second-nature to an expert in a given field of study, an elaboration based on these "obvious" things might lead only to confusion.

This manuscript is written with the aim that it will be useful to the widest audience possible and to the same person who wrote this work as an easy reference. While it might not be possible to convey what is inside to a grade one student, we hope to reach curious newcomers with minimal exposure to quantum field theory and general relativity. Knowledge of inflationary cosmology, the big field encompassing this work, is not assumed. Ideas including standard inflation, gauge-invariant cosmological perturbations, adiabatic regularization, nonminimally coupled inflation, among others, are introduced and developed along the way. We have tried our best to minimize forcing the reader to look somewhere else to understand what we wish to convey. Nonetheless, as we believe[1] in the value of further reading to widen one's horizon, relevant references are always included as a backup for those who need deeper understanding.

And in so trying to adhere to the above-mentioned aim, this manuscript has been written like a "student-friendly" book in physical appearance and the way the content is delivered (and not like a typical minimalistic research paper). Derivations are laid down carefully with all the relevant details. Important relationships and ideas are elaborated usually both from a quantitative and conceptual point of views. Statements that might lead to confusion are carefully explained and relevant footnotes are added to avoid possible conceptual pitfalls. To reinforce understanding particularly in some parts containing lengthy discussion and derivations, important equations are boxed and new concepts are written in a **bold-serif** format. Furthermore, some calculations are compartmentalized into worked out examples complete with title, to avoid long continuous discussion devoid of visual indication of what is being discussed.

[1] Needless to say, this belief is encoded in the usual requirement that a dissertation manuscript should include in-line citations.

To give a good bird's eye view to the reader of the content of each chapter, apart from the table of contents, each chapter opens with an outline, and a short introduction telling the reader what a given chapter is all about. Finally, to facilitate ease of reading, we have formatted this manuscript incorporating best practices in typography including optimal text width, relatively wide line spacing, conspicuous headings, etc.

Having said this, one cannot be so certain about the work that he has made; the judge of a painting is not the painter himself. Moreover, upon rereading some pages of this manuscript, the author of this manuscript could still see some parts inviting modification for better readability and pruning for a better fit in a unified whole. This work was written during a period dotted by tumultuous times when will could be the only source of water to quench the thirst of a dying plant. In spite of this, we have strived to produce a good one. Our hope is that in spite of its shortcomings, some people might find it useful. But for which the intention might not find the bins outside, it shall default to the soul who created this work; a painter can judge and appreciate his own painting if it is made primarily for himself.

Acknowledgment

> *Let us leave it to the flow of air on whether we have to thank people because they are doing their job. Irrespective of whatever decorations upon their names, we should not thank people because they simply exist. And certainly, we should not extend our gratitude to people because they are harmful.*

In the field of science it is hardly possible to find a research work not sitting on top of other research works, and this study is no exception. Furthermore, as we are humans whose logic circuitry can sometimes fuse well with idiocy and sometimes smoothly connect to reason, we owe our continuous improvement not only to pure reasonableness of life but also to human enabling factors helpful to live a good life and do good research. I am indebted to all the brilliant minds who set up and continue to improve the now complex but powerful knowledge structure of cosmology and particle physics, to the trees, walls, mountains, and sky to stare upon during my quite moments, and to all the good people many of whom might not have directly contributed to the completion of this work but in one way or another have added color to my life.

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CHAPTER

1

The Universe at Large and Its History

THE UNIVERSE IS FULL OF MAGICAL THINGS
PATIENTLY WAITING FOR OUR WITS TO GROW SHARPER

EDEN PHILLPOTTS
A SHADOW PASSES, 1919

1.1 History of the Universe
1.2 The Homogeneous Isotropic Universe
1.3 Friedmann Equations

Within the bounds of our senses and the "senses" of our tools, the Universe is undoubtedly the biggest thing known to us. Yet in spite of its size and complexity, it is comprehensible (or at least, this is what we choose to believe). In this chapter, we begin our journey of the incomprehensible comprehensibility of the Universe in relation to the subject and scope of this work.

In what follows, based on the standard Big Bang cosmology with inflation, we write down the chronology of the different epochs in the history of the Universe. This chronology is essential in establishing where this study stands in the spectrum laid down by time. After this history, we discuss a simple universe, a homogeneous isotropic system, that happens to be ours at large scales. Then we state the corresponding metric known as the FLRW metric, and derive the Friedmann and continuity equations governing the evolution of a homogeneous isotropic universe, from the Einstein field equations.

1.1 History of the Universe

Current experimental data tell us that in general, electromagnetic waves emitted by clusters of galaxies are redshifted. Such a stretching of wavelength can be attributed to the recession of heavenly bodies from us. Furthermore, the degree of redshift increases with distance from us, meaning that the farther they are, the faster they recede. If we believe that we are not in a special place in the Universe as what we otherwise initially thought, we reach a conclusion that the Universe is expanding.

If the Universe is expanding today and also yesterday, then if we extrapolate backward, we might be able to see it in a very compressed hot state during the very early times. Our current theoretical understanding of how nature works does not allow us to have a concrete and definite description that goes in accord with experiment, of this very early time when the Universe might be in the state of being a singularity. Nevertheless, we have enough to speculate and this "speculation" becomes more and more accurate as we go nearer to the present from the past.

And so it goes that in the past, about 13.7 billion years, the Universe starting from the very dense and hot state near the singularity, underwent a big bang. In what follows we describe the different epochs following this event. Our qualitative description is based on the standard Big Bang cosmology (ΛCDM Model) plus the theory of inflation (see below). Discussions of this chronology can be found scattered in refs. [1, 2, 3, 4].

Planck epoch (10^{-43} s after the Big Bang). There is a limit as to how far we can go back in time to describe what was going on. The approximate time $\sim 10^{-43}$ s (Planck time) may be that limit. During the Planck epoch, all the four fundamental interactions are thought to be unified. By being unified we mean that the gravitational, electromagnetic, weak, and strong interactions behave as one interaction. The energy scale permitting such a unification is of the order of 10^{19} GeV.

GUT (Grand Unification Theory) epoch ($\sim 10^{-43}$ s to $\sim 10^{-36}$ s after the Big Bang). At the end of the Planck epoch, gravity separated from the other three interactions. The energy scale of about 10^{16} GeV however, allowed the grand unification of the electroweak and strong nuclear interactions. (It is worth noting that general relativity is applicable for describing the dynamics of the Universe during the GUT epoch; i.e.,

below 10^{19} GeV). The Universe was composed of a soup of GUT particles like quarks, antiquarks, gluons, leptons, etc, that freely transform from one type of particle to another, and graviton. GUT particle interactions during this epoch might have violated the conservation of baryon number. This might have resulted in the asymmetry between matter and antimatter at the end of the period.

Inflationary epoch ($\sim 10^{-36}$ s to 10^{-32} s). The Universe went into a period of extremely rapid exponential growth. This process called **inflation**, smoothed out the Universe making it homogeneous. At the end of inflation, the particle responsible for such a process called **inflaton**, decayed into standard model particles. This **reheating** of the Universe filled it with quark-gluon plasma. Note that the placement of inflationary epoch before or after the electroweak epoch is not certain. Furthermore, in inflationary cosmology, the start of reheating after the end of inflation is considered as the beginning of the usual Big Bang expansion.

Electroweak epoch (10^{-32} s to 10^{-12} s). The strong nuclear interaction decoupled from the still-unified electroweak interaction. Sufficiently high energy enabled the production of large quantities of heavy electroweak bosons ($W^{\pm}$, Z^0) and Higgs bosons.

Quark, Hadron, and Lepton epochs (10^{-12} s to $\sim$ 3 minutes). At around 10^{-10} s, the electroweak interaction separated into electromagnetic and weak interactions. The interaction between the Higgs field through some symmetry-breaking process, resulted to many particles like quarks, leptons, etc, gaining mass. As the Universe continued to cool down, nucleosynthesis started—quarks combined to form mesons (e.g., π mesons) and baryons (e.g., protons and neutrons) and heavier baryons. Hadrons heavier than baryons decayed as the temperature continued to drop. Moreover, quark-anti-quark pairs annihilated leaving mainly residual quarks (that formed hadrons) from the quark-anti-quark asymmetry. However, the temperature was still high enough to support the existence of lepton-antilepton pairs. At around one second, neutrinos decoupled and became free-streaming. A little farther beyond this time, lepton and anti-leptons annihilated leaving mainly residual leptons from the lepton-antilepton asymmetry.

Radiation epoch ($\sim$ 10 s to $\sim$ 10 000 years). The annihilation of the particle-antiparticle pairs paved the way for the radiation epoch. Since there was only a slight asymmetry between particle and anti-particles, the Universe became dominated by radiation. The high radiation pressure prevented the formation of structures. During the early parts of the radiation era, big bang nucleosynthesis took place. Protons and neutrons combined to form the nucleus of light nucleons such as helium and deuterium.

Matter epoch ($\sim$ 10 000 years to present). At around 10 000 years after the Big Bang, the matter and radiation density became equal. This equality does not translate to equality between number densities of photons and massive particles. Photons during this time still far outnumbers massive particles for a significant combination of ions and electrons to form neutral atoms, to take place. The Universe was dominated by ions and radiation, that were continually exchanging energy. Beyond this time, the progressive expansion of the Universe stretched the wavelength of photons and reduced their number density thereby reducing the interaction rate between ions and electrons, and photons. At around 380 000 years after the Big Bang, photons decoupled and became free-streaming. The free-streaming photons became what we observe today as the **cosmic microwave background (CMB) radiation**.

Prior to **photon decoupling** , when matter dominated the Universe, structure formation started. For a given system of massive particles, given sufficiently high density, gravitational collapse can take place. Initially, such a collapse would happen but high radiation pressure would trigger the opposite—expanding the collapsed system. This took place in a repetitive manner that is, collapse and expansion, until the photons became scarce enough to interfere with structure formation.

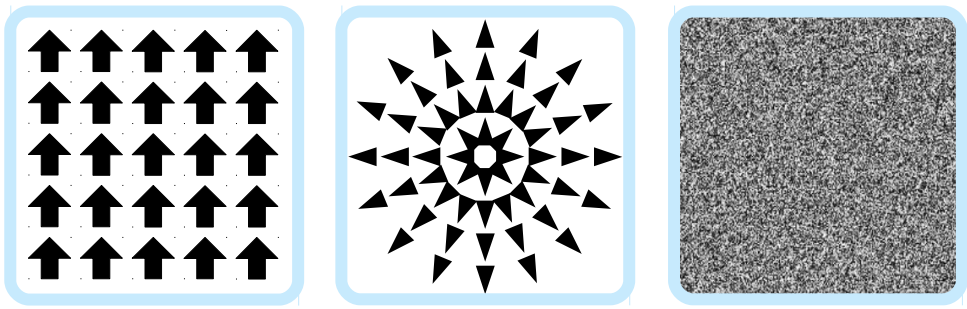
Structure formation was greatly facilitated by the presence of dark matter. They populated the denser regions corresponding to initial fluctuations left by inflation. These denser regions became even more dense through the attraction of more particles. The progressive gravitational collapse paved the way for galaxies and clusters that we now believed to be dominated by dark matter.

One point should be mentioned regarding CMB. When photons were tightly coupled to matter, dense "matter region" also implies dense "photon region". As such, when photons decoupled they carried with them the information of the inhomogeneities of the Universe. Since these inhomogeneities trace itself back to inflaton fluctuations, it can tell us a lot about the early Universe.

For the most part, the above-mentioned history (minus inflationary epoch) rests on the standard Big Bang cosmology that in turn, stands on the ground of particle physics, general relativity, and the so-called **four pillars**. These pillars include the (a) Hubble diagram "testifying" the expansion of the Universe, (b) prediction and detection of the CMB, (c) conformity between the predicted and observed abundance of light elements in the Universe, and (d) bottom-up structure formation. In other words, the striking agreement with experiment gives us a good reason to believe that it is a good model to describe the Universe. In spite of this, the standard Big Bang cosmology also brought on the table lots of questions aside from the answers it provided. The homogeneity of the Universe for instance, is something that one cannot just assume. For this problem, inflation comes to the rescue. We will return to this part in the next chapter and see how inflation solves many of the problems left behind by the standard Big Bang cosmology.

1.2 The Homogeneous Isotropic Universe

The **homogeneity** of a given system means uniformity of a set of properties ascribed to that system at all locations in that system for a given direction; a homogeneous system is translation invariant (see **Fig. 1.1**). **Isotropy** means uniformity of a set of properties ascribed to a given system at all directions at a given location in that system; an isotropic system is rotation invariant (about this given location). On a scale of few hundred Megaparsecs, sky surveys indicate that galaxies, clusters, and superclusters are uniformly distributed. Furthermore, the uniformity of CMB from all directions in the sky indicate that the Universe is also isotropic. *The assertion that all positions in the Universe are essentially equivalent, except for local irregularities, is known as the* **Cosmological Principle** [5].



homogeneous but not isotropic | **isotropic** but not homogeneous | **homogeneous** and **isotropic**

Figure 1.1: Homogeneous and/or isotropic system. A homogeneous system is translation invariant (left). An isotropic system is rotation invariant (middle). A homogeneous isotropic system is both translation and rotation invariant (right).

Given a homogeneous isotropic universe, we assign a spatial coordinate system x^i, $i = 1, 2, 3$. For an expanding universe like ours, it is more convenient to let x^i be a **comoving coordinate system**. With this coordinate system, the distance of two points in our homogeneous isotropic system as well as their locations, is constant. We can use a **scale factor** $a(t)$ to find time-evolving **physical distance** between two objects by multiplying $a(t)$ and the corresponding fixed comoving distance. The quantity $a(t)$ embodies the idea of how large or small a given region is with respect to time. The evolution of $a(t)$ is described by the so-called **Hubble parameter** defined by

Hubble Parameter

$$H \equiv \frac{\dot{a}}{a}, \tag{1.1}$$

where the overdot means differentiation with respect to t. Needless to say, the Hubble parameter is not necessarily constant (with time).

A homogeneous isotropic spacetime is characterized by the so-called **Friedmann-Lemaître-Robertson-Walker (FLRW) metric**. It is given by [6]

$$ds^2 = -dt^2 + a^2(t)\left[\delta_{ij}\mathrm{d}x^i\mathrm{d}x^j + K\frac{(\delta_{ij}x^i\mathrm{d}x^j)^2}{1 - K\delta_{ij}x^ix^j}\right], \tag{1.2}$$

where K tells us whether the three-dimensional (3D) spatial subspace of the 4D manifold is spherical ($K = 1$), hyperspherical ($K = -1$) or Euclidean ($K = 0$)[1]. In this work, beyond the next chapter (where we discuss the flatness problem in relation to the *general* Friedmann equation with $K \in \{-1, 0, 1\}$), unless otherwise specified, we always take $K = 0$, i.e., the 3D spatial submanifold is a (flat) **Euclidean space**. When K vanishes, the FLRW metric simplifies to

FLRW Metric

$$ds^2 = -dt^2 + a^2(t)\,\delta_{ij}\mathrm{d}x^i\mathrm{d}x^j. \tag{1.3}$$

Experimentally, based on 2015 Planck results, K is constrained as $\Omega_K = 0.000 \pm 0.005$, at $2\sigma \approx 95\%$ [99], where $\Omega_K \equiv -K/(a_0H_0)^2$, with the subscript zero indicating the present time.

The scalar curvature of the spacetime described by the metric (1.2) is given by

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right) + 6\frac{K}{a^2}. \tag{1.4}$$

Because the time derivative of H can be written as

$$\dot{H} = \frac{\ddot{a}}{a} - \frac{\dot{a}^2}{a^2}, \tag{1.5}$$

in terms of H, the scalar curvature can be expressed as

$$R = 6(\dot{H} + 2H^2) + 6\frac{K}{a^2}. \tag{1.6}$$

Note that when H is constant (and K vanishes) $R = 12H^2 =$ constant. In the limit of constant Hubble "constant" (as is nearly obeyed during inflation,) the 4D spacetime described by the FLRW metric becomes a **de Sitter spacetime**—*a positively curved maximally symmetric spacetime* [8].

[1] Since K is dimensionless, the comoving coordinate x^i has to be dimensionless as well. As a consequence, the scale factor a must then have a dimension of length to be consistent with the dimension of t. Note however, that when K vanishes, whatever is its dimension, we can freely choose a to be dimensionless and x^i to have a dimension of length.

1.3 Friedmann Equations

The time evolution of the scale factor and Hubble parameter is governed by the Einstein field equations given by

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + g_{\mu\nu}\Lambda = \frac{8\pi G}{c^4}T_{\mu\nu}, \tag{1.7}$$

where $R_{\mu\nu}$ is the Ricci tensor, $g_{\mu\nu}$ is metric tensor component, Λ is the cosmological constant, G is Newton's gravitational constant, c is the speed of light, and $T_{\mu\nu}$ is the symmetric energy-momentum tensor. For convenience we set $8\pi G = c = 1$. We also absorb the term involving the cosmological constant to $T_{\mu\nu}$ and simply rewrite the field equations as

$$R^{\mu}{}_{\nu} - \frac{1}{2}\delta^{\mu}_{\nu}R = T^{\mu}{}_{\nu}. \tag{1.8}$$

Now, consider a perfect fluid with energy-momentum tensor given by

$$T_{\mu\nu} = (\rho + p)U_{\mu}U_{\nu} + pg_{\mu\nu}, \tag{1.9}$$

where ρ and p are the energy density and pressure respectively, of the fluid and U^{μ} is its four velocity. Since we absorbed the cosmological constant into the energy momentum tensor, included in ρ and p are possibly non-vanishing energy density and pressure due to Λ. Furthermore, since we are at the moment looking into a homogeneous isotropic system, then the energy density and pressure are both independent of spatial coordinates; i.e., $\rho = \rho(t)$ and $p = p(t)$. These two are related by the equation of state given as

$$p = w\rho, \tag{1.10}$$

where $w = 0$ for non-relativistic matter or dust, $w = 1/3$ for radiation [9], and $w = -1$ for vacuum energy[2].

[2] This can be appreciated rather *informally* using a simple thought experiment. Consider a cylindrical tube equipped with a piston and inside is a vacuum. Pulling the piston will create more vacuum energy. Since vacuum energy density is constant, the additional vacuum energy generated by pulling the piston must have been supplied by the one who pulled the piston. So while the piston is being pulled, there must be a negative pressure against the piston. More quantitatively, for an adiabatic thermodynamic system, this constancy of the vacuum energy implies a pressure equal to negative of the energy density; i.e., $p = -\rho$.

We wish to write down the independent equations that can be derived from the field equations (1.8). For the left hand side, we need the components of the Ricci tensor.

$$R_{00} = -3\frac{\ddot{a}}{a} = -3(\dot{H} + H^2),$$
$$R_{ij} = g_{ij}\left(\frac{\ddot{a}}{a} + 2\frac{\dot{a}^2}{a^2} + \frac{2K}{a^2}\right) = g_{ij}\left(\dot{H} + 3H^2 + \frac{2K}{a^2}\right). \tag{1.11}$$

Needless to say, g_{ij} is the spatial metric resulting from rewriting the FLRW metric (1.2) as $\mathrm{d}s^2 = -\mathrm{d}t^2 + g_{ij}\mathrm{d}x^i\mathrm{d}x^j$. When K vanishes, $g_{ij} = a^2(t)\delta_{ij}$. We have made used of the definition of the Hubble parameter and (1.5) in order to expressed the components of the Ricci tensor in terms of the Hubble parameter.

For the right hand side of the field equations, we need the components of the energy-momentum tensor. To make things easy, we choose a frame where the fluid is at rest. We can then take $U^\mu = (U^0, 0, 0, 0)$ and impose the normalization condition $g_{\mu\nu}U^\mu U^\nu = -1$ to have $U^\mu = (1, 0, 0, 0)$. As such $T^\mu{}_\nu = \mathrm{diag}(-\rho, p, p, p)$. At this point we can see that since the metric, Ricci tensor, and energy-momentum tensor are all diagonal and the corresponding non-vanishing ij-components are all equal, then there are only two independent equations that we can obtain from the field equations.

For the 00-component of the field equations we have

$$R^0{}_0 - \frac{1}{2}R = -\rho,$$
$$+3(\dot{H} + H^2) - 3(\dot{H} + 2H^2) - \frac{3K}{a^2} = -\rho$$

(First) Friedmann Equation

$$\boxed{H^2 = \frac{\rho(t)}{3} - \frac{K}{a^2}.} \tag{1.12}$$

We call this the **first Friedmann equation** (more commonly known simply as the Friedmann equation). It relates the Hubble parameter describing the rate of expansion with the energy density.

For the ij-components of the field equations we have

$$R^i{}_j - \frac{1}{2}\delta^i_j R = T^i{}_j,$$

$$
\begin{aligned}
g^{ik}R_{kj} - \frac{1}{2}\delta^i_j R &= p\delta^i_j, \\
g^{ik}g_{kj}\left(\dot{H} + 3H^2 + \frac{2K}{a^2}\right) - 3\delta^i_j\left(\dot{H} + 2H^2 + \frac{K}{a^2}\right) &= p\delta^i_j, \\
-2\dot{H} - 3H^2 - \frac{K}{a^2} &= p, \\
-2\dot{H} - \rho + \frac{2K}{a^2} &= p, \\
\dot{H} &= -\frac{1}{2}(\rho + p) + \frac{K}{a^2}.
\end{aligned}
\tag{1.13}
$$

We note from (1.5) that $\ddot{a}/a = \dot{H} + H^2$. From the first Friedmann equation, we see that adding H^2 to both sides of the last of (1.13) amounts to adding $\rho/3$ and that terms involving K cancel. As such,

Second Friedmann Equation

$$\dot{H} + H^2 = \frac{\ddot{a}}{a} = -\frac{1}{6}(\rho + 3p). \tag{1.14}$$

We call it the **second Friedmann equation**. It involves the second derivative of the scale factor with respect to time. Whereas the first Friedmann equation tells us the "velocity" of expansion as dictated by the energy density, the second Friedmann equation tells us the "acceleration" of this expansion as dictated by energy density and pressure.

The first and second Friedmann equations constitute the set of two independent equations that can be derived from the Einstein field equations for a homogeneous isotropic universe with a perfect fluid as a source. Together with the equation of state, $p = w\rho$, and appropriate boundary conditions, the three equations tell us how such a universe will evolve with time.



Example 1. ***Continuity equation.*** The continuity equation relates the energy density and pressure as

Continuity Equation

$$\dot{\rho} = -3H(\rho + p). \tag{1.15}$$

Derive this relation from the first Friedmann equation and the result from ij-components of the Einstein field equations given by (1.13).

Solution. We take the derivative with respect to time of the first Friedmann equation.

$$2H\dot{H} = \frac{\dot{\rho}}{3} + \frac{2HK}{a^2} \qquad \Rightarrow \qquad \dot{H} = \frac{\dot{\rho}}{6H} + \frac{K}{a^2}\,. \tag{1.16}$$

Then, noting that $\dot{H} = -\frac{1}{2}(\rho+p) + \frac{K}{a^2}$ from (1.13) we find $\dot{\rho} = -3H(\rho+p)$, which was to be derived. Observe that this relation although we have made used of equations involving K, does not involve K. Furthermore, note that perhaps more fundamentally, it is a direct consequence of the covariant conservation equation for the energy-momentum tensor namely, $\nabla_\mu T^{\mu\nu} = 0$. What we have followed above then may be viewed as an alternative route leading to the continuity equation.



CHAPTER

2

Inflationary Universe

So the Scientific version of the Big Bang theory
is not really a theory of a bang,
it's really a theory of the aftermath of a bang.

Alan Guth
MIT Lecture on the Early Universe, 2013

2.1 Comoving Particle Horizon and Flatness Problems

2.2 Solution through Inflation

2.3 Single-Field Slow-Roll Inflation

Inflation is the current paradigm describing the very early stages of the Universe before the big bang. It is a complementary patch for the standard Big Bang cosmology that offers solution to two of the most puzzling problems of this theory namely, the horizon and flatness problems. In what follows, we explain these two problems and their solution through cosmic inflation. In so doing, we elaborate the "old" inflation theory proposed by Alan Guth. It contains the core ideas needed to solve the two mentioned problems but has a serious defect—inflation cannot be stopped smoothly. Then we explain how this defect is mended through the introduction of the slow-roll inflation.

2.1 Comoving Particle Horizon and Flatness Problems

The maximum physical distance covered by light from some initial time t_i (that we take as the "beginning" of the Universe) to some arbitrary t is simply $\int_{t_i}^{t} c\,\mathrm{d}\tilde{t}$. We divide the integrand by the scale factor to gain the corresponding maximum comoving distance:

$$\tau = \int_{t_i}^{t} \frac{c\,\mathrm{d}\tilde{t}}{a(\tilde{t})}\,. \tag{2.1}$$

The quantity τ in $\mathrm{d}\tau \equiv c\,\mathrm{d}t/a$ is called the **conformal time**. Evaluated from the beginning of the Universe to t, we call it the **comoving particle horizon**. The name *horizon* came from the idea that particles separated by a comoving distance greater than τ could not have communicated to each other in the past; there is a horizon separating spherical regions of radius τ.

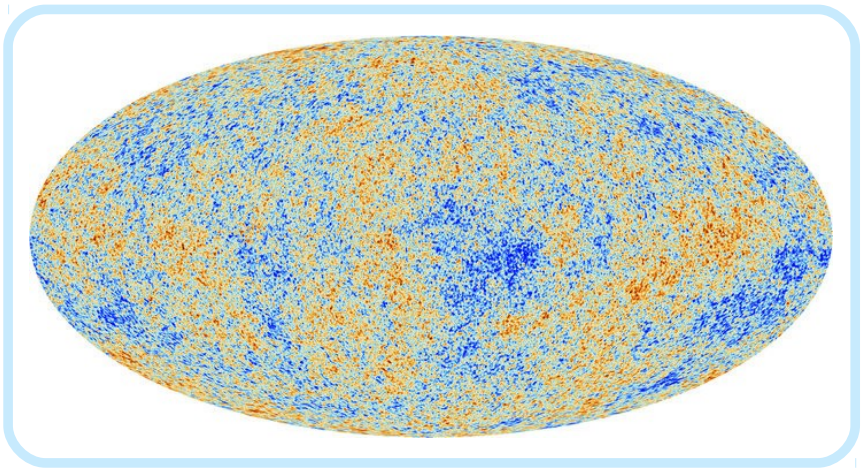


Figure 2.1: Planck all-sky CMB radiation map. The colormap shows the temperature fluctuation of ± 500 μK of the CMB radiation (red is hot and blue is cold) about a uniform background of 2.73 K. [Credit: ESA and the Planck Collaboration (used with permission)].

We run into trouble if we apply this concept to CMB radiation. Observations indicate that the CMB radiation has an isotropic temperature of 2.72548 $\pm$ 0.00057 K (see **Fig. 2.1**) [10]. Such a very small variation is quite intriguing

from the viewpoint of standard Big Bang cosmology because the regions corresponding to CMB radiation coming from two opposite directions in the sky for instance, could not have communicated before to have the same temperature. This is the **horizon problem**.

Another problem facing the standard Big Bang cosmology is the so-called **flatness problem**. To explain this we start with the notion of critical density defined as

$$\rho_c \equiv \frac{3H^2}{8\pi G} = 3H^2. \tag{2.2}$$

Needless to say, the critical density is not necessarily constant. The first Friedmann equation reads

$$H^2 = \frac{\rho}{3} - \frac{K}{a^2}. \tag{2.3}$$

When K vanishes, the energy density above is simply the critical density; a flat Universe has $\rho = \rho_c$. During the early times, matter and radiation dominate the Universe. Since radiation and matter energy densities are proportional to a^{-4} and a^{-3} respectively, then one can neglect K in the equation above. As such, as we go back to the earliest parts of the history of the Universe, the energy density approaches the critical density ρ_c; i.e.,

$$\lim_{t \to t_i} \rho = 3H^2 = \rho_c. \tag{2.4}$$

The total energy density ρ of the Universe can be written as a sum of that of matter, vacuum, and radiation.

$$\rho = \rho_{0,c} \left[\Omega_\Lambda + \Omega_m \left(\frac{a_0}{a} \right)^3 + \Omega_r \left(\frac{a_0}{a} \right)^4 \right], \tag{2.5}$$

The subscript 0 indicates the value today. The quantities Ω_Λ, Ω_m, and Ω_r are the *current* ratios of vacuum, matter, and radiation energy densities respectively, and the *current* critical density $\rho_{0,c}$. If we consider the time today, then $a = a_0$ and

$$\frac{\rho_0}{\rho_{0,c}} \equiv \Omega_0 = \Omega_\Lambda + \Omega_m + \Omega_r. \tag{2.6}$$

Based on the first Friedmann equation above, the difference between 1 and Ω_0

is proportional to K. We call this difference Ω_K.

$$\Omega_K \equiv 1 - \Omega_0 = -\frac{K}{(a_0 H_0)^2}. \tag{2.7}$$

The Planck Collaboration gives $\Omega_K = 0.000 \pm 0.005$, at $2\sigma \approx 95\%$; the Universe in other words, is flat today to within 0.5% [99].

To see why this is a problem we use the first Friedmann equation again.

$$\begin{aligned} H^2 &= \frac{\rho}{3} - \frac{K}{a^2} \\ 3K &= \rho a^2 - 3a^2 H^2; \qquad \rho_c = 3H^2 \\ 3K &= \rho a^2 \left(1 - \frac{\rho_c}{\rho}\right); \qquad \Omega \equiv \frac{\rho}{\rho_c} \\ 3K &= \rho a^2 (1 - \Omega^{-1}). \end{aligned} \tag{2.8}$$

According to usual standard Big Bang model, $a(t)$ increased significantly since the big bang. So if matter ($\rho \propto a^{-3}$) and radiation ($\rho \propto a^{-4}$) dominated in the past, ρa^2 must have decreased significantly while $(1 - \Omega^{-1})$ must have increased significantly. In a matter- or radiation-dominated universe, $\Omega = 1$ is thus an unstable fixed point. Even if the Universe were nearly flat in the beginning, we expect it to evolve to a non-flat state unless by nearly flat, we mean $(1 - \Omega^{-1})$ being unimaginably very closed to zero. This would be an extreme fitting, so to speak. Current observations simply contradict this idea. As a result, we have the flatness problem.



Example 1. ***Behavior of matter and radiation densities.*** Show that matter ($\rho_{\rm m}$) and radiation ($\rho_{\rm r}$) energy densities scale as $\rho_{\rm m} \propto a^{-3}$ and $\rho_{\rm r} \propto a^{-4}$ respectively.

Solution. From (1.15) of **Example 1.1** we have the continuity equation $\dot{\rho} = -3H(\rho + p)$. Since $p = w\rho$, this equation can be rewritten as $\dot{\rho} = -3(1 + w)H\rho$ which further implies

$$\dot{\rho} + 3(1 + w)\frac{\dot{a}}{a}\rho = 0,$$

$$\frac{1}{a^{3(1+w)}}\frac{\mathrm{d}}{\mathrm{d}t}(\rho a^{3(1+w)}) = 0. \tag{2.9}$$

For matter energy density $w = 0$. It follows that $\rho_{\mathrm{m}} \propto a^{-3}$. For radiation energy density $w = 1/3$. It follows that $\rho_{\mathrm{r}} \propto a^{-4}$.

2.2 Solution through Inflation

The horizon problem stems from the incredible homogeneity of the Universe. This is experimentally reflected to the homogeneity of the CMB radiation. We mentioned that two different regions of the Universe which are now separated by distance greater than the comoving horizon could not have communicated to each other to equilibrate their temperatures. Such improbability to communicate sounds self-explanatory and obvious but if we break this improbability, the horizon problem can be solved. Perhaps before, different patches of the Universe whose CMB radiation are now reaching us, were in causal contact.

Let us define another quantity before going right through the solution of the horizon problem. Let us call R_H given by

Comoving Hubble Radius

$$R_H \equiv \frac{1}{aH}, \tag{2.10}$$

the **comoving Hubble radius** (or simply, Hubble radius). We recall that the proper distance d is related to the comoving distance χ by $d = a(t)\chi$. As such,

$$\dot{d} = \dot{a}(t)\chi = (aH)\chi = \frac{\chi}{R_H}. \tag{2.11}$$

We see that the Hubble radius has a unit of time. If we consider $\dot{d}$ the recession velocity of a given region in the Universe a comoving distance χ from a certain reference location, then setting it equal to the speed of light c gives us $\chi = cR_H$. This equation tells us that the Hubble radius can be thought of as the comoving radius of a sphere whose edge is receding at the speed of light. Different regions separated by a comoving distance greater than the Hubble radius *cannot*

communicate now. This should be differentiated from the comoving particle horizon. Different regions separated by a comoving distance greater than the comoving particle horizon *could not have communicated before*.

Now, suppose there was a period of short but extremely rapid, nearly exponential expansion of the Universe driven by a negative pressure. Such a pressure may be attributed to vacuum energy ($w < 0$). The equation from **Section 1.3** given by $\dot{H} = -\frac{1}{2}(\rho + p)$, then tells us that if the pressure is $p = w\rho \approx -\rho$, then $\dot{H} \approx 0$. As such, $H \approx$ constant and because $\dot{a}/a = H$, then $a \propto e^{Ht}$ in agreement with what we have just said about the expansion being exponential. With the scale factor rising exponentially, the Hubble radius must be decreasing during that process of rapid expansion that we now call **inflation** [12, 13, 14, 15, 16, 16, 17, 18, 19, 20, 21]. Early on we may think, the observable universe might be inside the Hubble sphere (a sphere with Hubble radius). The space inside the Hubble sphere as we know, consists of causally connected regions. Because the visible universe was initially inside the Hubble sphere then there must have been a time for the different regions to even out their physical properties. These regions were "blown" by inflation out of the Hubble radius. After inflation, the Universe resumed its rather slow expansion. The Hubble radius started increasing again[1]. Those regions that became causally disconnected started entering the Hubble sphere again. And so it happens that those causally disconnected regions during the time of decoupling correspond to the same CMB radiation temperature. This is because they were in the same causally-connected region before. (One down and two more to go).

Inflation also offers a solution to the flatness problem. We saw in the previous section the fine-tuning of the initial condition needed to produce a nearly flat Universe today. The last of (2.8) namely,

$$3K = \rho a^2(1 - \Omega^{-1}), \tag{2.12}$$

tells us that if radiation or matter dominated in the past, then an increase in the scale factor means a decrease in ρa^2 that in turn, implies an increase in $(1 - \Omega^{-1})$. If the energy associated with inflation is neither of matter nor of radiation in origin but coming from some sort of energy that does *not* dilute with the expansion of space, then a short but extremely rapid exponential growth

[1] During radiation and matter dominations, $a \propto t^{\frac{1}{2}}$ and $a \propto t^{\frac{1}{3}}$ respectively. Thus, $R_H \propto t^{\frac{1}{2}}$ during radiation era and $R_H \propto t^{\frac{2}{3}}$ during matter era.

of a translates to decreasing $(1-\Omega^{-1})$. For sufficiently long enough period of inflation, we do not have to think of a specially designed initial condition for $(1-\Omega^{-1})$, since it will be pushed to nearly zero anyway. (Two down and one more to go).

How "much" inflation is enough to solve the horizon and flatness problems? We are going to answer this question based on some approximations involving the number of e-folds N required just to solve these two problems. This quantity is defined as

Number of e-folds

$$\mathrm{d}N \equiv \mathrm{d}\ln a, \tag{2.13}$$

implying that for the evolution of the scale factor from time t_1 to t_2, the number of e-folds is $N = \ln(a_2/a_1)$. In what follows, we are going to consider three values of time namely, the times at the start and end of inflation t_i and t_f respectively, and the time now t_0. The number of e-folds we are interested in is then $N = \ln(a_f/a_i)$.

Let us consider the horizon problem. We recall that the Hubble radius corresponds to a causality region whereby two particles separated by a comoving distance greater than R_H cannot communicate now. If two small regions separated by a proper distance $a_0 R_{H,0}$ share the same characteristics (eg., two CMB regions in the sky), then they must be inside a common Hubble sphere of proper radius $a_i R_{H,i}$ before inflation. Going back in time, the proper distance $a_0 R_{H,0}$ must be $a_0 R_{H,0}\frac{a_0}{a_f}$ at the end of inflation and $a_0 R_{H,0}\frac{a_f}{a_0}\frac{a_i}{a_f} = \frac{1}{H_0}\frac{a_f}{a_0}\frac{a_i}{a_f}$ at the start of inflation. Our condition then of being inside the Hubble sphere can be written as

$$\begin{aligned}
\frac{1}{H_0}\frac{a_f}{a_0}\frac{a_i}{a_f} &< \frac{1}{H_i}, \\
e^N > \frac{H_i}{H_0}\frac{a_f}{a_0} &\approx \frac{H_i}{H_0}\frac{T_0}{T_f}, \\
N &\gtrsim \ln\frac{T_0}{H_0} + \ln\frac{H_i}{T_{\mathrm{reh}}},
\end{aligned} \tag{2.14}$$

where T is temperature and in the last line, we have taken the temperature at the end of inflation T_f as approximately equal to the reheating temperature T_{reh}. We have $T_0 = 2.718\,\mathrm{K}$ and $H_0 = 67.8\,\mathrm{km/s/Mpc}$ [99] which in Planck

units are $T_0 = 0.234\,\text{meV}$ and $H_0 = 1.45 \times 10^{-30}\,\text{meV}$.

$$N \gtrsim 67 + \ln \frac{H_i}{T_{\text{reh}}}. \tag{2.15}$$

The reheating temperature so that there is no overproduction of gravitinos is $T_{\text{reh}} \lesssim 10^8$-$10^{10}\,\text{GeV}$ [22]. In effect the minimum number of e-folds is $N \gtrsim$ 70 - 100. To be clear, this number is model-dependent; it varies with the energy scale of inflation and mechanism of reheating. Oftentimes, the minimum value of N is taken as ~ 60 (see for instance, refs. [1, 6] for a detailed calculation) and when necessary, we will use this value instead of our more crude estimate above; the point of our estimation above is to arrive at a good order-of-magnitude result and to present the essentials of logic leading to it.

Incidentally, inflation does not only explain how to deal with the horizon and flatness problems. It also provides a mechanism to generate the seeds for structure formation—something that is lacking in the Standard Big Bang cosmology. During inflation quantum fluctuations were stretched and grew after crossing the shrinking Hubble sphere. The enhanced quantum fluctuations became the primordial cosmological perturbations that served as starting point—the seeds—of structures that we nowadays observe as galaxies and clusters of galaxies. (Three down)

Having been able to offer good solutions to the horizon and flatness problems, and provide a mechanism for generating primordial cosmological perturbations, inflation deserves some attention. We are going to discuss this concept in some length in the following section. Here, before leaving this section, we describe some specifics of what inflation technically is. There are three equivalent conditions for inflation [3]:

(i) decreasing comoving Hubble radius : $\dfrac{d}{dt}\left(\dfrac{1}{aH}\right) < 0$

(ii) accelerated expansion : $\dfrac{d^2a}{dt^2} > 0$

(iii) negative pressure : $p < 0$

The second condition follows from the first by simple differentiation. The third condition follows from the second through the second Friedmann equation.

$$\dot{H} + H^2 = \frac{\ddot{a}}{a} = -\frac{1}{6}(\rho + 3p). \tag{2.16}$$

If $\ddot{a} > 0$ then $p < -\rho/3 < 0$.

2.3 Single-Field Slow-Roll Inflation

Inflation can be considered as being driven by the scalar field called inflaton. We label this field as $\phi(t, \mathbf{x})$ and write down the corresponding action S. Such an action is a sum of the Einstein-Hilbert action and the matter term involving ϕ.

$$S = \frac{1}{2}\int \mathrm{d}^4x\sqrt{-g}\left[R - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V(\phi)\right]. \tag{2.17}$$

Here, g is the determinant of the metric, $g^{\mu\nu}$ is the inverse of the metric, and $V(\phi)$ is the potential[2]. The inflaton field as we can see, is minimally-coupled to gravity. For this section we are going to assume the following simplifications. First, we restrict ϕ to $\phi(t)$. Second, we take as our metric the FLRW metric (see **Section 1.2**). Deviations from these shall be considered later when we discuss perturbation starting at **Chapter 4**.

The energy-momentum tensor $T_{\mu\nu}$ corresponding to the inflaton is defined as

$$T_{\mu\nu} \equiv -\frac{2}{\sqrt{-g}}\frac{\delta S_\phi}{\delta g^{\mu\nu}}, \tag{2.18}$$

where S_ϕ is the matter part of the action. Its variation can be calculated as

$$\begin{aligned}
\delta S_\phi &= \int \mathrm{d}^4x\left[\delta\sqrt{-g}\left(-\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\,\partial_\nu\phi - V\right) - \frac{1}{2}\delta g^{\mu\nu}\partial_\mu\phi\,\partial_\nu\phi\right], \\
\delta\sqrt{-g} &= -\frac{1}{2}\sqrt{-g}\,g_{\alpha\beta}\,\delta g^{\alpha\beta}, \\
\delta S_\phi &= \int \mathrm{d}^4x\sqrt{-g}\,\delta g^{\alpha\beta}\left[\frac{1}{4}g_{\alpha\beta}\,\partial^\mu\phi\,\partial_\mu\phi + \frac{1}{2}g_{\alpha\beta}V(\phi) - \frac{1}{2}\partial_\alpha\phi\partial_\beta\phi\right].
\end{aligned} \tag{2.19}$$

Then

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta S_\phi}{\delta g^{\mu\nu}} = \partial_\mu\phi\partial_\nu\phi - g_{\mu\nu}\left[\frac{1}{2}\partial^\sigma\phi\,\partial_\sigma\phi + V(\phi)\right]. \tag{2.20}$$

[2] We are using the metric signature $(-+++)$ so the kinetic term has a minus sign instead of the usual plus sign in QFT literature.

For $\phi = \phi(t)$ we find that $T^{\mu}{}_{\nu}$ is diagonal—it is of the form $\mathrm{diag}(-\rho, p, p, p)$ where

Energy Density and Pressure

$$\begin{aligned} \rho(t) &= \tfrac{1}{2}\dot{\phi}(t)^2 + V(\phi), \\ p(t) &= \tfrac{1}{2}\dot{\phi}(t)^2 - V(\phi). \end{aligned} \tag{2.21}$$

The dynamics of inflaton is given by its equation of motion derivable from the action S. The corresponding Lagrangian density from S is

$$\mathcal{L} = \sqrt{-g}\left[\frac{1}{2}\dot{\phi}(t)^2 - V(\phi)\right]. \tag{2.22}$$

We use the Euler-Lagrange equation to derive the equation of motion.

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}}\right) &= 0, \\ -\sqrt{-g}\, V_{,\phi} - \frac{\partial}{\partial t}\left(\dot{\phi}\sqrt{-g}\right) &= 0; \qquad \sqrt{-g} = a^3 \\ -a^3 V_{,\phi} - 3a^2 \dot{a}\dot{\phi} - a^3\ddot{\phi} &= 0, \end{aligned}$$

Equation of Motion

$$\ddot{\phi}(t) + 3H\dot{\phi}(t) + V_{,\phi} = 0. \tag{2.23}$$

The dynamics of the geometry follows from the first and second Friedmann equations. From the first Friedmann equation we have

$$\begin{aligned} H^2 &= \frac{1}{3}\rho(t) \\ H^2 &= \tfrac{1}{3}\left[\tfrac{1}{2}\dot{\phi}(t)^2 + V(\phi)\right]. \end{aligned} \tag{2.24}$$

From the second Friedmann equation we have

$$\begin{aligned} \dot{H} + H^2 &= -\frac{1}{6}(\rho + 3p), \\ &= -\frac{1}{6}\left(\frac{\dot{\phi}^2}{2} + V + \frac{3\dot{\phi}^2}{2} - 3V\right), \end{aligned}$$

$$\dot{H} + H^2 = -\frac{1}{3}\left[\dot{\phi}(t)^2 - V(\phi)\right]. \tag{2.25}$$

We also find

$$\dot{H} = -\frac{1}{2}\dot{\phi}(t)^2. \tag{2.26}$$

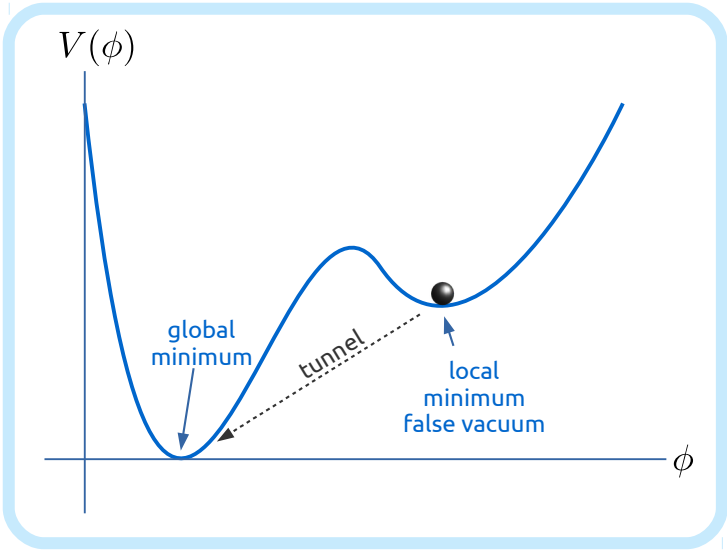


Figure 2.2: Inflation and false vacuum. Inflation happens when the inflaton is temporarily trapped in the false vacuum.

After attaining inflation, the next logical question is "When will it stop?" In the original formulation of inflation by Alan Guth, he considered many inflating bubbles [12]. We can think of these bubbles as expanding rapidly and then through the process of tunneling (see **Fig. 2.2**), reach the true vacuum. All the bubbles of true vacuum must then coalesce for the entire Universe to reach the true vacuum state. The following paper by Guth now working with Erick Weinberg, showed that the "bubbles will asymptotically fill an arbitrarily large fraction of space, yet they never percolate" [13]. In other words, inflation would continue and the Universe as a whole, would not reach the true vacuum.

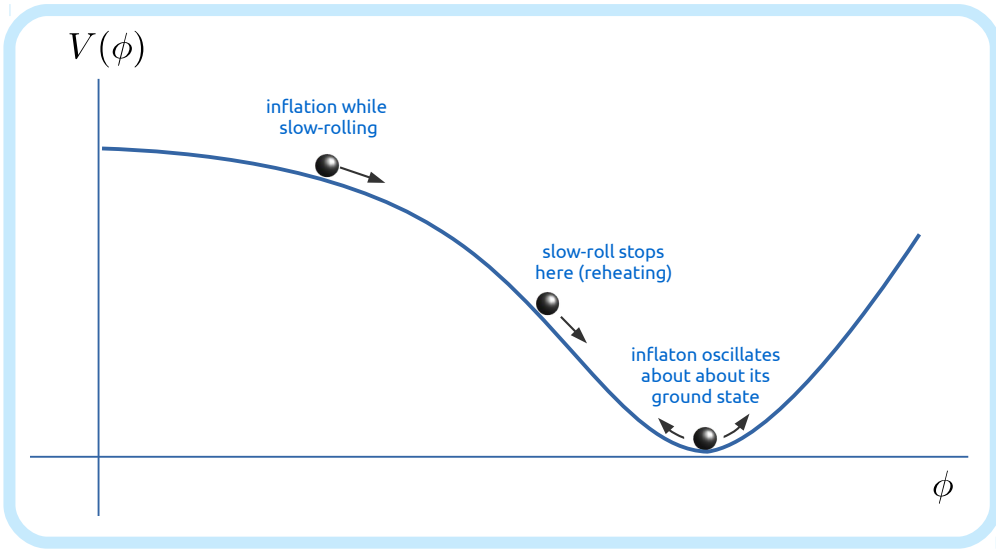


Figure 2.3: Slow-Roll Inflation. Inflation happens while the inflaton "slow-rolls" down the potential. The standard model particles are produced while the inflaton oscillates about its ground state.

The theory of inflation was rescued by Andrei Linde and independently by Andreas Albrecht and Paul Steinhardt through the proposition of **slow-roll inflation** [16], [17]. In this new type of inflation, instead of the need to tunnel to reach the true ground state, the inflaton rolls down the potential hill slowly (see **Fig. 2.3**). Such a slow-roll results to inflation. When the inflaton reaches the steep part of the potential hill, slow-roll ends; inflation also ends. Through coupling with the standard model particles, it decays. Because inflation is a rapid supercooled expansion, the succeeding decay of the inflaton reheats the Universe. We call such process **reheating** [23]. (Some authors when story-telling about the history of the Universe, prefer to take the beginning of the Big Bang as the end of inflation; that is, during reheating.)

Let us look into our set of equations to see the conformity of this new model to the above set of equations. When the inflaton slow-rolls, $\dot{\phi} \approx 0$ and (2.26) tells us that $H \approx$ constant, implying that the scale factor is exponentially increasing; thus, inflation happens. Note from (2.23),

$$\ddot{\phi}(t) + 3H\dot{\phi}(t) + V_{,\phi} = 0, \tag{2.27}$$

that the requirement $\dot{\phi} \approx 0$ may not be sufficient. If the first term namely, $\ddot{\phi}$, is large, slow-roll may halt prematurely. This can be remedied by a significant drag from the second term. For large enough potential, the first Friedmann equation tells us that the Hubble parameter will be also large. This can prevent the rapid variation of $\dot{\phi}$.

To be more quantitative about these matters, we introduce two Hubble slow-roll parameters. The **first slow-roll parameter** is defined as

First Slow-Roll Parameter

$$\epsilon \equiv -\frac{\dot{H}}{H^2}. \tag{2.28}$$

By virtue of (2.26) we find

$$\epsilon = \frac{\dot{\phi}^2}{2H^2}. \tag{2.29}$$

It is thus, a positive quantity. Inflation is characterized by $\epsilon < 1$. To see this, we note that $\dot{H} + H^2 = \ddot{a}/a$. As such,

$$\frac{\ddot{a}}{a} = H^2(1 - \epsilon). \tag{2.30}$$

When ϵ becomes unity, the accelerated expansion stops.

The **second slow-roll parameter** is defined as[3]

Second Slow-Roll Parameter

$$\eta \equiv \epsilon - \frac{1}{2H}\frac{\dot{\epsilon}}{\epsilon}. \tag{2.31}$$

This can be related to the inflaton field as follows.

$$\begin{aligned}
\eta &= \epsilon - \frac{1}{2H}\frac{\dot{\epsilon}}{\epsilon} \\
&= -\frac{\dot{H}}{H^2} + \frac{H}{2\dot{H}}\frac{d}{dt}\left(-\frac{\dot{H}}{H^2}\right) \\
&= -\frac{\dot{H}}{H^2} - \frac{H}{2\dot{H}}\left(\frac{\ddot{H}}{H^2} - \frac{2\dot{H}^2}{H^3}\right)
\end{aligned}$$

[3] It is also usual to define $\eta \equiv \dot{\varepsilon}/(\varepsilon H)$; see for instance, ref. [111].

$$= -\frac{\ddot{H}}{2\dot{H}H}; \qquad \dot{H} = -\frac{1}{2}\dot{\phi}^2$$

$$\eta = -\frac{\ddot{\phi}}{H\dot{\phi}}\,. \tag{2.32}$$

Looking at the equation of motion for ϕ, the smallness of $|\eta|$ corresponds to $|\ddot{\phi}| \ll |H\dot{\phi}|$. Small value of this second slow-roll parameter is required to prolong inflation. Together with the condition for ϵ, in summary, the two conditions for slow-roll inflation are

$$|\epsilon| \ll 1 \quad \text{and} \quad |\eta| \ll 1. \tag{2.33}$$

CHAPTER

3

ADM Decomposition

Everything that comes together falls apart. Everything.
The chair I'm sitting on. . . .
I'm gonna fall apart, . . .
And you're gonna fall apart. . . .
Things fall apart.

John Green, Looking for Alaska

3.1 Foliating the Manifold
3.2 Extrinsic Curvature
3.3 (3 + 1)-Decomposition of the Riemann Tensor
3.4 Action in Terms of the ADM Variables

The ADM formalism involves a method of foliating a four-dimensional manifold into three-dimensional spacelike leaves each corresponding to a unique value of time. It was proposed by Richard Arnowitt, Stanley Deser, and Charles W. Misner, as a Hamiltonian formulation of general relativity in 1959 (25). This sort of formulation and fragmentation of spacetime into 3D + 1D turns out to be indispensable in the decomposition of the action for inflation. For this reason, a thorough understanding is required.

Starting from the basic notion of spacetime foliation, we define the concepts of projection tensor and intrinsic and extrinsic curvatures in 3D space. The decomposition of the metric to 3D + 1D leads to a similar decomposition of the Riemann curvature tensor. This then enables writing the action in terms of 3D quantities—our main result in this chapter.

3.1 Foliating the Manifold

Consider a 4D spacetime (differentiable) manifold $\mathscr{M}$, with each point on $\mathscr{M}$ labeled by $y^a = (y^0, y^1, y^2, y^3)$ and is endowed with a metric

$$\mathrm{d}s^2 = \tilde{g}_{\mu\nu}\,\mathrm{d}y^\mu\,\mathrm{d}y^\nu, \tag{3.1}$$

where μ, ν run from 0 to 3. We follow the convention that the Greek indices $\alpha,\ \beta,\ \cdots = 0, 1, 2, 3$ while the Roman indices $a,\ b, \cdots = 1, 2, 3$. (We put a tilde over $g_{\mu\nu}$ to give way for $g_{\mu\nu}$ without a tilde in the discussion on ADM decomposition.) Let us divide this manifold into infinitely many non-intersecting 3D spacelike hypersurfaces with each point on $\mathscr{M}$ located on one and only one hypersurface (see **Fig. 3.1**). Each hypersurface is labeled by a constant t namely, $t = f(y^\mu)$, where f is a scalar function of y^μ describing a given hypersurface. Every hypersurface Σ_t is then embedded in $\mathscr{M}$ and is thus, a submanifold of $\mathscr{M}$. Furthermore, a tangent space $\mathscr{T}(\Sigma_t)$ at a point on Σ_t is a subspace of the corresponding tangent space $\mathscr{T}(\mathscr{M})$ at the same point viewed from $\mathscr{M}$.

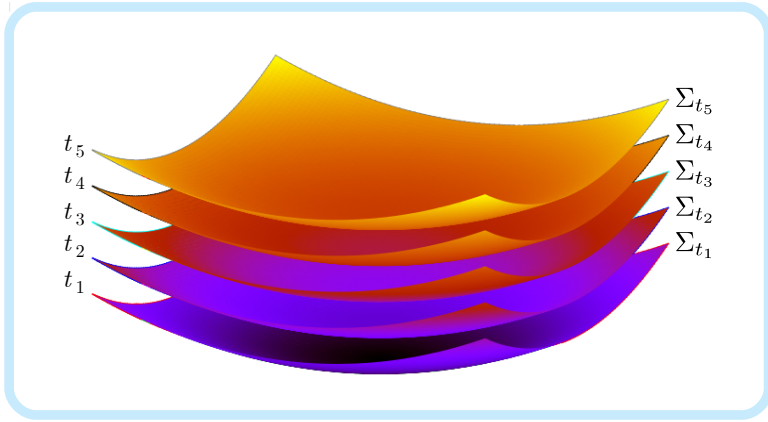


Figure 3.1: Foliating the Manifold. The manifold is foliated into many leaves with each leaf Σ_t corresponding to a fixed value of the parameter t. [code]

Let us coordinatize each hypersurface by x^i (where i runs from 1 to 3). Each point then on the manifold can be alternatively labeled by (t, x^i). The metric h_{ij} of Σ_t tells us how to measure distances in Σ_t. The corresponding 3D

metric is given by

$$ds^2_\Sigma = h_{ij}\, dx^i dx^j. \tag{3.2}$$



Example 1. Foliation of Euclidean space into concentric spheres. If we think of $\mathscr{M}$ as a 3D Euclidean space, then the foliation can be the division into infinitely many spheres centered at a chosen origin. The metric corresponding to $\mathscr{M}$ is then

$$ds^2 = \tilde{g}_{\mu\nu}\, dy^\mu dy^\nu = (dy^1)^2 + (dy^2)^2 + (dy^3)^2, \tag{3.3}$$

where (y^1, y^2, y^3) are the usual Cartesian coordinates (x, y, z). Here $\tilde{g}_{ab} = \text{diag}(1, 1, 1)$, where under this special circumstance, $\mu, \nu = 1, 2, 3$. The surface corresponding to constant r is Σ_r. If this surface is coordinatized by (θ, ϕ) then the corresponding metric is

$$\text{d}s^2_\Sigma = h_{ij} dx^i dx^j = r^2(d\theta^2 + \sin^2\theta d\phi^2). \tag{3.4}$$

Here $h_{ij} = (r^2, r^2 \sin^2\theta)$ where under this special circumstance $i, j = 1, 2$.



At each point on Σ_t, we can associate a normal vector $\mathbf{n}$ given by

$$n^\mu = \tilde{g}^{\mu\nu} n_\nu, \tag{3.5}$$

where

$$n_\nu \equiv -N \nabla_\nu t, \tag{3.6}$$

and N is the so-called **lapse function** defined as [26]

Lapse Function

$$N \equiv \frac{1}{\sqrt{-\tilde{g}^{\mu\nu} \nabla_\mu t \nabla_\nu t}}. \tag{3.7}$$

The scalar product $\mathbf{n}\cdot\mathbf{n} = -1$.

$$\tilde{g}_{\mu\nu}n^\mu n^\nu = \tilde{g}^{\mu\nu}n_\mu n_\nu = \tilde{g}^{\mu\nu}(-N\nabla_\mu t)(-N\nabla_\nu t) = -1. \tag{3.8}$$

The normal vector $\mathbf{n}$ is thus, timelike.

The normal vector n^μ finds it utility in the definition of the **projection tensor** $\gamma^\mu{}_\nu$ given by

Projection Tensor

$$\gamma^\mu{}_\nu \equiv \delta^\mu{}_\nu + n^\mu n_\nu. \tag{3.9}$$

This projection tensor projects a vector onto Σ_t. To convince ourselves of this, let us consider the projection of the normal vector n_μ onto Σ_t. This should vanish.

$$\gamma^\mu{}_\nu n^\nu = (\delta^\mu{}_\nu + n^\mu n_\nu)n^\nu = n^\mu + n^\mu \underbrace{(n^\nu n_\nu)}_{=-1} = 0. \tag{3.10}$$

A tangent vector w^i living in the tangent space at a point on Σ_t can be seen as a vector v^μ living in the tangent space at the same point on $\mathscr{M}$ by an observer in $\mathscr{M}$. The projection of v^μ onto Σ_t should be itself.

$$\gamma^\mu{}_\nu v^\nu = (\delta^\mu{}_\nu + n^\mu n_\nu)v^\nu = v^\mu + n^\mu \underbrace{n_\nu v^\nu}_{=0} = v^\nu. \tag{3.11}$$

The contraction $n_\nu v^\nu$ vanishes because n^μ is orthogonal to the tangent vector v^μ.

The projection property of the projection tensor tells us that it is a map from $\mathscr{M}$ to Σ_t. As we shall see, this is not simply a map but serves as a (spatial) metric for the spacelike hypersurface Σ_t. Let us lower the index μ in (3.9) to gain

3D metric

$$\gamma_{\mu\nu} = \tilde{g}_{\mu\nu} + n_\mu n_\nu. \tag{3.12}$$

Now, consider for instance, a tangent vector v^μ which lives in the tangent space of a point on Σ_t. Then,

$$\gamma_{\mu\nu}v^\mu = (\tilde{g}_{\mu\nu} + n_\mu n_\nu)v^\mu; \qquad n_\mu v^\mu = 0$$

$$\gamma_{\mu\nu}v^\mu = \tilde{g}_{\mu\nu}v^\mu.$$

The scalar product of two vectors u^μ and u^ν living in the tangent space $\mathscr{T}(\Sigma_t)$ of a point on Σ_t can also be computed using γ_{ab}. Indeed,

$$\gamma_{\mu\nu}u^\mu v^\nu = (\tilde{g}_{\mu\nu} + n_\mu n_\nu)u^\mu v^\nu; \qquad n_\mu v^\mu = 0$$
$$\gamma_{\mu\nu}u^\mu v^\nu = \tilde{g}_{\mu\nu}u^\mu u^\nu.$$

With $\gamma_{\mu\nu}$ being the metric of Σ_t, we can raise and lower indices of any tensor living in this manifold. Furthermore, we can also perform calculations of trace and scalar product involving tensors living in Σ_t or its corresponding set of other spaces (eg., tangent space) using $\gamma_{\mu\nu}$. One thing to keep in mind though, is, unlike that of $\tilde{g}_{\mu\nu}$ where $\tilde{g}^\mu{}_\nu = \delta^\mu_\nu$, raising one of the indices of $\gamma_{\mu\nu}$ does not "make" a Kronecker delta ($\gamma^\mu{}_\nu \neq \delta^\mu_\nu$). This is so because $\gamma^{\mu\nu}$ is not the inverse of $\gamma_{\mu\nu}$.

The idea that $\gamma_{\mu\nu}$ is a spatial metric for the hypersurface Σ_t may look like a little surprising since Σ_t is 3D while $\mathscr{M}$ is 4D. For one thing, $\gamma_{\mu\nu}$ has four indices that run from 0 to 3 instead of just 1 to 3. Actually this should not be very surprising if we think for instance, of a vector w^i living in the tangent space $\mathscr{T}(\Sigma_t)$ being "seen" as a vector v^μ living in the tangent space $\mathscr{T}(\mathscr{M})$. This is so because for a given point on Σ_t, $\mathscr{T}(\Sigma_t)$ is a subspace of $\mathscr{T}(\mathscr{M})$. We just need a suitable transformation or mapping to "extract" w^i from v^μ or, for the metric above, h_{ij} from $\gamma_{\mu\nu}$.

We introduce some more quantities that are useful in relating 4D and 3D quantities. The first one in the list is the so-called **time flow vector** t^μ. It is a 4D vector whose index can be raised or lowered by the metric $\tilde{g}_{\mu\nu}$. We motivate its formal definition by starting from a rather informal assignment:

$$t^\mu \equiv \frac{\partial y^\mu}{\partial t}. \tag{3.13}$$

It follows that

$$t^\mu \nabla_\mu t = 1, \tag{3.14}$$

which further implies $t^\mu n_\mu = -N$. We may then decompose the time flow vector into a sum of parallel and perpendicular parts with respect to the normal vector; that is, $t^\mu = t^\mu_\parallel + t^\mu_\perp$. In effect, $t^\mu_\parallel n_\mu = -N$ and $t^\mu_\perp n_\mu = 0$. Then the parallel

component must be Nn^μ. The perpendicular component is some vector N^a that we call the **shift function**. (Note here that by the notation N and N^μ, we do *not* mean $N^2 = N^\mu N_\mu$.)

With the parallel and perpendicular parts in hand, we can now formally define the time-flow vector as [27]

Time-Flow Vector

$$t^\mu \equiv Nn^\mu + N^\mu. \tag{3.15}$$

In comparison to the preliminary assignment above, this definition has the advantage of being coordinate-independent. New in this definition is the shift function that we have just mentioned above. Since it is perpendicular to n^μ it may be thought of as a projection of t^μ onto Σ_t. Indeed,

$$\begin{aligned} \gamma^\mu{}_\nu t^\nu &= (\delta^\mu_\nu + n^\mu n_\nu)(Nn^\nu + N^\nu), \\ &= Nn^\mu + N^\mu - n^\mu N + 0, \\ \gamma^\mu{}_\nu t^\nu &= N^\mu. \end{aligned} \tag{3.16}$$

Let us now find the relation between the 3D metrics γ_{ij} and $\gamma_{\mu\nu}$. Furthermore, we define the 3D version (N_i) of the shift function (N_μ) and also relate these two through coordinate transformation. We recall that $\mathscr{M}$ is coordinatized by y^μ while Σ_t is coordinatized by x^i. (Note that t is in general *not* y^0). We define the transformation matrix $M^\mu{}_i$ as

$$M^\mu{}_i \equiv \frac{\partial y^\mu}{\partial x^i}, \tag{3.17}$$

Then

$$\begin{aligned} h_{ij} &= M^\mu{}_i M^\nu{}_j \gamma_{\mu\nu} \\ N_i &= M^\mu{}_j N_\mu. \end{aligned} \tag{3.18}$$

We should have labeled N_i in the last equation above by a different symbol (say, $\bar{N}_i$) since observant eyes can see that $N_\mu = (N_0, N_i)$. The latter N_i is different from N_i in the last of (3.18) and is only the same in special circumstances. Literature usually follows this way of writing. Adding a bar or introducing many symbols may only complicate our notation. The meaning of a given symbol can become clear from the context of discussion.



Example 2. The induced metric. Let the manifold $\mathscr{M}$ be a 3D Euclidean space. Its metric is then

$$\mathrm{d}s^2 = \tilde{g}_{\mu\nu}\mathrm{d}y^\mu \mathrm{d}y^\nu = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2,$$

where (for this special circumstance again,) $a, b = 1, 2, 3$. We see that

$$\tilde{g}_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Let us foliate this into an infinite number of concentric 2-spheres each defined by $r^2 = x^2 + y^2 + z^2$, where r stands for radius. Each sphere is then a submanifold Σ_r endowed with a metric whose associated basis we have the freedom to choose. We may then write

$$\mathrm{d}s^2_\Sigma = h_{ij}\mathrm{d}x^i \mathrm{d}x^j = \gamma_{\mu\nu}\mathrm{d}y^\mu \mathrm{d}y^\nu,$$

where $x^i = (\theta, \phi)$, $y^\mu = (x, y, z)$, and

$$x = r\sin\theta\,\cos\phi,$$

$$y = r\sin\theta\,\sin\phi,$$

$$z = r\cos\theta.$$

Each sphere is thus labeled by a constant r and coordinatized by (θ, ϕ).

(a) Show that

$$\gamma_{\mu\nu} = \begin{pmatrix} 1 + \dfrac{x^2}{r^2} & \dfrac{xy}{r^2} & \dfrac{xz}{r^2} \\ \dfrac{xy}{r^2} & 1 + \dfrac{y^2}{r^2} & \dfrac{yz}{r^2} \\ \dfrac{xz}{r^2} & \dfrac{yz}{r^2} & 1 + \dfrac{z^2}{r^2} \end{pmatrix}.$$

(b) Using the brute-force method following the equation

$$h_{ij} = \frac{\partial y^\mu}{\partial x^i}\frac{\partial y^\nu}{\partial x^j}\gamma_{\mu\nu},$$

determine h_{ij}.

Solution.

(a) The normal at a given point on Σ_r is simply

$$n_\mu = (1)(\nabla_\mu r) = \left(\frac{x}{r}, \frac{y}{r}, \frac{z}{r}\right).$$

Since $\gamma_{\mu\nu} = \tilde{g}_{\mu\nu} + n_\mu n_\nu$ and $\tilde{g}_{\mu\nu} = \mathrm{diag}(1,1,1)$ then

$$\gamma_{\mu\nu} = \begin{pmatrix} 1+\frac{x^2}{r^2} & \frac{xy}{r^2} & \frac{xz}{r^2} \\ \frac{xy}{r^2} & 1+\frac{y^2}{r^2} & \frac{yz}{r^2} \\ \frac{xz}{r^2} & \frac{yz}{r^2} & 1+\frac{z^2}{r^2} \end{pmatrix}.$$

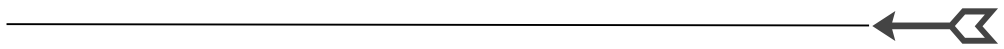
(b) We see that

$$\frac{\partial y^\mu}{\partial x^i} = \begin{pmatrix} r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ -r\sin\theta & 0 \end{pmatrix}.$$

then

$$h_{ij} = \left(\frac{\partial y^\mu}{\partial x^i}\right)^T \gamma_{\mu\nu} \left(\frac{\partial y^\nu}{\partial x^j}\right) = \begin{pmatrix} r^2 & 0 \\ 0 & r^2\sin^2\theta \end{pmatrix}.$$

The calculation leading to the last term using the brute-force method of matrix multiplication coupled with trigonometric simplification can be very tedious. It can be easily carried out using a suitable Computer Algebra System like Maxima.



We can also find the metric h_{ij} in the example above using a more direct method involving the substitution $(x,y,z) = (r\sin\theta\cos, r\sin\theta\sin\phi, r\cos\theta)$ in the expression $\mathrm{d}s^2 = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2$. Alternatively, we can use the more formal

notion of pullback in relating h_{ij} and $\tilde{g}_{\mu\nu}$. Consider a map $\Phi : \mathscr{M} \to \Sigma_t$. We can pull $\tilde{g}_{\mu\nu}$ onto Σ_t to gain the induced metric (of Σ_t) as

$$(\Phi^* \bar{g})_{ij} = h_{ij} = \frac{\partial y^\mu}{\partial x^i} \frac{\partial y^\nu}{\partial x^j} \tilde{g}_{\mu\nu}. \tag{3.19}$$

This often requires less tedious calculation than what is suggested by the relation $h_{ij} = M^\mu{}_i M^\nu{}_j \gamma_{\mu\nu}$ above (see the first of (3.18)) since $\tilde{g}_{\mu\nu}$ is usually given. Actually, we should have figured out the less cumbersome relation above from the latter through simple manipulation.

$$\begin{aligned} h_{ij} &= \frac{\partial y^\mu}{\partial x^i} \frac{\partial y^\nu}{\partial x^j} \gamma_{\mu\nu}, \\ &= \frac{\partial y^\mu}{\partial x^i} \frac{\partial y^\nu}{\partial x^j} (\tilde{g}_{\mu\nu} + n_\mu n_\nu), \\ &= \frac{\partial y^\mu}{\partial x^i} \frac{\partial y^\nu}{\partial x^j} \tilde{g}_{\mu\nu} + N^2 \frac{\partial y^\mu}{\partial x^i} \frac{\partial t}{\partial y^\mu} \frac{\partial y^\nu}{\partial x^j} \frac{\partial t}{\partial y^\mu}, \\ h_{ij} &= \frac{\partial y^\mu}{\partial x^i} \frac{\partial y^\nu}{\partial x^j} \tilde{g}_{\mu\nu}. \end{aligned} \tag{3.20}$$

Decomposing the Metric

We can now relate $\tilde{g}_{\mu\nu}$ with γ_{ij}, N_i, and N. To do this, we express $\mathrm{d}s^2$ in terms of (x^i, t).

$$\begin{aligned} \tilde{g}_{\mu\nu}\, \mathrm{d}y^\mu\, \mathrm{d}y^\nu &= \tilde{g}_{\mu\nu} \left(\frac{\partial y^\mu}{\partial t} \mathrm{d}t + \frac{\partial y^\mu}{\partial x^i} \mathrm{d}x^i \right) \left(\frac{\partial y^\nu}{\partial t} \mathrm{d}t + \frac{\partial y^\nu}{\partial x^j} \mathrm{d}x^j \right), \\ &= \tilde{g}_{\mu\nu}\, t^\mu t^\nu \mathrm{d}t^2 + \tilde{g}_{\mu\nu}\, M^\mu{}_i t^\nu \mathrm{d}x^i \mathrm{d}t + \tilde{g}_{\mu\nu}\, t^\mu M^\nu{}_j \mathrm{d}t \mathrm{d}x^j + \tilde{g}_{\mu\nu}\, M^\mu{}_i M^\nu{}_j \mathrm{d}x^i \mathrm{d}x^j, \\ &= t^\mu t_\mu \mathrm{d}t^2 + t_\mu M^\mu{}_i \mathrm{d}x^i \mathrm{d}t + t_\nu M^\nu{}_j \mathrm{d}t\, \mathrm{d}x^j + h_{ij} \mathrm{d}x^i \mathrm{d}x^j. \end{aligned} \tag{3.21}$$

The last term follows from the relation $h_{ij} = M^\mu{}_i M^\nu{}_j \tilde{g}_{\mu\nu}$. For the term $t^\mu t_\mu$ we have

$$\begin{aligned} t^\mu t_\mu &= (N n^\mu + N^\mu)(N n_\mu + N_\mu), \\ &= N^2 \underbrace{n^\mu n_\mu}_{-1} + N \underbrace{N^\mu n_\mu}_{=0} + N \underbrace{n^\mu N_\mu}_{=0} + N^\mu N_\mu, \\ &= -N^2 + N^\mu N_\mu, \end{aligned}$$

$$
\begin{aligned}
&= -N^2 + M^{\mu}{}_i N^i M_{\mu}{}^j N_j, \\
&= -N^2 + \delta_i^j N^i N_j, \\
t^{\mu} t_{\mu} &= -N^2 + N_k N^k. \qquad (3.22)
\end{aligned}
$$

For the term $t_\nu M^b{}_j$ we have

$$
\begin{aligned}
t_\nu M^\nu{}_j &= (N n_\nu + N_\nu) M^\nu{}_j; \qquad n_\nu \equiv -N \nabla_\nu t, \\
&= -N^2 \frac{\partial t}{\partial y^\nu} \frac{\partial y^\nu}{\partial x^j} + N_\nu M^\nu{}_j, \\
&= -N^2 \frac{\partial t}{\partial x^j} + N_j, \\
t_\nu M^\nu{}_j &= N_j. \qquad (3.23)
\end{aligned}
$$

Use the results from (3.22) and (3.23) to the last of (3.21).

$$
\begin{aligned}
\tilde{g}_{\mu\nu}\, \mathrm{d}y^\mu \mathrm{d}y^\nu &= (-N^2 + N_k N^k)\mathrm{d}t^2 + N_i\, \mathrm{d}x^i \mathrm{d}t + N_i\, \mathrm{d}t \mathrm{d}x^i + h_{ij}\, \mathrm{d}x^i \mathrm{d}x^j \\
\tilde{g}_{\mu\nu}\, \mathrm{d}y^\mu \mathrm{d}y^\nu &= -N^2 \mathrm{d}t^2 + h_{ij}(\mathrm{d}x^i + N^i \mathrm{d}t)(\mathrm{d}x^j + N^j \mathrm{d}t). \qquad (3.24)
\end{aligned}
$$

We can of course go to a coordinate system such that the left hand side above is simply $g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu$ and identify

ADM-Decomposed Metric

$$
g_{\mu\nu} = \begin{pmatrix} -N^2 + N_k N^k & N_i \\ N_i & h_{ij} \end{pmatrix}. \qquad (3.25)
$$

We should be reminded that $\tilde{g}_{\mu\nu}$ is not necessarily the same as $g_{\mu\nu}$. It is common however, to simply write $\tilde{g}_{\mu\nu}$ as $g_{\mu\nu}$. In the following chapters, when it is clear from the context what metric components we are talking about, we will omit the symbol tilde.

Inverse of the Decomposed Metric

Consider a block matrix $\mathbf{M}$ given by

$$
\mathbf{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}, \qquad (3.26)
$$

where $\mathbf{A}$ and $\mathbf{D}$ are square matrices of size $m \times m$ and $n \times n$ respectively, and $\mathbf{B}$ and $\mathbf{C}$ are rectangular matrices of size $m \times n$ and $n \times m$ respectively. The determinant of $\mathbf{M}$ is given by [28]

$$\det(\mathbf{M}) = \det(\mathbf{D})\ \det(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}). \tag{3.27}$$

Let us apply this equation to the calculation of the determinant $\det(g_{\mu\nu})$.

$$\begin{aligned}
\det(g_{\mu\nu}) &= \det(h_{ij})\det(-N^2 + N_k N^k - \mathbf{N}\mathbf{h}^{-1}\mathbf{N}^T); \\
&\qquad \mathbf{N} = (N_1\ N_2\ N_3), \quad \det h_{ij} = h \\
&= h\det(-N^2 + N_k N^k - N_i h^{ij} N_j), \\
\det(g_{\mu\nu}) &= -hN^2.
\end{aligned} \tag{3.28}$$

Then

$$\boxed{\sqrt{-g} = N\sqrt{h}.} \tag{3.29}$$

Suppose for the block matrix $\mathbf{M}$, the matrix $\mathbf{C^{-1}} + \mathbf{D}\mathbf{A}^{-1}\mathbf{B}$ is not singular, then [28]

$$\mathbf{M}^{-1} = \begin{pmatrix} (\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & -\mathbf{A}^{-1}\mathbf{B}(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & (\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1} \end{pmatrix}. \tag{3.30}$$

For the matrix $g_{\mu\nu}$ we see that

$$\begin{aligned}
g^{00} &= (-N^2 + N_k N^k - \mathbf{N}\mathbf{h}^{-1}\mathbf{N}^T)^{-1}, \\
&= (-N^2 + N_k N^k - N_k N^k)^{-1}, \\
g^{00} &= -\frac{1}{N^2}.
\end{aligned}$$

$$\begin{aligned}
g^{i0} &= \left[-\boldsymbol{h}^{-1}\mathbf{N}^T(-N^2)^{-1}\right]^i, \\
&= -h^{ij}N_j(-N^2)^{-1}, \\
g^{i0} &= \frac{N^i}{N^2}.
\end{aligned}$$

$$g^{i0} = g^{0i}.$$

$$\begin{aligned} g^{ij} &= \left[\left(\mathbf{h} - \mathbf{N}^T \cdot \frac{1}{-N^2 + N_k N^k} \cdot \mathbf{N}\right)^{-1}\right]^{ij}, \\ &= (-N^2 + N_k N^k)\left[h_{ij}(-N^2 + N_k N^k) - N_i N_j\right]^{-1}. \end{aligned} \tag{3.31}$$

We see on the other hand, that

$$\begin{aligned} &\left[h_{ik}(-N^2 + N_k N^k) - N_i N_k\right]\left[h^{kj} - \frac{N^k N^j}{N^2}\right], \\ &\quad = \delta_i^j(-N^2 + N_k N^k) - N_i N^j - \frac{N_i N^j}{N^2}(-N^2 + N_k N^k) + N_i N^j \frac{N_k N^k}{N^2}, \\ &\quad = \delta_i^j(-N^2 + N_k N^k). \end{aligned}$$

It follows that

$$g^{ij} = h^{ij} - \frac{N^i N^j}{N^2}. \tag{3.32}$$

The matrix inverse of $g_{\mu\nu}$ is then

$$g^{\mu\nu} = \frac{1}{N^2}\begin{pmatrix} -1 & N^i \\ N^i & N^2 h^{ij} - N^i N^j \end{pmatrix}. \tag{3.33}$$

3.2 Extrinsic Curvature

Previously, we introduced a projection tensor $\gamma^\mu{}_\nu$ defined as $\gamma^\mu{}_\nu \equiv \delta^\mu{}_\nu + n^\mu n_\nu$. It projects a 4D vector in (the tangent bundle[1] of) $\mathscr{M}$ onto (the corresponding tangent bundle of) Σ_t. The spatial metric associated with Σ_t as viewed from $\mathscr{M}$

[1] A tangent bundle is a collection of tangent spaces.

is $\gamma_{\mu\nu} = \tilde{g}_{\mu\nu} + n_\mu n_\nu$. Given that $\mathscr{M}$ is equipped with a metric $\mathrm{d}s^2 = \tilde{g}_{\mu\nu}\,\mathrm{d}y^\mu \mathrm{d}y^\nu$ and that Σ_t is equipped with a metric $\mathrm{d}s^2_\Sigma = h_{ij}\mathrm{d}x^i\mathrm{d}x^j$, there must exist a relationship between $\gamma_{\mu\nu}$ and h_{ij}. As already stated in the previous section, $h_{ij} = M^\mu{}_i M^\nu{}_j \gamma_{\mu\nu}$, where $M^\mu{}_i = \frac{\partial y^\mu}{\partial x^i}$.

The projection tensor need not be applicable to a $\binom{1}{0}$ tensor only. The projection of a tensor $T^{u_1 u_2 \cdots u_m}{}_{v_1 v_2 \cdots v_n}$ onto Σ_t is given by [29]

$$(\boldsymbol{\gamma}^*\mathbf{T})^{a_1 a_2 \cdots a_m}{}_{b_1 b_2 \cdots b_n} = \gamma^{a_1}{}_{u_1}\gamma^{a_2}{}_{u_2}\cdots\gamma^{a_m}{}_{u_m}\gamma^{v_1}{}_{b_1}\gamma^{v_2}{}_{b_2}\cdots\gamma^{v_n}{}_{b_n}T^{u_1 u_2 \cdots u_\rho}{}_{v_1 v_2 \cdots v_\sigma},$$

where $\boldsymbol{\gamma}^*$ is a map that pulls $\mathbf{T}$ onto Σ_t. The contraction of the pullback with the normal vector n^μ should be zero.

Consider a tensor ω^μ residing in (the tangent bundle of) Σ_t. We can take the covariant derivative of this tensor with respect to y^β namely, $\nabla_\beta\,\omega^\mu$, and project out the result onto Σ_t. The projection of this covariant derivative is what we define as the covariant derivative for the hypersurface Σ_t. That is,

Definition of 3D Covariant Derivative

$$D_\nu\,\omega^\mu \equiv \gamma^\mu{}_\alpha\gamma^\beta{}_\nu\nabla_\beta\,\omega^\alpha, \tag{3.34}$$

where D is a spatial covariant derivative operator. All our indices here run from 0 to 3. We can perform suitable mapping (less formally, coordinate transformation) to transform or map covariant derivative in the left hand side of (3.34) in order to match the coordinate chart of Σ_t.

The expression (3.34) upon careful inspection, seems problematic. If ω^μ lives in (the tangent bundle of) Σ_t we may not be able to just define its covariant derivative in $\mathscr{M}$. What we can actually do is extend ω^μ in $\mathscr{T}(\Sigma_t)$ to $\tilde{\omega}^\mu$ in $\mathscr{T}(\mathscr{M})$ in some neighborhood of Σ_t. Since we eventually project the result of the operation $\nabla_\nu\,\tilde{\omega}^\mu$ onto Σ_t, the extension to $\tilde{\omega}^\mu$ does not matter as long as $\tilde{\omega}^\mu = \omega^\mu$ at every point in Σ_t [29]. Technically then, (3.34) means,

$$D_\nu\,\omega^\mu = \gamma^\mu{}_\alpha\gamma^\beta{}_\nu\nabla_\beta\,\tilde{\omega}^\alpha. \tag{3.35}$$

In its "native" form for the space Σ_t,

$$D_i\,\omega^j = \frac{\partial y^\nu}{\partial x^i}\frac{\partial x^j}{\partial y^\mu}D_\nu\,\omega^\mu. \tag{3.36}$$

The extension of our definition for spatial covariant derivative for a general tensor $T^{a_1 a_2 \cdots a_m}{}_{b_1 b_2 \cdots b_n}$ on Σ_t is quite straightforward. We simply have to project the result of the action of ∇_α on the tensor onto Σ_t to get the corresponding spatial covariant derivative. Then we can perform suitable mapping to express the result in the coordinate chart of Σ_t.

$$D_\alpha T^{a_1 a_2 \ldots a_m}{}_{b_1 b_2 \ldots b_n} \equiv \gamma^\beta{}_\alpha \gamma^{a_1}{}_{p_1} \gamma^{a_2}{}_{p_2} \cdots \gamma^{a_m}{}_{p_m} \gamma^{q_1}{}_{b_1} \gamma^{q_2}{}_{b_2} \cdots \gamma^{q_n}{}_{b_n} T^{p_1 p_2 \cdots p_m}{}_{q_1 q_2 \cdots q_n},$$

$$D_k T^{i_1 \cdots i_m}{}_{j_1 \cdots j_n} = \frac{\partial y^\alpha}{\partial x^k} \frac{\partial x^{i_1}}{\partial y^{a_1}} \cdots \frac{\partial x^{i_m}}{\partial y^{a_m}} \frac{\partial y^{b_1}}{\partial x^{j_1}} \cdots \frac{\partial y^{b_n}}{\partial x^{j_n}} D_\alpha T^{a_1 \ldots a_m}{}_{b_1 \ldots b_n} \quad (3.37)$$

The definition given by (3.34) and its generalization given above allow us to relate the 3D Riemann curvature tensor to the 4D Riemann curvature tensor. We recall the definition of the Riemann curvature tensor in 4D as

$$R_{\mu\nu\alpha}{}^\beta v_\beta \equiv [\nabla_\mu, \nabla_\nu] v_\alpha. \quad (3.38)$$

where v_β is a tensor in (the cotangent bundle of) $\mathscr{M}$. Similarly, for the 3D case we have the definition

3D Riemann Tensor

$$ {}^{(3)}R_{\mu\nu\alpha}{}^\beta \omega_\beta \equiv [D_\mu, D_\nu] \omega_\alpha, \quad (3.39)$$

where ω_β is a tensor in (the cotangent bundle of) Σ_t and the action of D_μ on ω_α is defined by (3.34). In the coordinate system of Σ_t we have

$${}^{(3)}R_{ijkl} = \frac{\partial y^\mu}{\partial x^i} \frac{\partial y^\nu}{\partial x^j} \frac{\partial y^\alpha}{\partial x^k} \frac{\partial y^\beta}{\partial x^l} {}^{(3)}R_{abcd}. \quad (3.40)$$

The quantity ${}^{(3)}R^\mu{}_{\nu\alpha\beta}$ is the **intrinsic curvature** of the hypersurface Σ_t. The **extrinsic curvature** of Σ_t with respect to its embedding in $\mathscr{M}$ is defined as

Extrinsic Curvature

$$K_{\mu\nu} \equiv -\frac{1}{2} \pounds_{\mathbf{n}} \gamma_{\mu\nu}, \quad (3.41)$$

where $\pounds_{\mathbf{n}}$ is the Lie derivative operator. Since the Lie derivative of a tensor field measures the change of this field with respect to the flow of the vector field with respect to which the Lie derivative is evaluated, the extrinsic curvature

measures the change of the projection tensor as we travel along the normal vector field $\mathbf{n}$. The quantity $K_{\mu\nu}$ is often called the **second fundamental form** of the embedded manifold. The **first fundamental form** is the projection tensor $\gamma_{\mu\nu}$. Obviously, from the definition above, $K_{\mu\nu}$ is symmetric with respect to the exchange of the two indices μ and ν. [8]

Example 3. Extrinsic Curvature I. Show that $K_{\mu\nu}$ can be written in terms of the normal vector as

$$K_{\mu\nu} = -\gamma^{\alpha}{}_{\mu}\gamma^{\beta}{}_{\nu}n_{(\alpha;\beta)}, \tag{3.42}$$

where

$$n_{(\alpha;\beta)} \equiv \frac{1}{2}(n_{\alpha;\beta} + n_{\beta;\alpha}). \tag{3.43}$$

Solution. We manipulate the Lie derivative in the right hand side of (3.41).

$$\begin{aligned}
\pounds_{\mathbf{n}}\gamma_{\mu\nu} &= \gamma_{\mu\nu;\alpha}n^{\alpha} + \gamma_{\alpha\nu}n^{\alpha}{}_{;\mu} + \gamma_{\mu\alpha}n^{\alpha}{}_{;\nu}, \\
&= (\tilde{g}_{\mu\nu} + n_{\mu}n_{\nu})_{;\alpha}n^{\alpha} + (\gamma_{\alpha\nu}n^{\alpha})_{;\mu} - \gamma_{\alpha\nu;\mu}n^{\alpha} + (\gamma_{\mu\alpha}n^{\alpha})_{;\nu} - \gamma_{\mu\alpha;\nu}n^{\alpha}, \\
&= (n_{\mu}n_{\nu})_{;\alpha}n^{\alpha} - \gamma_{\alpha\nu;\mu}n^{\alpha} - \gamma_{\mu\alpha;\nu}n^{\alpha}, \\
&= n_{\mu;\alpha}n_{\nu}n^{\alpha} + n_{\mu}n_{\nu;\alpha}n^{\alpha} - n_{\alpha;\mu}n_{\nu}n^{\alpha} - n_{\alpha}n_{\nu;\mu}n^{\alpha} \\
&\quad - n_{\mu;\nu}n_{\alpha}n^{\alpha} - n_{\mu}n_{\alpha;\nu}n^{\alpha}; \qquad (n_{\alpha}n^{\alpha} = -1) \\
&= n_{\mu;\alpha}n_{\nu}n^{\alpha} + n_{\mu}n_{\nu;\alpha}n^{\alpha} + n_{\nu;\mu} + n_{\mu;\nu}, \\
&= n_{\mu;\alpha}(\gamma^{\alpha}{}_{\nu} - \delta^{\alpha}{}_{\nu}) + n_{\nu;\alpha}(\gamma^{\alpha}{}_{\mu} - \delta^{\alpha}{}_{\mu}) + n_{\nu;\mu} + n_{\mu;\nu}, \\
&= \gamma^{\alpha}{}_{\nu}n_{\mu;\alpha} + \gamma^{\alpha}{}_{\mu}n_{\nu;\alpha}, \\
&= \gamma^{\alpha}{}_{\nu}\delta^{\beta}{}_{\mu}n_{\beta;\alpha} + \gamma^{\alpha}{}_{\mu}\delta^{\beta}{}_{\nu}n_{\beta;\alpha}; \qquad (n^{\beta}n_{\beta;\alpha} = 0), \\
\pounds_{\mathbf{n}}\gamma_{\mu\nu} &= 2\gamma^{\alpha}{}_{\mu}\gamma^{\beta}{}_{\nu}n_{(\alpha;\beta)},
\end{aligned} \tag{3.44}$$

from which follows the expression we wish to show.

Example 4. Extrinsic Curvature II. Show that $K_{\mu\nu}$ can be written in terms of the normal vector as

$$K_{\mu\nu} = -\gamma^{\alpha}{}_{\mu}\gamma^{\beta}{}_{\nu}n_{\alpha;\beta}. \tag{3.45}$$

Solution. Referring to **Example 3**, the absence of parentheses simply means that since the covariant derivative of the normal vector can be decomposed into symmetric and antisymmetric parts, $n_{\alpha;\beta} = n_{(\alpha;\beta)} + n_{[\alpha;\beta]}$, where $n_{[\alpha;\beta]} = \frac{1}{2}(n_{\alpha;\beta} - n_{\beta;\alpha})$, we need only to prove that $\gamma^{\alpha}{}_{\mu}\gamma^{\beta}{}_{\nu}n_{[\alpha;\beta]} = 0$, in order to establish the expression above for $K_{\mu\nu}$.

Let us then prove this by first rewriting the left hand side as $\gamma_{\alpha\mu}\gamma_{\beta\nu}\, n^{[\alpha;\beta]}$. Then

$$\begin{aligned}
\gamma_{\alpha\mu}\,\gamma_{\beta\nu}\, n^{[\alpha;\beta]} &= \tilde{g}_{\alpha\mu}\,\tilde{g}_{\beta\nu}\, n^{[\alpha;\beta]}, \\
&= \frac{1}{2}(\tilde{g}_{\alpha\mu}\,\tilde{g}_{\beta\nu} - \tilde{g}_{\beta\mu}\,\tilde{g}_{\alpha\nu})n^{[\alpha;\beta]}, \\
&= \frac{1}{2}(n_{[\mu;\nu]} - n_{[\nu;\mu]}), \\
\gamma_{\alpha\mu}\,\gamma_{\beta\nu}\, n^{[\alpha;\beta]} &= 0.
\end{aligned} \tag{3.46}$$

Hence, $K_{\mu\nu} = -\gamma^{\alpha}{}_{\mu}\gamma^{\beta}{}_{\nu}n_{\alpha;\beta}$.

Example 5. Extrinsic Curvature III. Show that

$$K_{\mu\nu} = -\gamma^{\alpha}{}_{\mu}\nabla_{\alpha}\, n_{\nu}. \tag{3.47}$$

Solution. From **Example 4** we have

$$\begin{aligned}
K_{\mu\nu} &= -\gamma^{\alpha}{}_{\mu}\gamma^{\beta}{}_{\nu}n_{\alpha;\beta}, \\
&= -(\delta^{\alpha}{}_{\mu} + n^{\alpha}n_{\mu})\gamma^{\beta}{}_{\nu}n_{\alpha;\beta}; \qquad ((n^{\alpha}n_{\alpha})_{;\beta} = 0) \\
&= -\gamma^{\alpha}{}_{\nu}\nabla_{\alpha}\, n_{\mu},
\end{aligned}$$

$$K_{\mu\nu} = -\gamma^{\alpha}{}_{\mu}\nabla_{\alpha} n_{\nu}. \tag{3.48}$$

The last line follows from the symmetry property of $K_{\mu\nu}$.

Example 6. Extrinsic Curvature IV. Show that $K_{\mu\nu}$ is purely spatial.

Solution. It is purely spatial if its projection on the spacelike hypersurface is itself. Note the **idempotence** of the projection tensor. This means double projection is effectively an identity operation; i.e., $\gamma^{\mu}{}_{\beta}\gamma^{\alpha}{}_{\mu} = \gamma^{\alpha}{}_{\beta}$. With this idea and the relation we proved in **Example 5**, let us calculate the projection of $K_{\mu\nu}$ onto Σ_t.

$$\begin{aligned} \gamma^{\mu}{}_{\beta}K_{\mu\nu} &= -\gamma^{\mu}{}_{\beta}\gamma^{\alpha}{}_{\mu}\nabla_{\alpha}n_{\nu}, \\ &= -\gamma^{\alpha}{}_{\beta}\nabla_{\alpha}n_{\nu}, \\ \gamma^{\mu}{}_{\beta}K_{\mu\nu} &= K_{\beta\nu}. \end{aligned} \tag{3.49}$$

Hence, it is purely spatial. With $K_{\mu\nu}$ being a tensor living in Σ_t, we can calculate its trace as $\gamma^{\mu\nu}K_{\mu\nu} = K$. We can also lower and raise its indices using $\gamma_{\mu\nu}$.

Example 7. Extrinsic Curvature V. Starting from the definition of the extrinsic curvature given by (3.41) show that

$$K_{ij} = -\frac{1}{2N}(\dot{h}_{ij} - D_i N_j - D_j N_i). \tag{3.50}$$

Solution. The definition states that $K_{\mu\nu} \equiv -\frac{1}{2}\pounds_{\mathbf{n}}\gamma_{\mu\nu}$. From the definition of the time-flow vector given by (3.15), we know that $\mathbf{t} \equiv N\mathbf{n} + \mathbf{N}$. (Note that N is not the magnitude of $\mathbf{N}$.) As such, $\pounds_{\mathbf{t}}\gamma_{\mu\nu} = \pounds_{N\mathbf{n}}\gamma_{\mu\nu} + \pounds_{\mathbf{N}}\gamma_{\mu\nu}$. Let us try to take out the lapse function N from the Lie-derivative expression in the right hand side.

$$\pounds_{N\mathbf{n}}\gamma_{\mu\nu} = Nn^{\alpha}\gamma_{\mu\nu;\alpha} + (Nn^{\alpha})_{;\mu}\gamma_{\alpha\nu} + (Nn^{\alpha})_{;\nu}\gamma_{\mu\alpha},$$

$$
\begin{aligned}
&= Nn^{\alpha}\gamma_{\mu\nu;\alpha} + n^{\alpha}_{;\mu}\gamma_{\alpha\nu} + n^{\alpha}_{;\nu}\gamma_{\mu\alpha} + N_{;\mu}n^{\alpha}\gamma_{\alpha\nu} + N_{;\nu}n^{\alpha}\gamma_{\mu\alpha},\\
&= N\pounds_{\mathbf{n}}\gamma_{\mu\nu} + N_{;\mu}n^{\alpha}\gamma_{\alpha\nu} + N_{;\nu}n^{\alpha}\gamma_{\mu\alpha},\\
\pounds_{N\mathbf{n}}\gamma_{\mu\nu} &= N\pounds_{\mathbf{n}}\gamma_{\mu\nu}. \qquad (3.51)
\end{aligned}
$$

With this result the expression for the extrinsic curvature becomes

$$
K_{\mu\nu} = -\frac{1}{2N}(\pounds_{\mathbf{t}}\gamma_{\mu\nu} - \pounds_{\mathbf{N}}\gamma_{\mu\nu}). \qquad (3.52)
$$

Consider the Lie derivative with respect to the time-flow vector.

$$
\begin{aligned}
\pounds_{\mathbf{t}}\gamma_{\mu\nu} &= t^{\alpha}\gamma_{\mu\nu;\alpha} + t^{\alpha}{}_{;\mu}\gamma_{\alpha\nu} + t^{\alpha}{}_{;\nu}\gamma_{\mu\alpha}\\
\pounds_{\mathbf{t}}\gamma_{\mu\nu} &= t^{\alpha}\gamma_{\mu\nu,\alpha} + t^{\alpha}{}_{,\mu}\gamma_{\alpha\nu} + t^{\alpha}{}_{,\nu}\gamma_{\mu\alpha}. \qquad (3.53)
\end{aligned}
$$

To get K_{ij} we need to contract $K_{\mu\nu}$ with $M^{\mu}{}_{i}M^{\nu}{}_{j}$. Noting that $t^{\alpha} = \partial y^{\alpha}/\partial t$ we have

$$
\begin{aligned}
M^{\mu}{}_{i}M^{\nu}{}_{j}\pounds_{\mathbf{t}}\gamma_{\mu\nu} &= \frac{\partial y^{\mu}}{\partial x^{i}}\frac{\partial y^{\nu}}{\partial x^{j}}\frac{\partial y^{\alpha}}{\partial t}\frac{\partial \gamma_{\mu\nu}}{\partial y^{\alpha}} + \frac{\partial y^{\mu}}{\partial x^{i}}\frac{\partial y^{\nu}}{\partial x^{j}}\frac{\partial^2 y^{\alpha}}{\partial y^{\mu}\partial t}\gamma_{\alpha\nu} + \frac{\partial y^{\mu}}{\partial x^{i}}\frac{\partial y^{\nu}}{\partial x^{j}}\frac{\partial^2 y^{\alpha}}{\partial y^{\nu}\partial t}\gamma_{\mu\alpha},\\
&= \frac{\partial y^{\mu}}{\partial x^{i}}\frac{\partial y^{\nu}}{\partial x^{j}}\frac{\gamma_{\mu\nu}}{\partial t} + \frac{\partial y^{\nu}}{\partial x^{j}}\frac{\partial^2 y^{\alpha}}{\partial t\partial x^{i}}\gamma_{\alpha\nu} + \frac{\partial y^{\mu}}{\partial x^{i}}\frac{\partial^2 y^{\alpha}}{\partial t\partial x^{j}}\gamma_{\mu\alpha},\\
&= \frac{\partial}{\partial t}\left(\frac{\partial y^{\mu}}{\partial x^{i}}\frac{\partial y^{\nu}}{\partial x^{j}}\gamma_{\mu\nu}\right),\\
M^{\mu}{}_{i}M^{\nu}{}_{j}\pounds_{\mathbf{t}}\gamma_{\mu\nu} &= \dot{h}_{ij}. \qquad (3.54)
\end{aligned}
$$

The second Lie derivative in the equation for $K_{\mu\nu}$ given by (3.52) is $\pounds_{\mathbf{N}}\gamma_{\mu\nu}$. It involves the shift function which resides in the tangent bundle of Σ_t and the metric for Σ_t. As such, the expansion of the Lie derivative should involve the spatial covariant derivative operator D_{μ} instead of ∇_{μ}.

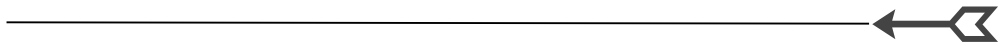
$$
\begin{aligned}
\pounds_{\mathbf{N}}\gamma_{\mu\nu} &= N^{\alpha}D_{\alpha}\gamma_{\mu\nu} + (D_{\mu}N^{\alpha})\gamma_{\alpha\nu} + (D_{\nu}N^{\alpha})\gamma_{\mu\alpha},\\
&= (D_{\mu}N^{\alpha})\gamma_{\alpha\nu} + (D_{\nu}N^{\alpha})\gamma_{\mu\alpha},\\
&= D_{\mu}N_{\nu} + D_{\nu}N_{\mu},\\
M^{\mu}{}_{i}M^{\nu}{}_{j}\pounds_{\mathbf{N}}\gamma_{\mu\nu} &= D_{i}N_{j} + D_{j}N_{i}. \qquad (3.55)
\end{aligned}
$$

Combining the last two results above for the two Lie derivatives $\pounds_{\mathbf{t}}\gamma_{\mu\nu}$ and $\pounds_{\mathbf{N}}\gamma_{\mu\nu}$ we find

$$K_{ij} = M^{\mu}{}_{i}M^{\nu}{}_{j}K_{\mu\nu} = -\frac{1}{2N}(M^{\mu}{}_{i}M^{\nu}{}_{j}\pounds_{\mathbf{t}}\gamma_{\mu\nu} - M^{\mu}{}_{i}M^{\nu}{}_{j}\pounds_{\mathbf{N}}\gamma_{\mu\nu})$$

$$K_{ij} = -\frac{1}{2N}(\dot{h}_{ij} - D_iN_j - D_jN_i), \tag{3.56}$$

which was to be shown.



3.3 (3 + 1)-Decomposition of the Riemann Tensor

We are now in position to decompose the 4D Riemann curvature tensor and curvature scalar to 3D + 1D. (This is what we mean by the (3 + 1)-decomposition). Consider a tensor ω_α living in (the cotangent bundle of) Σ_t. Then, by definition,

$$\begin{aligned}
D_\nu\,\omega_\alpha &= \gamma^{\rho}{}_{\nu}\gamma^{\sigma}{}_{\alpha}\nabla_\rho\,\omega_\sigma,\\
D_\mu D_\nu\,\omega_\alpha &= D_\mu(\gamma^{\rho}{}_{\nu}\gamma^{\sigma}{}_{\alpha}\nabla_\rho\,\omega_\sigma),\\
&= \gamma^{\lambda}{}_{\mu}\gamma^{\tau}{}_{\nu}\gamma^{\xi}{}_{\alpha}\nabla_\lambda(\gamma^{\rho}{}_{\tau}\gamma^{\sigma}{}_{\xi}\nabla_\rho\,\omega_\sigma),\\
&= \gamma^{\lambda}{}_{\mu}\gamma^{\tau}{}_{\nu}\gamma^{\xi}{}_{\alpha}\gamma^{\rho}{}_{\tau}\gamma^{\sigma}{}_{\xi}\nabla_\lambda\nabla_\rho\,\omega_\sigma + \gamma^{\lambda}{}_{\mu}\gamma^{\tau}{}_{\nu}\gamma^{\xi}{}_{\alpha}\nabla_\lambda(\gamma^{\rho}{}_{\tau}\gamma^{\sigma}{}_{\xi})\nabla_\rho\,\omega_\sigma,\\
D_\mu D_\nu\,\omega_\alpha &= \gamma^{\lambda}{}_{\mu}\gamma^{\rho}{}_{\nu}\gamma^{\sigma}{}_{\alpha}\nabla_\lambda\nabla_\rho\,\omega_\sigma + \gamma^{\lambda}{}_{\mu}\gamma^{\tau}{}_{\nu}\gamma^{\xi}{}_{\alpha}\nabla_\lambda(\gamma^{\rho}{}_{\tau}\gamma^{\sigma}{}_{\xi})\nabla_\rho\,\omega_\sigma.
\end{aligned} \tag{3.57}$$

The third line can be confusing since one may think that

$$D_\mu D_\nu\,\omega_\alpha = \gamma^{\rho}{}_{\mu}\gamma^{\sigma}{}_{\nu}\gamma^{\lambda}{}_{\alpha}\,\nabla_\rho\nabla_\sigma\,\omega_\lambda. \tag{3.58}$$

Unfortunately, this seemingly more convenient expression is in contradiction with the way we defined spatial covariant derivative above. The action of D_ν on ω_α is a projection of the action of ∇_ν on ω_α; that is, $D_\nu\,\omega_\alpha = \gamma^{\rho}{}_{\nu}\gamma^{\sigma}{}_{\alpha}\nabla_\rho\,\omega_\sigma$. Moreover, the action of D_μ on $D_\nu\,\omega_\alpha$ should be a projection of the action of ∇_μ on $D_\nu\,\omega_\alpha$ with all indices μ, ν, and α taken into account.

For the second term in the right hand side of the last equation above for

$D_\mu D_\nu\, \omega_\alpha$, we have

$$\begin{aligned}
&\gamma^\lambda{}_\mu \gamma^\tau{}_\nu \gamma^\xi{}_\alpha \gamma^\rho{}_\tau \nabla_\lambda (n^\sigma n_\xi) + \gamma^\lambda{}_\mu \gamma^\tau{}_\nu \gamma^\xi{}_\alpha \gamma^\sigma{}_\xi \nabla_\lambda (n^\rho n_\tau),\\
&\quad = \gamma^\lambda{}_\mu \gamma^\rho{}_\nu \gamma^\xi{}_\alpha (n_\xi \nabla_\lambda n^\sigma + n^\sigma \nabla_\lambda n_\xi) + \gamma^\lambda{}_\mu \gamma^\tau{}_\nu \gamma^\sigma{}_\alpha (n_\tau \nabla_\lambda n^\rho + n^\rho \nabla_\lambda n_\tau),\\
&\quad = 0 + \gamma^\lambda{}_\mu \gamma^\rho{}_\nu \gamma^\xi{}_\alpha n^\sigma \nabla_\lambda n_\xi + 0 + \gamma^\lambda{}_\mu \gamma^\tau{}_\nu \gamma^\sigma{}_\alpha n^\rho \nabla_\lambda n_\tau,\\
&\quad = -\gamma^\rho{}_\nu \gamma^\xi{}_\alpha n^\sigma K_{\mu\xi} - \gamma^\tau{}_\nu \gamma^\sigma{}_\alpha n^\rho K_{\mu\tau},\\
&\quad = -\gamma^\rho{}_\nu n^\sigma K_{\mu\alpha} - \gamma^\sigma{}_\alpha n^\rho K_{\mu\nu}. \qquad (3.59)
\end{aligned}$$

In effect, we can rewrite the expression for $D_\mu D_\nu\, \omega_\alpha$ above as

$$D_\mu D_\nu\, \omega_\alpha = \gamma^\lambda{}_\mu \gamma^\rho{}_\nu \gamma^\sigma{}_\alpha \nabla_\lambda \nabla_\rho\, \omega_\sigma - (\gamma^\rho{}_\nu n^\sigma K_{\mu\alpha} + \gamma^\sigma{}_\alpha n^\rho K_{\mu\nu}) \nabla_\rho\, \omega_\sigma. \qquad (3.60)$$

The term involving $K_{\mu\nu}$ being symmetric in the indices μ and ν, vanishes when we calculate $[D_\mu, D_\nu]\omega_\alpha$. As such, we omit this irrelevant term.

$$D_\mu D_\nu\, \omega_\alpha \supset \gamma^\lambda{}_\mu \gamma^\rho{}_\nu \gamma^\sigma{}_\alpha \nabla_\lambda \nabla_\rho \omega_\sigma - \gamma^\rho{}_\nu n^\sigma K_{\mu\alpha} \nabla_\rho \omega_\sigma. \qquad (3.61)$$

Since ω_σ lives in (the cotangent bundle of) Σ_t and n^σ is normal to Σ_t, then $n^\sigma \omega_\sigma = 0$. It follows that

$$\begin{aligned}
D_\mu D_\nu\, \omega_\alpha &\supset \gamma^\lambda{}_\mu \gamma^\rho{}_\nu \gamma^\sigma{}_\alpha \nabla_\lambda \nabla_\rho\, \omega_\sigma + \gamma^\rho{}_\nu K_{\mu\alpha} \omega_\sigma \nabla_\rho\, n^\sigma,\\
&= \gamma^\lambda{}_\mu \gamma^\rho{}_\nu \gamma^\sigma{}_\alpha \nabla_\lambda \nabla_\rho\, \omega_\sigma - K_{\mu\alpha} K_\nu{}^\sigma \omega_\sigma. \qquad (3.62)
\end{aligned}$$

Interchanging the indices μ and ν and renaming some dummy indices give us

$$\begin{aligned}
D_\nu D_\mu\, \omega_\alpha &\supset \gamma^\lambda{}_\nu \gamma^\rho{}_\mu \gamma^\sigma{}_\alpha \nabla_\lambda \nabla_\rho\, \omega_\sigma - K_{bc} K_\mu{}^\sigma \omega_\sigma,\\
&= \gamma^\rho{}_\nu \gamma^\lambda{}_\mu \gamma^\sigma{}_\alpha \nabla_\rho \nabla_\lambda\, \omega_\sigma - K_{bc} K_\mu{}^\sigma \omega_\sigma. \qquad (3.63)
\end{aligned}$$

We can now calculate the 3D Riemann curvature tensor using the last two results above that constitute $[D_\mu, D_\nu]\omega_\alpha$. Expanding this commutator and renaming some dummy indices, we find

$$[D_\mu, D_\nu]\omega_\alpha = \gamma^\rho{}_\mu \gamma^\sigma{}_\nu \gamma^\lambda{}_\alpha [\nabla_\rho, \nabla_\sigma]\omega_\lambda - K_{\mu\alpha} K_\nu{}^\lambda \omega_\lambda + K_{bc} K_\mu{}^\lambda \omega_\lambda. \qquad (3.64)$$

By definition, $[D_\mu, D_\nu]\omega_\alpha = {}^{(3)}R_{\mu\nu\alpha}{}^{\lambda}\omega_\lambda$ and $[\nabla_\mu, \nabla_\nu]\omega_\alpha = R_{\mu\nu\alpha}{}^{\lambda}\omega_\lambda$. We then find the so-called **Gauss-Codazzi Equation**:

Gauss-Codazzi Equation

$$ {}^{(3)}R_{\mu\nu\alpha}{}^{\beta} = \gamma^{\rho}{}_{\mu}\gamma^{\sigma}{}_{\nu}\gamma^{\lambda}{}_{\alpha}R_{\rho\sigma\lambda}{}^{\beta} - K_{\mu\alpha}K_{\nu}{}^{\beta} + K_{\nu\alpha}K_{\mu}{}^{\beta}. \tag{3.65}$$

It relates the 4D curvature tensor with the 3D curvature tensor.

The next thing to do is perform contraction of indices to relate the 4D curvature to the 3D curvature scalar.

$$\begin{aligned}
{}^{(3)}R_{\mu\nu\alpha}{}^{\nu} &= \gamma^{\rho}{}_{\mu}\gamma^{\sigma}{}_{\nu}\gamma^{\lambda}{}_{\alpha}R_{\rho\sigma\lambda}{}^{\nu} - K_{\mu\alpha}K_{\nu}{}^{\nu} + K_{bc}K_{\mu}{}^{\nu},\\
{}^{(3)}R_{\mu\alpha} &= \gamma^{\rho}{}_{\mu}\gamma^{\sigma}{}_{\nu}\gamma^{\lambda}{}_{\alpha}R_{\rho\sigma\lambda}{}^{\nu} - KK_{\mu\alpha} + K_{bc}K_{\mu}{}^{\nu},\\
\gamma^{\mu\alpha}\,{}^{(3)}R_{\mu\alpha} &= \gamma^{pc}\gamma^{q}{}_{\nu}\gamma^{\lambda}{}_{\alpha}R_{\rho\sigma\lambda}{}^{\nu} - K^2 + K_{bc}K^{\alpha\nu},\\
{}^{(3)}R &= \gamma^{pr}\gamma^{q}{}_{\nu}R_{\rho\sigma\lambda}{}^{\nu} - K^2 + K_{\mu\nu}K^{\mu\nu},\\
&= (\tilde{g}^{\rho\lambda} + n^{\rho}n^{\lambda})(\delta^{\sigma}{}_{\nu} + n^{\sigma}n_{\nu})R_{pqr}{}^{\nu} - K^2 + K_{\mu\nu}K^{\mu\nu},\\
&= R + n^{\rho}n^{\lambda}R_{\rho\lambda} + \tilde{g}^{\rho\lambda}n^{\sigma}n_{\nu}R_{\rho\sigma\lambda}{}^{\nu} + 0 - K^2 + K_{\mu\nu}K^{\mu\nu},\\
{}^{(3)}R &= R + 2R_{\mu\nu}n^{\mu}n^{\nu} - K^2 + K_{\mu\nu}K^{\mu\nu}.
\end{aligned} \tag{3.66}$$

The zero in the second to the last line is due to the antisymmetry of Riemann tensor namely, $R_{\rho\sigma\lambda}{}^{\nu} = -R_{\sigma\rho\lambda}{}^{\nu}$.

Let us further simplify the equation above for ${}^{(3)}R$ so that it is written solely in terms of R and $K_{\mu\nu}$ (and its contraction). For the term $R_{\mu\nu}\,n^{\mu}n^{\nu}$ we have

$$\begin{aligned}
R_{\mu\nu}\,n^{\mu}n^{\nu} &= R^{\alpha}{}_{\mu\alpha\nu}\,n^{\mu}n^{\nu},\\
&= ([\nabla_\alpha, \nabla_\nu]n^{\alpha})n^{\nu},\\
&= (\nabla_\alpha\nabla_\nu\, n^{\alpha})n^{\nu} - (\nabla_\nu\nabla_\alpha\, n^{\alpha})n^{\nu},\\
R_{\mu\nu}\,n^{\mu}n^{\nu} &= -(\nabla_\mu\, n^{\nu})(\nabla_\nu\, n^{\mu}) + (\nabla_\mu\, n^{\mu})(\nabla_\nu\, n^{\nu}) + \text{div. terms}.
\end{aligned} \tag{3.67}$$

For the first term in the right hand side, we use the relation $K_{\mu\nu} = -\gamma^{\alpha}{}_{\mu}\nabla_\alpha\, n_\nu$ established in **Example 5**. Note that this relation does *not* imply $K_{\mu\nu} = -\nabla_\mu\, n_\nu$! However, assuming that this holds yields $(\nabla_\mu\, n^{\nu})(\nabla_\nu\, n^{\mu}) = K_{\mu\nu}K^{\mu\nu}$,

which as we shall see, turns out to be correct. One proper way to reach this end is to express $\nabla_\mu n^\nu$ as $\gamma^\nu{}_\alpha \nabla_\mu n^\alpha$ and $\nabla_\nu n^\mu$ as $\gamma^\mu{}_\beta \nabla_\nu n^\beta$, noting that $n^\alpha \nabla_\mu n_\alpha = 0$. Then swap the two metric coefficients to get two extrinsic curvatures; that is, $(\nabla_\mu n^\nu)(\nabla_\nu n^\mu) = (\gamma^\mu{}_\beta \nabla_\mu n^\alpha)(\gamma^\nu{}_\alpha \nabla_\nu n^\beta) = K_\beta{}^\alpha K_\alpha{}^\beta = K_{\mu\nu} K^{\mu\nu}$. Similarly, for the second term in the right hand side of the equation above for $R_{\mu\nu} n^\mu n^\nu$, noting that $K_{\mu\nu}$ can be raised or lowered by either $\tilde{g}_{\mu\nu}$ or $\gamma_{\mu\nu}$, we have

$$\begin{aligned} \tilde{g}^{\mu\nu} K_{\mu\nu} &= -\gamma^\alpha{}_\mu \nabla_\alpha (\tilde{g}^{\mu\nu} n_\nu), \\ &= -\gamma^\alpha{}_\mu \nabla_\alpha n^\mu, \\ &= -(\delta^\alpha{}_\mu + n^\alpha n_\mu) \nabla_\alpha n^\mu, \\ \tilde{g}^{\mu\nu} K_{\mu\nu} &= -\nabla_\mu n^\mu = K. \end{aligned} \tag{3.68}$$

With the last two results above, the equation for $R_{\mu\nu} n^\mu n^\nu$ given by (3.67) can now be written as

$$R_{\mu\nu} n^\mu n^\nu = -K_{\mu\nu} K^{\mu\nu} + K^2, \tag{3.69}$$

where we have omitted the divergence terms. Upon substitution in the equation for ${}^{(3)}R$ given by the last of (3.66), we finally have

$$\boxed{{}^{(3)}R = R + K^2 - K_{\mu\nu} K^{\mu\nu}.} \tag{3.70}$$

In the coordinate system of Σ_t, this becomes ${}^{(3)}R = R + K^2 - K_{ij} K^{ij}$.

3.4 Action in Terms of the ADM Variables

In **Section 2.3** we introduced an action for inflation involving a single scalar field that is minimally coupled with gravity. It reads

$$\boxed{S = \frac{1}{2} \int \mathrm{d}^4 y \sqrt{-\tilde{g}} \left[R - \tilde{g}^{\mu\nu} \nabla_\mu \phi \, \nabla_\nu \phi - 2V(\phi) \right].} \tag{3.71}$$

The symbol tilde indicates that the integral is defined on the spacetime manifold $\mathscr{M}$ coordinatized by $y^\alpha = (y^0, y^1, y^2, y^3)$. The corresponding metric is $\mathrm{d}s^2 =$

$\tilde{g}_{\mu\nu}\mathrm{d}y^\mu\mathrm{d}y^\nu$. (This metric needless to say, is not necessarily the FLRW metric introduced in **Chapter 2**.)

In this section, we wish to express the action above in terms of the ADM variables introduced in the previous sections. In order to do so, we foliate $\mathscr{M}$ into spatial hypersurfaces (Σ_t) with each leaf labeled by a constant t. Such a foliation is possible for globally hyperbolic spacetimes[2] that cover most of the spacetimes of interest in cosmology and astrophysics [29]. The submanifold Σ_t apart from the label t, is coordinatized by $x^i = (x^1, x^2, x^3)$ and has an induced metric $\gamma_{\mu\nu} = \tilde{g}_{\mu\nu} + n_\mu n_\nu$, where $n_\mu \equiv -N\nabla_\mu t$. We can measure distances along Σ_t by using the metric $\mathrm{d}s^2_\Sigma = \gamma_{\mu\nu}\,\mathrm{d}y^\mu\mathrm{d}y^\nu$, which in turn, can be written in a manifestly 3D form given by $\mathrm{d}s^2_\Sigma = h_{ij}\,\mathrm{d}x^i\mathrm{d}x^j$. The induced metric h_{ij} is related to $\gamma_{\mu\nu}$ by $h_{ij} = M^\mu{}_i M^\nu{}_j \gamma_{\mu\nu}$.

In the ADM decomposition as what we have found out in **Section 3.1**, the metric can be written as $\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu\mathrm{d}x^\nu = -N^2\mathrm{d}t^2 + h_{ij}(N^i + \mathrm{d}x^i\mathrm{d}t)(N^j + \mathrm{d}x^j\mathrm{d}t)$. It then follows that

$$
\begin{aligned}
g_{\mu\nu} &= \begin{pmatrix} -N^2 + N_k N^k & N_i \\ N_i & h_{ij} \end{pmatrix}, \\
g^{\mu\nu} &= \frac{1}{N^2}\begin{pmatrix} -1 & N^i \\ N^i & N^2 h^{ij} - N^i N^j \end{pmatrix}, \\
\sqrt{-g} &= N\sqrt{h}
\end{aligned}
\tag{3.72}
$$

The invariant volume element in the integral above is then $\mathrm{d}^4y\sqrt{-\tilde{g}} = \mathrm{d}t\mathrm{d}x^i\sqrt{-g} = \mathrm{d}t\mathrm{d}x^i N\sqrt{h}$.

From **Sec. 3.3**, we know that the Ricci scalar can be decomposed as $R = {}^{(3)}R - K^2 + K_{ij}K^{ij}$, where K_{ij} is the extrinsic curvature that is related to the lapse and shift functions as

$$
K_{ij} = -\frac{1}{2N}(\dot{h}_{ij} - D_i N_j - D_j N_i). \tag{3.73}
$$

The lapse function is often absorbed into K_{ij} to form a new quantity that we label as E_{ij}, that does not explicitly depend on N; more specifically, $E_{ij} \equiv$

[2] A spacetime is globally hyperbolic if it has no naked singularity and no closed causal curve. [30]

$-NK_{ij}$. In effect,

$$E_{ij} = -\frac{1}{2}(\dot{h}_{ij} - D_i N_j - D_j N_i), \qquad E = E^i{}_i, \tag{3.74}$$

and the Ricci scalar in the action above becomes $R = {}^{(3)}R + N^{-2}(E_{ij}E^{ij} - E^2)$.

With all of the above considerations, all that is left is the kinetic term. We expand it using the expression for the inverse metric above.

$$\begin{aligned}\tilde{g}^{\mu\nu}\nabla_\mu\phi\,\nabla_\nu\phi &= g^{00}\dot{\phi}^2 + 2g^{0i}\dot{\phi}\,\partial_i\phi + g^{ij}\partial_i\phi\partial_j\phi,\\ &= -N^{-2}\dot{\phi}^2 + 2N^{-2}N^i\dot{\phi}\,\partial_i\phi + h^{ij}\partial_i\phi\,\partial_j\phi - N^{-2}N^iN^j\partial_i\phi\,\partial_j\phi,\\ &= -N^{-2}(\dot{\phi} - N^i\partial_i\phi)^2 + h^{ij}\partial_i\phi\,\partial_j\phi. \end{aligned}\tag{3.75}$$

With this last piece in hand, the action in terms of the ADM variables can be written as

$$S = \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{h}\Big[N\,{}^{(3)}R - 2NV + N^{-1}(E_{ij}E^{ij} - E^2) + N^{-1}(\dot{\phi} - N^i\phi_{,i})^2 - Nh^{ij}\phi_{,i}\phi_{,j}\Big]. \tag{3.76}$$

A gauge choice (see the next chapter) where $\phi = \phi(t)$, removes the terms involving spatial derivatives inside the square brackets.

ADM-Decomposed Action

$$S = \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{h}\Big[N\,{}^{(3)}R - 2NV + N^{-1}(E_{ij}E^{ij} - E^2) + N^{-1}\dot{\phi}^2\Big]. \tag{3.77}$$

CHAPTER

Decomposition of the Action for General Single-Field Inflation

4

GENERALITY IS, INDEED,
AN INDISPENSABLE INGREDIENT OF REALITY;
FOR MERE INDIVIDUAL EXISTENCE OR ACTUALITY
WITHOUT ANY REGULARITY WHATEVER IS A NULLITY.
CHAOS IS PURE NOTHING.

CHARLES SANDERS PEIRCE, THE MONIST, 1905

4.1 Action for General Single-Field Inflation
4.2 Gauge Choice
4.3 Hamiltonian Constraints
4.4 First-Order Solutions
4.5 The Second-Order Action

There is a plethora of inflation models out there ranging from single-field to multiple-field types of inflation. In this work, owing to its relative simplicity and so far, consistency with experiments, we elect the former. Even with this choice however, we are facing a multitude of possibilities. What we do is take a more general approach — ambitious enough to cover general single-field slow-roll inflation and modest enough to consider only those within the jurisdiction of general relativity. Specifically, we extend the action laid down in **Chapter 2** from a Lagrangian involving kinetic-plus-potential terms to function-of-kinetic-and-inflaton terms. The end result of this chapter, is a second-order action (from which one can obtain power spectra,) blessed with appropriate gauge choice and ADM decomposed metric.

4.1 Action for General Single-Field Inflation

We recall from **Section 3.4** the action for slow-roll single-field inflation model given by[1]

$$S = \frac{1}{2}\int d^4x\sqrt{-g}\,\left[R - g^{\mu\nu}\nabla_\mu\phi(x)\nabla_\nu\phi(x) - 2V(\phi)\right], \tag{4.1}$$

where V is the potential, R is the scalar curvature, and g is the determinant of the metric $\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu\mathrm{d}x^\nu$. The matter term in the action is a sum of the kinetic term

$$X \equiv -\frac{1}{2}g^{\mu\nu}\nabla_\mu\phi(x)\nabla_\nu\phi(x), \tag{4.2}$$

and the potential term $-V(\phi)$; that is, $X - V$. We generalize this action within the framework of general relativity by elevating the matter term to a general function of the kinetic term and the inflaton field, and call such a function $P(X,\phi)$. (As we shall see later, P stands for "pressure.") Specifically, we write the new action as [113, 110, 33]

Action for General Single-Field Inflation

$$S = \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{-g}\,[R + 2P(\phi, X)]. \tag{4.3}$$

Needless to say, when $P = X - V$, it reduces to the more familiar action given by (4.1) above.

All of the observations made as of writing this work, involving CMB, baryon acoustic oscillation (BAO), and large-scale surveys, among others, are consistent with slow-roll single-field inflation (see refs. [34, 99, 35, 36, 37] for information about these concepts and the experimental measurement results). We may not need relatively more complex theories involving multi-fields and in this work, we choose to focus on single-field inflation. The action above is general enough to encompass a wide variety of models including kinetically-driven inflation, natural inflation, polynomial chaotic inflation, etc [38]. Its generality

[1] From hereon, we loosen the tight notation used in the previous chapter. For instance, we omit the symbol tilde on top of $g_{\mu\nu}$ for the metric components not expressed in the ADM variables. We also write the spatial covariant derivative as ∇_i instead of D_i used in the previous chapter.

allows us to make model-independent calculations involving important inflationary observables such as power spectra, spectral tilt, tensor-to-scalar ratio, etc., (see **Chapter 5**) within the framework of general relativity and slow-roll single-field inflation.

Background Equations

We wish to derive the background equations of motion from the general action given by the last boxed equation above. Our main working relation is the Einstein field equation,

$$R^{\mu}{}_{\nu} - \frac{1}{2}\delta^{\mu}{}_{\nu}R = T^{\mu}{}_{\nu}. \tag{4.4}$$

The energy-momentum tensor in the right hand side is given by the definition

$$T_{\mu\nu} \equiv -\frac{2}{\sqrt{-g}}\frac{\delta S_{\phi}}{\delta g^{\mu\nu}}. \tag{4.5}$$

For the variation of the action, we have

$$\begin{aligned}
\delta S_{\phi} &= \int \mathrm{d}^4x \left(\delta\sqrt{-g}P + \sqrt{-g}P_{,X}\frac{\delta X}{\delta g^{\mu\nu}}\delta g^{\mu\nu}\right); \qquad \delta\sqrt{-g} = -\frac{1}{2}\sqrt{-g}g_{\mu\nu}\delta g^{\mu\nu} \\
&= \int \mathrm{d}^4x \left(-\frac{1}{2}\sqrt{-g}\, g_{\mu\nu}\, P + \sqrt{-g}P_{,X}\frac{\delta X}{\delta g^{\mu\nu}}\right)\delta g^{\mu\nu}, \\
&= -\frac{1}{2}\int \mathrm{d}^4x\, \sqrt{-g}\, \left(g_{\mu\nu}\, P + P_{,X}\phi_{,\mu}\phi_{,\nu}\right)\delta g^{\mu\nu},
\end{aligned} \tag{4.6}$$

from which follows

$$\frac{\delta S_{\phi}}{\delta g^{\mu\nu}} = -\frac{\sqrt{-g}}{2}(g_{\mu\nu}\, P + P_{,X}\, \phi_{,\mu}\, \phi_{,\nu}). \tag{4.7}$$

We can now write down the energy-momentum tensor as

$$\begin{aligned}
T_{\mu\nu} &= (g_{\mu\nu}P + P_{,X}\, \phi_{,\mu}\, \phi_{,\nu}), \\
T^{\mu}{}_{\nu} &= (\delta^{\mu}{}_{\nu}P + P_{,X}\, \phi^{,\mu}\, \phi_{,\nu}).
\end{aligned} \tag{4.8}$$

For the background equation of motion, the scalar field is simply a function of time [$\phi = \phi(t)$] and the spacetime is endowed with the FLRW metric. We

find that the energy-momentum tensor above takes a diagonal form similar to that of a perfect fluid in its rest frame. For the case in hand, we label the corresponding components as $T^{\mu}{}_{\nu} = \text{diag}(-\rho, p, p, p)$ where as usual, ρ is energy density while p is pressure. For the 00-component, noting that $X = \frac{1}{2}\dot{\phi}(t)^2$, we get

$$T^{0}{}_{0} \equiv -\rho = P - 2XP_{,X}. \tag{4.9}$$

For the ij-components, we have

$$T^{i}{}_{j} = P\delta^{i}_{j} = p\delta^{i}_{j}. \tag{4.10}$$

This justifies the use of the term "pressure" for the function $P(\phi, X)$ in the action.

Going back to the Einstein equation with the source term in hand, and the geometric part given by (1.11), we find for the 00-component as

First Friedmann Equation

$$\rho = 3H^2. \tag{4.11}$$

For the $ij-$components, we find (see (1.13))

Second Friedmann Equation

$$\dot{H} + H^2 = -\tfrac{1}{6}(\rho + 3p). \tag{4.12}$$

These two equations are the same Friedmann equations we derived in **Chapter 1** except that now, we have more general equations for energy density and pressure.

Hubble and Sound Flow Parameters

It will be useful for a more compact notation later in our derivations, to define the "speed of sound" c_s as

$$c_s^2 \equiv \frac{\mathrm{d}P}{\mathrm{d}\rho}. \tag{4.13}$$

Because $-\rho = P - 2XP_{,X}$ then $\mathrm{d}\rho/\mathrm{d}X = P_{,X} + 2XP_{,XX}$ and c_s can be written as

Speed of Sound

$$c_s^2 = \frac{P_{,X}}{P_{,X} + 2XP_{,XX}}. \tag{4.14}$$

The value of the speed of sound represents the speed of propagation of the scalar field. For the case where $P = X - V$, we find that it is simply unity, corresponding to the speed of light.

During inflation, the Hubble parameter and the speed of sound are nearly constant. Their small variation is measured by the slow-roll and sound flow parameters ϵ and δ respectively.

$$\epsilon \equiv -\frac{\dot{H}}{H^2} = \frac{XP_{,X}}{H^2} \quad \text{and} \quad \delta \equiv \frac{\dot{c}_s}{Hc_s}. \tag{4.15}$$

These parameters can vary as well and so are their variations, *ad infinitum*. We anticipate that each successive variation becomes smaller and smaller. For precise calculations of inflationary observables however, the corresponding chain of variations with respect to time become important. Although we need to stop somewhere, there is apparently a need to conveniently represent them. This leads to the introduction of *Hubble* and *sound flow functions*. Let $\{\epsilon_n\}$ and $\{\delta_n\}$, where $n = 0, 1, 2, \cdots$, be the sets of Hubble and sound flow functions respectively. They are recursively defined as [39, 40]

Hubble and Sound-Flow Functions

$$\epsilon_{n+1} \equiv \frac{\mathrm{d}\ln\epsilon_n}{\mathrm{d}N} \quad \text{and} \quad \delta_{n+1} \equiv \frac{\mathrm{d}\ln\delta_n}{\mathrm{d}N}, \tag{4.16}$$

where

$$\epsilon_0 \equiv \frac{H_i}{H} \quad \text{and} \quad \delta_0 \equiv \frac{c_{s,i}}{c_s}, \tag{4.17}$$

with the subscript i indicating the value of the corresponding variables above at the start of inflation. The quantity N stands for the number of e-folds with $\mathrm{d}N \equiv \mathrm{d}\ln a$. In terms of the Hubble parameter, the two definitions above are

equivalent to

$$\dot{\epsilon}_n = H\epsilon_n\epsilon_{n+1} \quad \text{and} \quad \dot{\delta}_n = H\delta_n\delta_{n+1}. \tag{4.18}$$

These relations allow us to easily see that the set of Hubble and sound flow functions (apart from sign) include the usual slow-roll parameter ϵ and the sound flow parameter δ; more specifically,

$$\epsilon_1 = \epsilon \quad \text{and} \quad \delta_1 = -\delta. \tag{4.19}$$

Furthermore, the other slow-roll parameter η defined in **Chapter 2** can be written as

$$\eta = \epsilon_1 - \tfrac{1}{2}\,\epsilon_2. \tag{4.20}$$

Rewriting the Action in Terms of ADM Variables

In the ADM decomposition, the metric is given by

ADM-Decomposed Metric

$$\mathrm{d}s^2 = g_{\mu\nu}\,\mathrm{d}x^\mu \mathrm{d}x^\nu = -N^2dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt), \tag{4.21}$$

where h_{ij} is the spatial metric of the spatial hypersurfaces in the 3+1 foliation of spacetime, N is the lapse function[2] indicating the proper time for a co-moving observer that has lapsed in relation to the coordinate time t, and N^i is the shift function indicating the projection of the time flow vector onto a spatial hypersurface (see **Chapter 3** for more details). Expressed in terms of the ADM variables, the action (4.1) as what we found in the previous chapter, can be written as

$$\begin{aligned} S = \frac{1}{2}\int \mathrm{d}t\,\mathrm{d}^3\mathbf{x}\,\sqrt{h}\Big[N\,{}^{(3)}R - 2NV + N^{-1}(E_{ij}E^{ij} - E^2) \\ + N^{-1}(\dot{\phi} - N^i\phi_{,i})^2 - Nh^{ij}\phi_{,i}\phi_{,j}\Big], \end{aligned} \tag{4.22}$$

[2] Unfortunately, the same symbol N is used for the lapse function and the number of e-folds. It should be clear from context which one we are referring to whenever we mention N in our discussion.

where

$$E_{ij} \equiv \tfrac{1}{2}(\dot{h}_{ij} - \nabla_i N_j - \nabla_j N_i)\,, \qquad E = E^i{}_i\,. \tag{4.23}$$

Note that ∇_i is covariant differentiation with respect to the spatial metric h_{ij}. We will not be repeating the calculation in **Chapter 3** for the more general action given by (4.3). It is sufficient for us to simply state the result. In terms of the ADM variables we have

ADM-Decomposed Action

$$S = \frac{1}{2}\int \mathrm{d}t\, \mathrm{d}^3\mathbf{x}\, \sqrt{h} N \left[{}^{(3)}R + \frac{1}{N^2}(E_{ij}E^{ij} - E^2) + 2P(\phi, X) \right]. \tag{4.24}$$

4.2 Gauge Choice

Appropriate choice of gauge can greatly simplify one route of calculation in comparison to another. When performing calculation using the ADM variables, the spatial metric is the one that often takes the center stage. It is then good to choose the components of the metric such that its spatial part carries much of the burden of the quantities we are interested in, but takes a form that is as simple as possible. Such a form can be realized through coordinate transformation.

Owing to its symmetric nature, the metric in four dimensional spacetime has 10 components. If we perturb the metric from the spatially flat FLRW background, there are also 10 resulting perturbation variables. Derivations can be simplified if these perturbation variables can be divided into groups that can be treated independent of each other (at least to first order). This is where the **scalar-vector-tensor (SVT) decomposition** comes in. With this sort of division, the **decomposition theorem** [1, 41] tells us that we can work on the scalar perturbation without having to mind the tensor perturbations and vice-versa. The scalar perturbation as we know, is the simplest of the three. It is directly related to matter and hence, to structure formation. The tensor perturbations on the other hand, correspond to primordial gravitational waves. Much of the details of calculations in this work involve the scalar perturbation.

The derivations for the tensor perturbations follow closely the same pathway and hence, can simply be omitted. For the most part, we ignore the vector perturbations. They decay with the expansion of the universe and hence, can be neglected.

With SVT decomposition in mind, we write the metric as

$$ds^2 = (1+2\Phi)\mathrm{d}t^2 + 2aB_i\mathrm{d}x^i\mathrm{d}t + a^2(t)[\delta_{ij}(1-2\Psi) + 2C_{ij}]\mathrm{d}x^i\mathrm{d}x^j, \quad (4.25)$$

where

$$B_i = B_{,i} + D_i; \qquad \partial^i D_i = 0, \quad (4.26)$$

$$C_{ij} = 2C_{,ij} + 2C_{(i,j)} + F_{ij}; \qquad \partial^i C_i = 0, \quad \partial^i F_{ij} = F^i{}_i = 0. \quad (4.27)$$

As we can see, the vector B_i is decomposed into a derivative of a scalar and a transverse vector. Furthermore, the tensor part C_{ij} is decomposed into derivatives of a scalar and a transverse vector, and a transverse traceless tensor. The derivative operator above with raised index should not be taken too seriously; it is just given by $\partial^i \equiv \delta^{ij}\partial_j$. The accounting in the table below tells us that we have four scalars, two transverse vectors, and one transverse traceless tensor, totaling to 10 independent perturbations (see **Table 4.1**).

Perturbation	Symbol	Independent Components
scalar	$\Phi,\ B,\ C,\ \Psi$	4
vector	$B_i,\ C_i$	(3 – 1) + (3 – 1) = 4
tensor	F_{ij}	6 – 3 – 1 = 2

Table 4.1: The 10 independent metric perturbations. The metric perturbations classified as scalar, vector, and tensor. The vector perturbations are all transverse while the tensor perturbation is transverse and traceless.

Concentrating on the scalar perturbations, the metric above reduces to

$$ds^2 = -(1+2\Phi)\mathrm{d}t^2 + 2aB_{,i}\mathrm{d}x^i\mathrm{d}t + a^2(t)[\delta_{ij}(1-2\Psi) + 2C_{,ij}]\mathrm{d}x^i\mathrm{d}x^j. \quad (4.28)$$

This metric is invariant under a set of two coordinate transformations given as

$$\begin{aligned} t &\rightarrow t + \alpha \\ x^i &\rightarrow x^i + \beta^{,i}, \end{aligned} \tag{4.29}$$

where α and β are scalars with magnitudes that are assumed to be small including their derivatives. Note that we have only two degrees of freedom here instead of four for the four-dimensional spacetime. The vector degree of freedom has been intentionally excluded because we are focusing only on scalars. The resulting transformations of these scalars can be easily derived from the invariance of the metric. For instance, consider the 00-component.

$$\begin{aligned} g_{00}(x) &= g'_{\mu\nu}(x') \frac{\partial x'^{\mu}}{\partial t} \frac{\partial x'^{\nu}}{\partial t} \\ &= g'_{00}(1+\dot{\alpha})^2 + 2g'_{0i}(1+\dot{\alpha})(\dot{\beta}^{,i}) + g'_{ij}(\dot{\beta}^{,i}\dot{\beta}^{,j}) \\ &= -(1+2\Phi')(1+\dot{\alpha})^2 + 2aB'_{,i}(1+\dot{\alpha})(\dot{\beta}^{,i}) \\ g_{00}(x) &= -1 - 2\Phi' - 2\dot{\alpha}. \end{aligned} \tag{4.30}$$

In going from the second line to the third line, we recognized that the last term in the second line is second order in β so we have discarded it. Now, since $g_{00} = -(1+2\Phi)$, we find

$$\Phi' = \Phi - \dot{\alpha}. \tag{4.31}$$

Using the same approach, we see that

$$\begin{aligned} B' &= B + \frac{\alpha}{a} - a\dot{\beta} \\ \Psi' &= \Psi + H\alpha \\ C' &= C - \beta. \end{aligned} \tag{4.32}$$

The above transformations involve the geometric part of the Einstein equation. The source part (also usually called the matter part,) involves the energy-momentum tensor $T_{\mu\nu}$. The components of $T_{\mu\nu}$ transform according to the usual

tensor transformation relation

$$T_{\mu\nu}(x) = \frac{\partial x'^{\rho}}{\partial x^{\mu}} \frac{\partial x'^{\sigma}}{\partial x^{\nu}} T'_{\rho\sigma}(x'). \tag{4.33}$$

In the first chapter, we considered only the spatially independent components of the energy-momentum tensor namely, $\mathrm{diag}(-\bar{\rho}, \bar{p}, \bar{p}, \bar{p})$. We now put a bar over them to emphasize that they are background quantities corresponding to a homogeneous isotropic universe. In this chapter and beyond, $T_{\mu\nu}$ stands for the full energy-momentum tensor including the perturbations; e.g., $T^0{}_0$ is $-\bar{\rho}(t) - \delta\rho(t, \mathbf{x})$. As such, the transformation above applies not only to the background quantities but to the perturbations as well. In fact, since we are done laying down the basics about the background quantities in the first two chapters, our main focus now is on the perturbations.

Consider the 00-component of $T_{\mu\nu}$. It transforms as

$$\begin{aligned} T^0{}_0 &= \frac{\partial x^0}{\partial x'^{\mu}} \frac{\partial x'^{\nu}}{\partial x^0} T'^{\mu}{}_{\nu} \\ T^0{}_0 &= \frac{\partial x^0}{\partial x'^0} \frac{\partial x'^0}{\partial x^0} T'^0{}_0 + \frac{\partial x^0}{\partial x'^0} \frac{\partial x'^i}{\partial x^0} T'^0{}_i + \frac{\partial x^0}{\partial x'^i} \frac{\partial x'^0}{\partial x^0} T'^i{}_0 + \frac{\partial x^0}{\partial x'^i} \frac{\partial x'^j}{\partial x^0} T'^i{}_j. \end{aligned} \tag{4.34}$$

The second term in the right hand side is second order in the perturbation variable because $\partial x'^i / \partial x^0 = \dot{\beta}^{,i}$ and $T^0{}_i$ is originally zero in the unperturbed system so it is at least first order. The same goes for the third term. The last term is likewise second order because the product of the two partial derivative terms is $\alpha_{,i}\dot{\beta}^{,j}$. We are then left with

$$\begin{aligned} \bar{\rho}(t) + \delta\rho(t, \mathbf{x}) &= (1 - \dot{\alpha})(1 + \dot{\alpha})[\bar{\rho}'(t) + \delta\rho'(t, \mathbf{x})], \\ \bar{\rho}(t) + \delta\rho(t, \mathbf{x}) &= \bar{\rho}'(t') + \delta\rho'(t, \mathbf{x}') \end{aligned} \tag{4.35}$$

Since $\bar{\rho}\,'(t') = \bar{\rho}(t) + \alpha\dot{\rho}(t)$, then

$$\boxed{\delta\rho' = \delta\rho - \alpha\dot{\bar{\rho}}.} \tag{4.36}$$

This equation tells us that matter perturbation can be made to vanish using our freedom to choose α. Likewise, some of the components of the metric perturbations can be eliminated. This can complicate a lot of things when performing calculations related to physical observables. For this reason, it is

good to define a quantity with a good combination of matter and geometric parts such that a transformation of the former is compensated by the resulting transformation of the latter. We denote one such "gauge-invariant" quantity as $\zeta(t, \mathbf{x})$ and define it as (see ref. [42] for other "gauge-invariant" variables.)

Gauge-Invariant Scalar Perturbation

$$\zeta(t, \mathbf{x}) \equiv -\Psi(t, \mathbf{x}) - \frac{H}{\dot{\bar{\rho}}(t)}\delta\rho(t, \mathbf{x}). \tag{4.37}$$

Here, H is the usual time-dependent Hubble parameter.

The quantity $\zeta(t, \mathbf{x})$ involves the Newtonian potential Ψ and the density perturbation $\delta\rho$. During inflation, the dominant component of the universe is inflaton so $\delta\rho$ involves inflaton fluctuations. These fluctuations that started out inside the Hubble sphere, went out of the horizon, became classical, and seeded the large scale structures that we nowadays see as galaxies and clusters of galaxies. The quantity $\zeta(t, \mathbf{x})$ encodes the primordial fluctuations in a gauge-invariant way. We call it the **primordial cosmological perturbation**.



Example 1. Gauge-Invariance of ζ. Show that $\zeta(t, \mathbf{x})$ is gauge-invariant under the transformation given by (4.29).

Solution. From (4.29) and the second of (4.32) we have

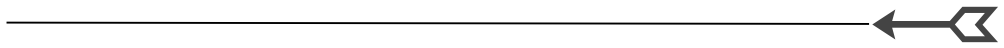
$$\begin{aligned} \Psi &\rightarrow \Psi + H\alpha, \\ t &\rightarrow t + \alpha, \\ \delta\rho &\rightarrow \delta\rho - \dot{\bar{\rho}}\alpha. \end{aligned} \tag{4.38}$$

Under time translation the scale factor, its derivative, and the derivative of the energy density transform as

$$\begin{aligned} a &\rightarrow a + \alpha\dot{a}, \\ \dot{a} &\rightarrow \dot{a} + \alpha\ddot{a} + \dot{\alpha}\dot{a}, \\ \dot{\bar{\rho}} &\rightarrow \dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}}. \end{aligned} \tag{4.39}$$

Then

$$
\begin{aligned}
-\zeta &= \Psi + \frac{H}{\dot{\bar{\rho}}}\delta\rho \\
-\zeta' &= \Psi + H\alpha + \frac{\dot{a} + \alpha\ddot{a} + \dot{\alpha}\dot{a}}{(\dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}})(a + \alpha\dot{a})}(\delta\rho - \dot{\bar{\rho}}\alpha) \\
&= \Psi + H\alpha + \frac{H + \alpha\ddot{a}/a + \dot{\alpha}H}{(\dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}})(1 + \alpha H)}(\delta\rho - \dot{\bar{\rho}}\alpha) \\
&= \Psi + H\alpha + \frac{H + \alpha\ddot{a}/a + \dot{\alpha}H - H^2\alpha}{(\dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}})}(\delta\rho - \dot{\bar{\rho}}\alpha) \\
&= \Psi + H\alpha + \frac{H + \alpha(\dot{H} + H^2) + \dot{\alpha}H - H^2\alpha}{(\dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}})}(\delta\rho - \dot{\bar{\rho}}\alpha) \\
&= \Psi + H\alpha + \frac{H + \alpha\dot{H} + \dot{\alpha}H}{(\dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}})}(\delta\rho - \dot{\bar{\rho}}\alpha) \\
&= \Psi + H\alpha + \frac{H\delta\rho - H\alpha\dot{\bar{\rho}}}{\dot{\bar{\rho}}(1 + \alpha\ddot{\bar{\rho}}/\dot{\bar{\rho}})} \\
-\zeta' &= \Psi + \frac{H}{\dot{\bar{\rho}}}\delta\rho = \zeta \qquad \blacksquare
\end{aligned}
\tag{4.40}
$$



We have effectively laid down all the necessary things we need to fix a gauge for our calculations. In so doing, we recall that in the ADM decomposition, the metric is given by

$$ds^2 = -N^2\mathrm{d}t^2 + h_{ij}(dx^i + N^i\mathrm{d}t)(\mathrm{d}x^j + N^j\mathrm{d}t). \tag{4.41}$$

As we shall see later, the lapse and shift functions N and N^i respectively, are Lagrange multipliers in the Hamiltonian formulation. They can thus be "taken out" of the Einstein Hilbert action involving the inflaton because of the separate constraint equations that we can write involving these Lagrange multipliers. As such, the focus goes to the spatial part of the metric. We choose h_{ij} to contain the gauge-invariant variables $\zeta(t, \mathbf{x})$ and the transverse traceless

tensor perturbation that we denote as γ_{ij}. We may then write our choice as

Spatial Metric

$$h_{ij} = a^2(t)e^{2\zeta(x)}\left(e^{\gamma}\right)_{ij}, \quad (\partial^i\gamma_{ij} = 0,\, \gamma^i{}_i = 0). \tag{4.42}$$

With this choice of the spatial metric, we have effectively removed one of the scalar perturbations from the metric; see (4.25). With two scalars in the coordinate transformations at our disposal (namely, α and β), we use the remaining one to fix the inflaton fluctuation to zero; that is,

$$\delta\phi(x) = 0. \tag{4.43}$$

The last two relations above constitute what we call the **comoving gauge**. In this gauge, calculations can be greatly simplified in two complementary ways. First, the background field $\phi = \phi(t)$ is used instead of the more cumbersome general inflaton function $\phi(x)$. Terms of the form $g^{\mu\nu}\phi_{,\mu}\phi_{,\nu}$ for instance, simply evaluates to $-\frac{1}{2}\dot{\phi}(t)^2$ (to zero-order) when $\phi = \phi(t)$. Second, within the framework of ADM decomposition (where the indispensable metric is not $g_{\mu\nu}$ but h_{ij}), the gauge-invariant scalar and tensor perturbations are "rightfully" encoded in the spatial metric.

The form of h_{ij} encoding the scalar and tensor perturbations is suggestive of only two important quantities worthy of consideration namely, $\zeta(x)$ and $\gamma_{ij}(x)$. Considering the form of the ADM decomposed metric, $\mathrm{d}s^2 = -N\mathrm{d}t^2 + h_{ij}(\mathrm{d}x^i + N^i\mathrm{d}t)(dx^j + N^j\mathrm{d}t)$, there is certainly no other place where another tensor perturbation could be found. However, there could be other scalar perturbations aside from $\zeta(x)$ in h_{ij}; namely, those encoded in N and N^i. One cannot remove them using coordinate transformation since the two scalars α and β have already been used up in choosing the comoving gauge. Fortunately, in the Hamiltonian formulation (that we use here), N^i and N are subject to Hamiltonian constraints. Because of these constraints, the scalar parts of the lapse and shift functions can be expressed in terms of $\zeta(x)$. Thus, there is one and only one scalar that survives namely, $\zeta(x)$.

4.3 Hamiltonian Constraints

Derivation of the Hamiltonian

We derive the Hamiltonian (density) corresponding to the Lagrangian (density) in the action given by (4.24)[3].

$$\mathcal{L} = \frac{1}{2}\sqrt{h}N\left[{}^{(3)}R + N^{-2}(E_{ij}E^{ij} - E^2) + 2P\right]. \tag{4.44}$$

Since E_{ij} is related to the extrinsic curvature K_{ij} as $K_{ij} = -E_{ij}/N$ then

Lagrangian Density

$$\mathcal{L} = \frac{1}{2}\sqrt{h}N\left({}^{(3)}R + K_{ij}K^{ij} - K^2 + 2P\right). \tag{4.45}$$

From this Lagrangian we define the canonical momentum π^{ij} as

$$\pi^{ij} \equiv \frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}}. \tag{4.46}$$

The Hamiltonian is naturally written in terms of the canonical momentum instead of the extrinsic curvature. The extrinsic curvature can be related with the canonical momentum by rewriting it in terms of h_{ij}. From the definitions of the extrinsic curvature and the time flow vector t^μ, given by (3.41) and (3.15) respectively,

$$\begin{aligned} K_{\mu\nu} &\equiv -\frac{1}{2}\pounds_{\mathbf{n}}\gamma_{\mu\nu}, \\ t^\mu &\equiv N^\mu + Nn^\mu, \end{aligned} \tag{4.47}$$

we find

$$K_{\mu\nu} = \frac{1}{2N}\left(\pounds_{\mathbf{N}}\gamma_{\mu\nu} - \pounds_{\mathbf{t}}\gamma_{\mu\nu}\right). \tag{4.48}$$

Expressed in the spatial coordinates x^i (see **Example 7** of **Sec. 3.2**),

$$K_{ij} = \frac{1}{2N}\left(\pounds_{\mathbf{N}}h_{ij} - \dot{h}_{ij}\right). \tag{4.49}$$

[3] In so doing we follow the logic given in ref. [26].

As such, we see from the definition of the canonical momentum that

$$\frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}} = \frac{\sqrt{h}N}{2}\left(0 + 2K_{kl}\frac{\partial K^{kl}}{\partial \dot{h}_{ij}} - 2K\frac{\partial K}{\partial \dot{h}_{ij}}\right),$$
$$\pi^{ij} = \frac{\sqrt{h}N}{2}\left(-\frac{K_{ij}}{N} - 2K\frac{\partial K}{\partial \dot{h}_{ij}}\right). \tag{4.50}$$

For the second term inside the pair of parentheses in the last line involving the derivative of K, we have

$$K = K^{l}{}_{l} = \frac{1}{N}\left(\frac{1}{2}\pounds_{\mathbf{N}}h^{l}{}_{l} - \frac{1}{2}h^{kl}\dot{h}_{kl}\right),$$
$$\frac{\partial K}{\partial \dot{h}_{ij}} = -\frac{h^{ij}}{2N}. \tag{4.51}$$

The expression for π^{ij} can then be written as

$$\boxed{\frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}} = \pi^{ij} = -\tfrac{1}{2}\sqrt{h}(K^{ij} - Kh^{ij}).} \tag{4.52}$$

With the canonical momentum in hand, we can now perform Legendre transformation to calculate the Hamiltonian. We have

$$\mathcal{H} = \pi^{ij}\dot{h}_{ij} - \mathcal{L}; \qquad K_{ij} = \frac{1}{N}\left(\frac{1}{2}\pounds_{\mathbf{N}}h_{ij} - \frac{1}{2}\dot{h}_{ij}\right),$$
$$\mathcal{H} = -\pi^{ij}(2NK_{ij} - \pounds_{\mathbf{N}}h_{ij}) - \tfrac{1}{2}\sqrt{h}N[{}^{(3)}R + K_{ij}K^{ij} - K^2 + 2P]. \tag{4.53}$$

Let us evaluate the Lie derivative in the expression above.

$$\pounds_{\mathbf{N}}h_{ij} = \nabla_k h_{ij}N^k + h_{kj}\nabla_i N^k + h_{ik}\nabla_j N^k,$$
$$= h_{kj}\nabla_i N^k + h_{ik}\nabla_j N^k,$$
$$\pounds_{\mathbf{N}}h_{ij} = \nabla_i N_j + \nabla_j N_i. \tag{4.54}$$

Then the Hamiltonian can be written as

$$\mathcal{H} = -\pi^{ij}[2NK_{ij} - \nabla_i N_j - \nabla_j N_i] - \tfrac{1}{2}\sqrt{h}N[{}^{(3)}R + K_{ij}K^{ij} - K^2 + 2P],$$

$$\mathcal{H} = \tfrac{1}{2}\sqrt{h}N[-{}^{(3)}R - K_{ij}K^{ij} + K^2 - 2P - 4h^{-1/2}\pi^{ij}K_{ij}] + \pi^{ij}(\nabla_i N_j + \nabla_j N_i). \tag{4.55}$$

The terms involving K and K_{ij} in the last of (4.55) can be expressed in terms of π with the help of (4.52). We start with the term $K_{ij}K^{ij}$.

$$\begin{aligned} K_{ij} &= -2h^{-1/2}\pi_{ij} + Kh_{ij}, \\ K_{ij}K^{ij} &= (-2h^{-1/2}\pi_{ij} + Kh_{ij})(-2h^{-1/2}\pi^{ij} + Kh^{ij}), \\ &= 4\frac{\pi_{ij}\pi^{ij}}{h} - 2\frac{K\pi^{ij}h_{ij}}{\sqrt{h}} - 2\frac{K\pi_{ij}h^{ij}}{\sqrt{h}} + K^2 h_{ij}h^{ij}, \\ K_{ij}K^{ij} &= h^{-1}(4\pi_{ij}\pi^{ij} - 4h^{1/2}K\pi + 3hK^2). \end{aligned} \tag{4.56}$$

From the first of (4.56) we see that

$$K = -2h^{-1/2}\pi + 3K,$$

$$\boxed{K = \frac{\pi}{\sqrt{h}}.} \tag{4.57}$$

Use this to the last of (4.56).

$$K_{ij}K^{ij} = h^{-1}\left(4\pi_{ij}\pi^{ij} - 4\pi^2 + 3\pi^2\right),$$

$$\boxed{K_{ij}K^{ij} = h^{-1}\left(4\pi_{ij}\pi^{ij} - \pi^2\right).} \tag{4.58}$$

Next we calculate $\pi^{ij}K_{ij}$.

$$\begin{aligned} \pi^{ij}K_{ij} &= \pi^{ij}\left(-2\frac{\pi^{ij}}{\sqrt{h}} + Kh_{ij}\right), \\ &= -2h^{-1/2}\pi^{ij}\pi_{ij} + K\pi, \\ \pi^{ij}K_{ij} &= -2h^{-1/2}\pi^{ij}\pi_{ij} + h^{-1/2}\pi^2. \end{aligned} \tag{4.59}$$

Use the results from the last equations of (4.57) - (4.59) in the expression

for the Hamiltonian given by the last of (4.55).

$$\begin{aligned} &- K_{ij}K^{ij} + K^2 - 4h^{-1/2}\pi^{ij}K_{ij} \\ &\quad = -h^{-1}\left(4\pi_{ij}\pi^{ij} - \pi^2\right) + h^{-1}\pi^2 + 8h^{-1}\pi^{ij}\pi_{ij} - 4h^{-1}\pi^2, \\ &\quad = 4h^{-1}\pi_{ij}\pi^{ij} - 2h^{-1}\pi^2. \end{aligned} \tag{4.60}$$

The Hamiltonian then becomes

$$\mathcal{H} = \tfrac{1}{2}\sqrt{h}N\left[-{}^{(3)}R + 4h^{-1}\pi_{ij}\pi^{ij} - 2h^{-1}\pi^2 - 2P\right] + \pi^{ij}(\nabla_i N_j + \nabla_j N_i). \tag{4.61}$$

Consider the last term above.

$$\begin{aligned} \pi^{ij}\nabla_i N_j &= \nabla_i(\pi^{ij}N_j) - N_j\nabla_i\pi^{ij}, \\ \tfrac{1}{2}\pi^{ij}(\nabla_i N_j + \nabla_j N_i) &= \nabla_i(\pi^{ij}N_j) - N_j\nabla_i\pi^{ij}, \\ \pi^{ij}(\nabla_i N_j + \nabla_j N_i) &= 2\nabla_i(\pi^{ij}N_j) - 2N_j\nabla_i\pi^{ij}. \end{aligned} \tag{4.62}$$

The first term in the right hand side is a total derivative and can be removed by integration. We use this result in the expression for $\mathcal{H}$ given above.

Hamiltonian Density

$$\mathcal{H} = \tfrac{1}{2}\sqrt{h}N\left[-{}^{(3)}R + 4h^{-1}\pi_{ij}\pi^{ij} - 2h^{-1}\pi^2 - 2P\right] - 2N_j\nabla_i\pi^{ij}. \tag{4.63}$$

This is our sought-for expression for the Hamiltonian.

Equations of Constraints

Let us look back at our expression for the Lagrangian given by (4.45). This equation together with the relations for K_{ij}, tells us that it is independent of $\dot{N}$ and $\dot{N}_i$. Symbolically,

$$\begin{aligned} \pi_N &= \frac{\partial \mathcal{L}}{\partial \dot{N}} = 0, \\ \pi_N^i &= \frac{\partial \mathcal{L}}{\partial \dot{N}_i} = 0. \end{aligned} \tag{4.64}$$

For the first equation above, one may think that $\mathcal{L} = \mathcal{L}(N, \dot{N})$. The Euler-Lagrange equation then tells us that $\partial\mathcal{L}/\partial N = 0$. Likewise, $\partial\mathcal{L}/\partial N_i = 0$. Thus, the lapse and shift functions are Lagrange multipliers. Consequently, the time derivatives of π_N and π^i_N vanish. But the time derivative of momentum is simply the derivative of the Hamiltonian with respect to the conjugate variable of the momentum. It follows that

$$\frac{\partial\mathcal{H}}{\partial N} = 0, \qquad \frac{\partial\mathcal{H}}{\partial N^i} = 0. \tag{4.65}$$

These are the primary constraints for N and N_i within the framework of Hamiltonian formalism.

Consider the first constraint above. Using the expression for the Hamiltonian given by (4.63), we find

$$\frac{\partial\mathcal{H}}{\partial N} = \frac{1}{2}\sqrt{h}\left[-{}^{(3)}R + 4h^{-1}\pi_{ij}\pi^{ij} - 2h^{-1}\pi^2 - 2P\right] - \sqrt{h}NP_{,X}\frac{\partial X}{\partial N}. \tag{4.66}$$

Since $X \equiv -\frac{1}{2}g^{\mu\nu}\phi_{,\mu}(y)\phi_{,\nu}(y)$ and $\phi = \phi(t)$, in our chosen gauge, we need to only consider the 00 component of $g^{\mu\nu}$ in the calculation of the derivative of X in the last term.

$$\frac{\partial X}{\partial N} = -2\frac{X}{N}. \tag{4.67}$$

In effect,

$$\frac{\partial\mathcal{H}}{\partial N} = \tfrac{1}{2}\sqrt{h}\left[-{}^{(3)}R + 4h^{-1}\pi_{ij}\pi^{ij} - 2h^{-1}\pi^2 - 2P\right] + 2\sqrt{h}P_{,X}X. \tag{4.68}$$

The first constraint above then becomes

First Constraint

$$-{}^{(3)}R + 4h^{-1}\pi_{ij}\pi^{ij} - 2h^{-1}\pi^2 - 2P + 4P_{,X}X = 0. \tag{4.69}$$

For the second constraint we have

Second Constraint

$$\nabla_i\pi^{ij} = 0. \tag{4.70}$$

Some people prefer to work using E_{ij}. Let us go back to the use of K_{ij} and

eventually turn to E_{ij}. We have

$$
\begin{aligned}
{}^{(3)}R - K_{ij}K^{ij} + K^2 + 2P - 4P_{,X}X = 0,\\
\nabla_i(K^{ij} - Kh^{ij}) = 0.
\end{aligned}
\tag{4.71}
$$

Since $K_{ij} = -E_{ij}/N$ and $K = -E/N$, the equations of constraint for N and N_i can be written as

Constraint Equations

$$
\begin{aligned}
{}^{(3)}R - \frac{1}{N^2}(E_{ij}E^{ij} - E^2) + 2P - 4P_{,X}X = 0,\\
\nabla_i\left[\frac{1}{N}(E^i{}_j - \delta^i_j E)\right] = 0.
\end{aligned}
\tag{4.72}
$$

Note that these equations can be easily derived from the vanishing variations of the action with respect to N and N_i. It is with the aim to have a deeper insight into the Hamiltonian formulation that we had followed a zigzag road.

Had we not considered this zigzag road, we could have just derived the last two equations above from the action and called them equations of motion. In fact, of course, we can simply call them as such. There is a shallow difference however, that may lead to confusion if proper care is not taken into account. Consider for instance, the Klein-Gordon action for a free field ϕ with mass m in Minkowski space given as

$$
S = \int \mathrm{d}^4x \left(-\tfrac{1}{2}\phi^{,\mu}\phi_{,\mu} - \tfrac{1}{2}m^2\phi^2\right). \tag{4.73}
$$

(Note that we are working with the metric signature $(-,+,+,+)$ so the sign in front of the first term is not wrong!) The corresponding equation of motion is given by

$$
(\partial_\mu\partial^\mu - m^2)\phi(x) = 0. \tag{4.74}
$$

Following suitable boundary conditions, after integration by parts, we can put the action in the form

$$
S = \tfrac{1}{2}\int \mathrm{d}^4x \left(\partial_\mu\partial^\mu\phi - m^2\phi\right)\phi, \tag{4.75}
$$

and yet we know that we cannot just take $S = 0$ due to the equation of motion

above. The case for the equation of constraint is different. We have the action involving N and N^i that are treated as Lagrange multipliers corresponding to equations of constraint of the form $f(\zeta, \dot{\zeta}) = 0$, where ζ is the expansion variable of N and N^i. (We will be more precise about this later.) Any term resulting from the manipulation of the action by way of integration by parts for instance, that is proportional to $f(\zeta, \dot{\zeta})$ can be readily eliminated. In other words, the constraint equations and the action are tied together as one system of equations.

4.4 First-Order Solutions

The advantage of using the ADM formulation is that one can regard ϕ and h_{ij} as the dynamical variables while taking N and N^i as Lagrange multipliers [43]. Given the gauge choice where the spatial metric is given by[4] $h_{ij} = a^2(t)\delta_{ij}e^{2\zeta(t,\mathbf{x})}$ and $\phi = \phi(t)$ (because $\delta\phi(t, \mathbf{x}) = 0$), it is natural to ask about the resulting form of N and N^i in the equations of constraint given by (4.72). If the deviation from the space-independent background is small, we can perform the following perturbative expansion

$$\begin{aligned} N &= 1 + N^{(1)} + N^{(2)} + \cdots, \\ N_i &= \psi_{,i} + \tilde{N}_i, \end{aligned} \tag{4.76}$$

and neglect higher-order terms that are not necessary for our desired level of approximation. The quantity $\psi_{,i}$ in the equation above is irrotational while $\tilde{N}_i$ is divergence-free (i.e., $\tilde{N}_{i,i} = 0$). These two have the following expansions:

$$\begin{aligned} \psi &= \psi^{(1)} + \psi^{(2)} + \cdots, \\ \tilde{N}_i &= \tilde{N}_i^{(1)} + \tilde{N}_i^{(2)} + \cdots \end{aligned} \tag{4.77}$$

The quantities $\tilde{N}_i$, ψ, and N admit expansions in powers of ζ. We can set the equations of constraint to zero order-by-order with respect to the variable ζ. [3]

[4] We are currently setting aside the tensor perturbation and focusing on the scalar perturbation.

The solutions to the equations of constraint (4.72) have already been calculated in refs. [113, 110]. These are given by

First-Order Solutions of the Constraint Equations

$$N^{(1)} = \frac{\dot{\zeta}}{H}, \qquad \tilde{N}_i^{(1)} = 0, \qquad \psi^{(1)} = -\frac{\zeta}{H} + \chi, \tag{4.78}$$

where χ is a solution of the differential equation

$$\delta^{ij}\partial_i\partial_j\chi = a^2\frac{\epsilon}{c_s^2}\dot{\zeta}, \tag{4.79}$$

with ϵ being the slow-roll parameter defined in **Chapter 3** and is given by (2.28)

$$\epsilon \equiv -\frac{\dot{H}}{H^2} = \frac{XP_{,X}}{H^2}, \tag{4.80}$$

and c_s is the speed of sound given by (4.14)

$$c_s^2 = \frac{P_{,X}}{2XP_{,XX} + P_{,X}}. \tag{4.81}$$

It is our task to show the explicit calculation for the solutions above.

We start with the first of (4.78) and focus on the term $E_{ij}E_{ij} - E^2$ in the first constraint equation. We should be reminded from (4.23) that

$$E_{ij} = \frac{1}{2}\left(\dot{h}_{ij} - \nabla_i N_j - \nabla_j N_i\right), \tag{4.82}$$

or, in a more compact form,

$$E_{ij} = \tfrac{1}{2}\dot{h}_{ij} - N_{(i;j)}. \tag{4.83}$$

The derivative of the spatial metric given by (4.42) can simply be written as

$$\begin{aligned}\dot{h}_{ij} &= 2a\dot{a}(1+2\zeta)\delta_{ij} + 2a^2\dot{\zeta}\delta_{ij},\\ \dot{h}_{ij} &= 2a^2[H(1+2\zeta) + \dot{\zeta}]\delta_{ij}.\end{aligned} \tag{4.84}$$

The inverse of the spatial metric and its time derivative can be easily calculated

from the expression for h_{ij}.

$$\begin{aligned} h^{ij} &= a^{-2}(1-2\zeta)\delta^{ij}, \\ \dot{h}^{ij} &= -2a^{-3}\dot{a}(1-2\zeta)\delta^{ij} - 2a^{-2}\dot{\zeta}\delta^{ij}, \\ \dot{h}^{ij} &= -\frac{2}{a^2}[H(1-2\zeta)+\dot{\zeta}]\delta^{ij}. \end{aligned} \tag{4.85}$$

(It may be a simple matter but observations suggest that pedantic people can easily get confused with δ^{ij}. It is nothing but the Kronecker delta; we have simply put the indices upstairs in the right hand side of the first of (4.85) to match the position of that in the left hand side.) Let us try to "raise" the two indices of $\dot{h}_{ij}$ in the third of (4.85).

$$\begin{aligned} h^{ik}h^{jl}\dot{h}_{kl} &= (a^{-2})(1-2\zeta)\delta^{ik}(a^{-2})(1-2\zeta)\delta^{jl}(2a^2)[H(1+2\zeta)+\dot{\zeta}]\delta_{kl}, \\ &= 2a^{-2}(1-4\zeta)[H(1+2\zeta)+\dot{\zeta}]\delta^{ij}, \\ &= 2a^{-2}[H(1-2\zeta)+\dot{\zeta}]\delta^{ij}, \\ h^{ik}h^{jl}\dot{h}_{kl} &= -\dot{h}^{ij}. \end{aligned} \tag{4.86}$$

The last line tells us that $\dot{h}_{ij}$ is not a tensor (as we should have expected) in the spatial hypersurface in the ADM decomposition. We are fortunate to have been able to see that we can raise its two indices like a tensor except for a change of sign.

Let us then calculate the product $E_{ij}E^{ij}$. To do this, we need an expression for E^{ij}.

$$\begin{aligned} E^{ij} &= h^{ik}h^{jl}E_{kl}, \\ E^{ij} &= h^{ik}h^{jl}\left[\tfrac{1}{2}\dot{h}_{kl} - N_{(k;l)}\right], \\ E^{ij} &= -\tfrac{1}{2}\dot{h}^{ij} - N^{(i;j)}. \end{aligned} \tag{4.87}$$

Contracting this with E_{ij} we find

$$\begin{aligned} E_{ij}E^{ij} &= -\left[\tfrac{1}{2}\dot{h}_{ij} - N_{(i;j)}\right]\left[\tfrac{1}{2}\dot{h}^{ij} + N^{(i;j)}\right], \\ &= -\tfrac{1}{4}\dot{h}_{ij}\dot{h}^{ij} + \tfrac{1}{2}\dot{h}^{ij}N_{(i;j)} - \tfrac{1}{2}\dot{h}_{ij}N^{(i;j)} + N_{(i;j)}N^{(i;j)}, \end{aligned}$$

$$= -\tfrac{1}{4}\dot{h}_{ij}\dot{h}^{ij} + \tfrac{1}{2}\dot{h}^{ij}N_{(i;j)} + \tfrac{1}{2}\dot{h}^{ij}N_{(i;j)} + N_{(i;j)}N^{(i;j)},$$

$$E_{ij}E^{ij} = -\tfrac{1}{4}\dot{h}_{ij}\dot{h}^{ij} + \dot{h}^{ij}N_{(i;j)} + N_{(i;j)}N^{(i;j)}. \tag{4.88}$$

For the first term in the right hand side of the last equation above, we use the last lines of (4.84) and (4.85).

$$\dot{h}_{ij}\dot{h}^{ij} = 2a^2[H(1+2\zeta)+\dot{\zeta}]\delta_{ij}\left(-\frac{2}{a^2}\right)[H(1-2\zeta)+\dot{\zeta}]\delta^{ij},$$

$$\dot{h}_{ij}\dot{h}^{ij} = -12(H^2 + H\dot{\zeta} + H\dot{\zeta}),$$

$$\dot{h}_{ij}\dot{h}^{ij} = -12(H^2 + 2H\dot{\zeta}). \tag{4.89}$$

In effect, the last of (4.88) turns out to be

$$E_{ij}E^{ij} = 3(H^2 + 2H\dot{\zeta}) + \dot{h}^{ij}N_{(i;j)} + N_{(i;j)}N^{(i;j)}. \tag{4.90}$$

Next, we calculate E^2. Because $E = E^i{}_i = h^{ik}E_{ki}$ then we are able to derive

$$E = a^{-2}(1-2\zeta)\delta^{ik}\left[\tfrac{1}{2}\dot{h}_{ki} - N_{(k;i)}\right],$$

$$= \tfrac{1}{2}a^{-2}(1-2\zeta)\delta^{ik}(2a^2)\left[H(1+2\zeta)+\dot{\zeta}\right]\delta_{ki} - h^{ik}N_{(k;i)},$$

$$E = 3(H+\dot{\zeta}) - h^{ik}N_{(k;i)}. \tag{4.91}$$

Taking the square of this, we find

$$E^2 = 9(H^2 + 2H\dot{\zeta}) - 6(H+\dot{\zeta})h^{ik}N_{(k;i)} + h^{ik}h^{jl}N_{(i;k)}N_{(j;l)}. \tag{4.92}$$

We can now calculate the quantity $E_{ij}E^{ij} - E^2$.

$$E_{ij}E^{ij} - E^2 = -6(H^2 + 2H\dot{\zeta}) + \dot{h}^{ij}N_{(i;j)} + N_{(i;j)}N^{(i;j)},$$
$$+ 6(H+\dot{\zeta})h^{ij}N_{(i;j)} - h^{ik}h^{jl}N_{(i;k)}N_{(j;l)}. \tag{4.93}$$

For the second term in the right hand side, we have from (4.85),

$$\dot{h}^{ij} = -\frac{2}{a^2}[H(1-2\zeta)+\dot{\zeta}]\delta^{ij},$$

$$\dot{h}^{ij} = -2Hh^{ij} - \frac{2}{a^2}\dot{\zeta}\delta^{ij},$$
$$\dot{h}^{ij}N_{(i;j)} = \left(-2Hh^{ij} - \frac{2}{a^2}\dot{\zeta}\delta^{ij}\right)N_{(i;j)},$$
$$\dot{h}^{ij}N_{(i;j)} = -2Hh^{ij}N_{(i;j)} - \frac{2}{a^2}\dot{\zeta}\delta^{ij}N_{(i;j)}. \tag{4.94}$$

Because of the expansion

$$N_i = \psi_{1,i} + \psi_{2,i} + \cdots + \tilde{N}_i^{(1)} + \tilde{N}_i^{(2)} + \cdots \tag{4.95}$$

we see that the second term in the right hand side of the last of (4.94) is second order. Then to first order,

$$\dot{h}^{ij}N_{(i;j)} = -2Hh^{ij}N_{(i;j)}. \tag{4.96}$$

Following the same reasoning, we see that the last terms in the first and second lines of (4.93) are second order. Furthermore, the product $\dot{\zeta}N_{(i;j)}$ is second order. To first order then, (4.93) can be written as

$$E_{ij}E^{ij} - E^2 = -6(H^2 + 2H\dot{\zeta}) - 2Hh^{ij}N_{(i;j)} + 6Hh^{ij}N_{(i;j)}. \tag{4.97}$$

Consider the covariant derivative in the right hand side. We have

$$\Gamma^i_{jk} = \frac{1}{2}h^{il}(h_{lj,k} + h_{kl,j} - h_{jk,l}). \tag{4.98}$$

Because $h_{ij} = a^2(1+2\zeta)\delta_{ij}$ and $h^{ij} = a^{-2}(1-2\zeta)\delta^{ij}$ the quantity Γ^i_{jk} is first order in ζ. We thus find that $N_{i;j} = N_{i,j}$ to first order. It follows that (4.97) can be written as

$$E_{ij}E^{ij} - E^2 = -6(H^2 + 2H\dot{\zeta}) + 4Hh^{ij}N_{(i,j)}. \tag{4.99}$$

Consider the last term above. Because $\tilde{N}_{i,i} = 0$ then

$$\begin{aligned} h^{ij}N_{(i,j)} &= \tfrac{1}{2}h^{ij}(\psi^{(1)}_{,ij} + \psi^{(1)}_{,ji}), \qquad \psi^{(1)}_{,ij} = \psi^{(1)}_{,ji} \\ h^{ij}N_{(i,j)} &= h^{ij}\psi^{(1)}_{,ij}. \end{aligned} \tag{4.100}$$

But $h^{ij} = a^2(1-2\zeta)\delta^{ij}$ and $\zeta\psi^{(1)}$ is second order. Then,

$$h^{ij}N_{(i,j)} = a^{-2}\delta^{ij}\psi^{(1)}_{,ij}. \tag{4.101}$$

Using this to (4.99) gives us

$$E_{ij}E^{ij} - E^2 = -6(H^2 + 2H\dot{\zeta}) + 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij}. \tag{4.102}$$

Substitute the result above in the first equation of constraint,

$${}^{(3)}R - \frac{1}{N^2}(E_{ij}E^{ij} - E^2) + 2P - 4P_{,X}X = 0. \tag{4.103}$$

In this equation the scalar curvature to first order in ζ is given by (try Maxima)

$${}^{(3)}R = -\frac{4}{a^2}\nabla^2\zeta. \tag{4.104}$$

As such, using this equation together with (4.99), in (4.103) gives us

$$-\frac{4}{a^2}\nabla^2\zeta + 2P - 4XP_{,X} - \frac{1}{N^2}\left[-6(H^2 + 2H\dot{\zeta}) + 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij}\right] = 0. \tag{4.105}$$

The last term in the left hand side can be written as

$$-(1 - 2N^{(1)})\left[-6(H^2 + 2H\dot{\zeta}) + 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij}\right], \tag{4.106}$$

which to first order, is simply

$$-12N^{(1)}H^2 + 12H\dot{\zeta} - 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij}. \tag{4.107}$$

It follows that

$$-\frac{4}{a^2}\nabla^2\zeta + 2P - 4XP_{,X} - 12N^{(1)}H^2 + 12H\dot{\zeta} - 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij} = 0. \tag{4.108}$$

Note that the quantity P also depends on N. Its corresponding expansion can result to a complicated expression for $N^{(1)}$. The way out of this complication is to simply take

$$N^{(1)} = \frac{\dot{\zeta}}{H}, \tag{4.109}$$

and see if we will be able to arrive at the other desired results.

With (4.109) at hand, (4.108) becomes

$$-\frac{4}{a^2}\nabla^2\zeta + 2P - 4XP_{,X} - 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij} = 0. \tag{4.110}$$

Let us focus now on the second and third terms above involving P. We can think of X as $X = X^{(0)} + \delta X$, where $X^{(0)}$ is zero-order while δX is first-order. Then, ignoring in the mean time the argument ϕ of P, we see that

$$\begin{aligned} P(X^{(0)} + \delta X) &= P(X^{(0)}) + (\delta X)P(X^{(0)})_{,X}, \\ XP_{,X} &= (X^{(0)} + \delta X)\left[P(X^{(0)})_{,X} + (\delta X)P(X^{(0)})_{,XX}\right], \\ XP_{,X} &= X^{(0)}P_{,X} + (\delta X)P_{,X} + (\delta X)X^{(0)}P_{,XX}. \end{aligned} \tag{4.111}$$

Then

$$2P - 4XP_{,X} = 2P(X^{(0)}) - 4X^{(0)}P_{,X} - 2(\delta X)P_{,X} - 4(\delta X)X^{(0)}P_{,XX}. \tag{4.112}$$

If we simply write $X^{(0)}$ as X and ignore the zero-order terms in (4.110), we find

$$-\frac{4}{a^2}\nabla^2\zeta - 2(\delta X)P_{,X} - 4(\delta X)XP_{,XX} - 4Ha^{-2}\delta^{ij}\psi^{(1)}_{,ij} = 0. \tag{4.113}$$

We recall the definition of X and the expression for the inverse of the metric in the ADM formalism.

$$X \equiv -\frac{1}{2}g^{\mu\nu}\phi_{,\mu}\phi_{,\nu}, \qquad g^{\mu\nu} = \frac{1}{N^2}\begin{pmatrix} -1 & N^i \\ N^i & N^2h^{ij} - N^iN^j \end{pmatrix}. \tag{4.114}$$

Then $g^{\mu\nu} = g^{\mu\nu(0)} - 2N^{(1)}g^{\mu\nu(0)}$ and $\delta X = -2N^{(1)}X$. (Note that we can ignore N^i because $\phi = \phi(t)$.) By virtue of (4.109), this variation of X can be expressed as

$$\delta X = -2\frac{\dot{\zeta}}{H}X. \tag{4.115}$$

To first-order then, (4.113) can be written as

$$-\frac{1}{a^2}\nabla^2\zeta+\frac{\dot{\zeta}}{H}XP_{,X}+2\frac{\dot{\zeta}}{H}X^2P_{,XX}-\frac{H}{a^2}\nabla^2\psi^{(1)}=0;\ \nabla^2\equiv\delta^{ij}\partial_i\partial_j$$

$$\nabla^2\psi^{(1)}=-\frac{\nabla^2\zeta}{H}+\frac{a^2}{H^2}\left(XP_{,X}+2X^2P_{,XX}\right)\dot{\zeta}. \tag{4.116}$$

Let us see if this is correct. Equations (4.78) and (4.79) tell us that

$$\psi^{(1)}=-\frac{\zeta}{H}+\chi;\qquad \nabla^2\chi=a^2\frac{\epsilon}{c_s^2}\dot{\zeta} \tag{4.117}$$

Use the expressions for ϵ and c_s given by (4.80) and (4.81) respectively, in the second equation above and use the resulting equation in the expression for $\nabla^2\psi^{(1)}$.

$$\nabla^2\psi^{(1)}=-\frac{\nabla^2\zeta}{H}+\frac{a^2}{H^2}\left(XP_{,X}+2X^2P_{,XX}\right)\dot{\zeta}. \tag{4.118}$$

This is exactly (4.116). Thus, subject to some initial or boundary conditions, (4.116) holds and implies (4.117).

Let us now move on to show that $\partial^2\tilde{N}_i^{(1)}=0$. For this, we need the second equation of constraint given by (4.72) namely,

$$\nabla_i\left[N^{-1}(E^i{}_j-\delta^i_jE)\right]=0. \tag{4.119}$$

The covariant derivative above can simply be taken as ordinary derivative because the Christoffel symbol is first order in ζ. Let us then expand the expression above.

$$-N^{-2}\partial_iN(E^i{}_j-\delta^i_jE)+N^{-1}\partial_i(E^i{}_j-\delta^i_jE)=0;\qquad N\approx1+N^{(1)},$$

$$-(1-2N^{(1)})\partial_iN(E^i{}_j-\delta^i_jE)+(1-N^{(1)})\partial_i(E^i{}_j-\delta^i_jE)=0,$$

$$-\partial_iN(E^i{}_j-\delta^i_jE)+(1-N^{(1)})\partial_i(E^i{}_j-\delta^i_jE)=0. \tag{4.120}$$

We note that $N^{(1)}\partial_iN$ is second order so in going from the second to the third line, we have removed the terms containing this product.

Let us calculate E_{ij} and E.

$$\begin{aligned}
E_{ij} &= \tfrac{1}{2}\dot{h}_{ij} - N_{i,j},\\
&= a^2[H(1+2\zeta)+\dot{\zeta}]\delta_{ij} - N_{(i,j)},\\
E_{ij} &= h_{ij}H + a^2\dot{\zeta}\delta_{ij} - N_{(i,j)},\\
E^i{}_j &= h^{ik}[h_{kj}H + a^2\dot{\zeta}\delta_{kj} - N_{(k,j)}],\\
&= \delta^i_j H + a^2\dot{\zeta}a^{-2}(1-2\zeta)\delta^{ik}\delta_{kj} - a^{-2}(1-2\zeta)\delta^{ik}N_{(k,j)},\\
E^i{}_j &= \delta^i_j H + \dot{\zeta}\delta^i_j - a^{-2}\delta^{ik}N_{(k,j)},\\
E &= 3H + 3\dot{\zeta} - a^{-2}\delta^{ik}N_{(k,i)}.
\end{aligned} \tag{4.121}$$

The difference $E^i{}_j - \delta^i_j E$ can now be calculated from the last two lines.

$$E^i{}_j - \delta^i_j E = -2H\delta^i_j - 2\delta^i_j\dot{\mathcal{R}} - a^{-2}\delta^{ik}N_{(k,j)} + a^{-2}\delta^i_j\delta^{kl}N_{(k,l)}. \tag{4.122}$$

Consider the first term in the last of (4.120), namely, $-\partial_i N(E^i{}_j - \delta^i_j E)$. Since $\partial_i N$ is at least first order, to first order, we can only multiply it with $-2H\delta^i_j$ above. Mathematically,

$$\begin{aligned}
-\partial_i N(E^i{}_j - \delta^i_j E) &= 2\partial_i N H\delta^i_j,\\
&= 2\partial_i N^{(1)} H\delta^i_j,\\
&= 2\partial_i\frac{\dot{\zeta}}{H}H\delta^i_j,\\
-\partial_i N(E^i{}_j - \delta^i_j E) &= 2\partial_j\dot{\zeta}.
\end{aligned} \tag{4.123}$$

For the second term in the last of (4.120), we have

$$\begin{aligned}
\partial_i(E^i{}_j - \delta^i_j E) &= -2\partial_j\dot{\zeta} - a^{-2}\partial^k N_{(k,j)} + a^{-2}\delta^{kl}\partial_j N_{(k,l)},\\
&= -2\partial_j\dot{\zeta} - \frac{a^{-2}}{2}\partial^2\tilde{N}^{(1)}_j - a^{-2}\psi^{(1)}_{,iij} + a^{-2}\psi^{(1)}_{,iij},\\
&= -2\partial_j\dot{\zeta} - \frac{a^{-2}}{2}\partial^2\tilde{N}^{(1)}_j,
\end{aligned}$$

$$(1-N^{(1)})\partial_i(E^i{}_j-\delta^i_j E)=-2\partial_j\dot{\zeta}-\frac{a^{-2}}{2}\partial^2\tilde{N}^{(1)}_j. \tag{4.124}$$

Adding the last expressions in (4.123) and (4.124) gives us

$$\partial^2\tilde{N}^{(1)}_i=0. \tag{4.125}$$

Under appropriate choice of boundary condition, one can simply set $\tilde{N}^{(1)}_i=0$. This finishes our derivation of the first-order solutions.

4.5 The Second-Order Action

The action expressed in terms of the ADM variables can be expanded as

$$S=S^{(0)}+S^{(1)}+S^{(2)}+S^{(3)}+\cdots, \tag{4.126}$$

where $S^{(n)}$ means to order $\mathcal{O}(\zeta^n)$. The zero-order action corresponds to the background, while $S^{(2)}$ and $S^{(3)}$ correspond to the free part and interaction part respectively. The free part is necessary in the calculation of the power spectrum while the interaction part is needed in the derivation of non-Gaussianity. The least important part is $S^{(1)}$ which vanishes by virtue of the first-order equations of constraint.

$$S=S^{(0)}+S^{(2)}+S^{(3)}+\cdots. \tag{4.127}$$

For the most part, we are only interested in the calculation of the power spectrum and its regularization. As such, the "background" and free parts suffice for our purposes.

In this section we wish to calculate $S^{(2)}$. In so doing, we recall that the action given by (4.24) involves N and N^i. Having calculated these quantities in terms of ζ up to first order, one may ask if we need an expression for N and N^i up to $\mathcal{O}(\zeta^2)$ and perform another round of laborious derivation similar to that of the previous section. Careful inspection tells us that the answer is no. It was pointed out in ref. [43] that *the second-order terms in N, N^i multiply the constraints evaluated to first order, which vanish due to the first-order expressions for N and N^i*. In fact, going beyond $n=2$, detailed calculations in

ref. [110] indicate that for $S^{(n)}$, $n \geq 3$, one only needs knowledge of N and N^i up to $N^{(n-2)}$ and $N^{i(n-1)}$. It follows that even at $n = 3$, we need only the expansion for N and N^i up to first order.[5]

With this matter settled, we proceed to the calculation proper. From the action given by (4.24),

$$S = \frac{1}{2}\int d^4x \left\{\sqrt{h}N\left[{}^{(3)}R + 2P(\phi, X)\right] + \sqrt{h}N^{-1}\left(E_{ij}E^{ij} - E^2\right)\right\}, \quad (4.128)$$

we identify the Lagrangian as

$$\mathcal{L} = \tfrac{1}{2}\sqrt{h}N\left[{}^{(3)}R + 2P(\phi, X)\right] + \tfrac{1}{2}\sqrt{h}N^{-1}\left(E_{ij}E^{ij} - E^2\right). \quad (4.129)$$

We wish to show that the second-order action is given by [113, 110]

$$S^{(2)} = \int \mathrm{d}t\, \mathrm{d}^3x\, \frac{a^2\epsilon}{c_s^2}\left(a\dot{\zeta}^2 - \frac{c_s^2}{a}\zeta_{,i}\zeta^{,i}\right), \quad (4.130)$$

where (see (4.13) for the definition of c_s^2)

$$\epsilon \equiv -\frac{\dot{H}}{H^2} = \frac{XP_{,X}}{H^2}, \qquad c_s^2 = \frac{P_{,X}}{2XP_{,XX} + P_{,X}}. \quad (4.131)$$

We start with the factor $\sqrt{h}N$ in the Lagrangian. Since the 3D metric is given by $h_{ij} = a^2e^{2\zeta}\delta_{ij}$, then $\sqrt{h} = a^3e^{3\zeta}$. On the other hand, the lapse function can be written as $N = 1 + \alpha$, with $\alpha \equiv N^{(1)}$ (we denote $N^{(1)}$ as simply α to avoid confusion with N and N^i).

$$\sqrt{h}N = a^3e^{3\zeta}(1 + \alpha). \quad (4.132)$$

For the 3D scalar curvature we find[6] (using e.g., Maxima)

$${}^{(3)}R = -2a^{-2}e^{-2\zeta}\left[2\nabla^2\zeta + (\partial_i\zeta)(\partial^i\zeta)\right] \quad (4.133)$$

[5] We do not reproduce here the (already) detailed calculations in ref. [110] nor the explicit cancellations of many terms due to the equation of constraint. Including vanishing terms that pretend not to be, would simply fill the pages with extraordinary long equations.

[6] This expression for the curvature just like that for other quantities in this section is truncated up to second order because the aim is the second-order action.

Here, we follow the convention $\partial_i = \partial^i$ and $\nabla^2 = \delta^{ij}\partial_i\partial_j$. We have raised one of the indices in the last term inside the square brackets to emphasized the implied summation.

Next we consider the term $P(\phi(t), X)$. Note that the scalar field in our chosen gauge is function of time only. As such,

$$X \equiv -\frac{1}{2}g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} = -\frac{1}{2}g^{00}\dot{\phi}^2 = \frac{1}{2}N^{-2}\dot{\phi}^2. \tag{4.134}$$

The quantity X can now be expanded as follows.

$$\begin{aligned} X = X^{(0)} + \Delta X &= \frac{1}{2}\dot{\phi}^2(1+\alpha)^{-2}, \\ &= \frac{1}{2}\left(\dot{\phi}^2 - 2\alpha\dot{\phi}^2 + 3\alpha^2\dot{\phi}^2\right), \\ X = X^{(0)} &+ (-2\alpha + 3\alpha^2)X^{(0)}. \end{aligned} \tag{4.135}$$

We identify $\Delta X = (-2\alpha + 3\alpha^2)X^{(0)}$. Taking $P^{(0)} = P(X^{(0)})$ and using this expression for ΔX we can expand P as

$$\begin{aligned} P(X^{(0)} + \Delta X) &= P^{(0)} + P^{(0)}_{,X}\Delta X + \frac{1}{2}P^{(0)}_{,XX}(\Delta X)^2, \\ &= P^{(0)} + P^{(0)}_{,X}(-2\alpha + 3\alpha^2)X^{(0)} + \frac{1}{2}P^{(0)}_{,XX}[(-2\alpha + 3\alpha^2)X^{(0)}]^2, \\ P(X^{(0)} + \Delta X) &= P^{(0)} + P^{(0)}_{,X}(-2\alpha + 3\alpha^2)X^{(0)} + \frac{1}{2}P^{(0)}_{,XX}(4\alpha^2)[X^{(0)}]^2. \end{aligned} \tag{4.136}$$

Let us clean up our notation and simply denote $P^{(0)}$ and $X^{(0)}$ by P and X respectively. Furthermore, we denote the derivative of P with respect to X by a prime. Then,

$$P(X + \Delta X) = P - 2\alpha X P' + \alpha^2(3XP' + 2X^2P''). \tag{4.137}$$

We have all the necessary equations to calculate the first term in the Lagrangian. We start with $\sqrt{h}N\,{}^{(3)}R$. In the calculation that follows, we use the sub-calculation results given by (4.132) and (4.133).

$$\sqrt{h}N\,{}^{(3)}R = -2ae^{\zeta}(1+\alpha)\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right]; \qquad \alpha = \frac{\dot{\zeta}}{H},$$

$$
\begin{aligned}
&= \frac{-2a}{H} e^{\zeta}(H+\dot{\zeta})\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right], \\
&= -\frac{2}{H}\frac{d}{dt}\left(ae^{\zeta}\right)\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right], \\
&\supset 2\left(-\frac{\dot{H}}{H^2}\right)\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right]e^{\zeta} + \frac{2}{H}ae^{\zeta}\left[2\nabla^2\dot{\zeta} + 2(\partial_i\dot{\zeta})(\partial^i\zeta)\right], \\
&\supset 2a\epsilon\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right]e^{\zeta} + \frac{2}{H}ae^{\zeta}\left[-2(\partial_i\dot{\zeta})(\partial^i\zeta) + 2(\partial_i\dot{\zeta})(\partial^i\zeta)\right], \\
&= 2a\epsilon\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right]e^{\zeta}, \\
&\supset 2a\epsilon\left[-2(\partial_i\zeta)^2 + (\partial_i\zeta)^2\right]e^{\zeta}, \\
\sqrt{h}N\,{}^{(3)}R &\supset -2a\epsilon(\partial_i\zeta)^2\left(1+\zeta+\cdots\right)
\end{aligned}
\tag{4.138}
$$

Then,

$$
\boxed{\sqrt{h}N\,{}^{(3)}R \supset -2a\epsilon(\partial_i\zeta)^2 + \mathcal{O}(\zeta^3).} \tag{4.139}
$$

For the term $\sqrt{h}NP$, we use (4.132) and (4.137).

$$
\begin{aligned}
\sqrt{h}NP &= a^3e^{3\zeta}N\left[P - 2\alpha XP' + \alpha^2(3XP' + 2X^2P'')\right], \\
\sqrt{h}NP &= a^3e^{3\zeta}\left[P - 2\alpha XP' + \alpha^2(3XP' + 2X^2P'') + \alpha P - 2\alpha^2XP'\right].
\end{aligned}
\tag{4.140}
$$

Note from the first and second of (4.131) that $H^2\epsilon/c_s^2 = XP' + 2X^2P''$.

$$
\sqrt{h}NP = a^3e^{3\zeta}\left[P + \alpha(P - 2XP') + \alpha^2H^2\frac{\epsilon}{c_s^2}\right]. \tag{4.141}
$$

Because $\dot{H} = -\frac{1}{2}(\rho + P)$ and $\rho = 3H^2$ then $P = -2\dot{H} - 3H^2$. Furthermore, $XP' = \epsilon H^2 = -\dot{H}$. In effect, $P - 2XP' = P + 2\dot{H} = -3H^2$. We can then rewrite the expression above as

$$
\sqrt{h}NP = a^3e^{3\zeta}\left[-2\dot{H} - 3H^2(1+\alpha) + \alpha^2H^2\frac{\epsilon}{c_s^2}\right]. \tag{4.142}
$$

Note that $(a^3e^{3\zeta})^{\cdot} = 3a^3(H+\dot{\zeta})e^{3\zeta}$. As such,

$$a^3e^{3\zeta}\dot{H} \supset -3a^3e^{3\zeta}H(H+\dot{\zeta}) = -3a^3e^{3\zeta}H^2(1+\alpha). \tag{4.143}$$

and the equation above can be written as

$$\sqrt{h}NP = a^3e^{3\zeta}\left[3H^2(1+\alpha) + \alpha^2H^2\frac{\epsilon}{c_s^2}\right]. \tag{4.144}$$

We leave the exponential function above unexpanded to ease taking of derivatives in case we need to perform integration by parts later.

Let us now move on to the second term of the Lagrangian given by (4.129) namely, $\sqrt{h}N^{-1}(E_{ij}E^{ij} - E^2)$. The factor $\sqrt{h}N^{-1}$ can be expanded as

$$\sqrt{h}N^{-1} = a^3e^{3\zeta}(1+\alpha)^{-1}, \tag{4.145}$$

where the exponential factor has not been expanded in anticipation of the exponential factor in the terms $E_{ij}E^{ij} - E^2$. For the term $E_{ij}E^{ij} - E^2$, recall from (4.83) that

$$E_{ij} = \frac{1}{2}\dot{h}_{ij} - N_{(i;j)}, \qquad N_{(i;j)} = \frac{1}{2}(N_{i;j} + N_{j;i}). \tag{4.146}$$

Noting that $E^{ij} = h^{ik}h^{lj}E_{kl}$, then the contraction $E_{ij}E^{ij}$ can be written as

$$\begin{aligned}
E_{ij}E^{ij} &= \left[\frac{1}{2}\dot{h}_{ij} - N_{(i;j)}\right]\left[\frac{1}{2}\dot{h}^{ij} - N^{(i;j)}\right], \\
&= -\frac{1}{4}\dot{h}_{ij}\dot{h}^{ij} + \frac{1}{2}\dot{h}^{ij}N_{(i,j)} - \frac{1}{2}\dot{h}_{ij}h^{ik}h^{lj}N_{k;l} + h^{ik}h^{lj}N_{(i;j)}N_{k;l}, \\
E_{ij}E^{ij} &= -\frac{1}{4}\dot{h}_{ij}\dot{h}^{ij} + \dot{h}^{ij}N_{(i,j)} + h^{ik}h^{lj}N_{(i;j)}N_{k;l}.
\end{aligned} \tag{4.147}$$

Because $\dot{h}_{ij} = 2a^2e^{2\zeta}(H+\dot{\zeta})\delta_{ij}$ and $\dot{h}^{ij} = -2a^{-2}e^{-2\zeta}(H+\dot{\zeta})\delta^{ij}$ then

$$-\frac{1}{4}\dot{h}_{ij}\dot{h}^{ij} = 3(H+\dot{\zeta})^2. \tag{4.148}$$

For the covariant derivative of N_i, we need the 3D Christoffel symbol.

$$\begin{aligned}\Gamma^k_{ij} &= \frac{1}{2}h^{kl}\left(h_{li,j} + h_{jl,i} - h_{ij,l}\right)\\ &= \frac{1}{2}a^{-2}e^{2\zeta}\delta^{kl}\left(2a^2e^{2\zeta}\delta_{li}\zeta_{,j} + 2a^2e^{2\zeta}\delta_{jl}\zeta_{,i} - 2a^2e^{2\zeta}\delta_{ij}\zeta_{,l}\right)\\ &= \delta^{kl}(\delta_{li}\zeta_{,j} + \delta_{jl}\zeta_{,i} - \delta_{ij}\zeta_{,l})\\ \Gamma^k_{ij} &= \delta^k_i\zeta_{,j} + \delta^k_j\zeta_{,i} - \delta_{ij}\zeta^{,k}. \end{aligned} \tag{4.149}$$

Note in the last term that the index k has been raised following the notation $\zeta^{,k} = \delta^{ik}\zeta_{,i}$. The covariant derivative is then given by

$$\begin{aligned}N_{(i;j)} &= N_{(i,j)} - \Gamma^k_{ij}N_k,\\ N_{(i;j)} &= N_{(i,j)} - \left(\delta^k_i\zeta_{,j} + \delta^k_j\zeta_{,i} - \delta_{ij}\zeta^{,k}\right)N_k. \end{aligned} \tag{4.150}$$

Because N_i is first-order, the second term in the right hand side above is second-order.

With the expression for the covariant derivative in hand, we can now calculate the contraction $\dot{h}^{ij}N_{(i;j)}$ in the expression for $E_{ij}E^{ij}$ above.

$$\begin{aligned}\dot{h}^{ij}N_{(i;j)} &= -2a^{-2}e^{-2\zeta}(H+\dot{\zeta})\delta^{ij}N_{(i,j)}\\ &\quad + 2a^{-2}e^{-2\zeta}(H+\dot{\zeta})\delta^{ij}\left(\delta^k_i\zeta_{,j} + \delta^k_j\zeta_{,i} - \delta_{ij}\zeta^{,k}\right)N_k,\\ &= -2a^{-2}e^{-2\zeta}(H+\dot{\zeta})\delta^{ij}N_{(i,j)} - 2a^{-2}e^{-2\zeta}(H+\dot{\zeta})\zeta^{,i}N_i,\\ \dot{h}^{ij}N_{(i;j)} &= -2a^{-2}e^{-2\zeta}(H+\dot{\zeta})\delta^{ij}N_{(i,j)} - 2a^{-2}e^{-2\zeta}H\zeta^{,i}N_i. \end{aligned} \tag{4.151}$$

The last term in the expression for $E_{ij}E^{ij}$ is $h^{ik}h^{lj}N_{(i;j)}N_{k;l}$. The calculation goes as

$$\begin{aligned}h^{ik}h^{lj}N_{(i;j)} &= a^{-4}e^{-4\zeta}\delta^{ik}\delta^{lj}\left[N_{(i,j)} - \left(\delta^p_i\zeta_{,j} + \delta^p_j\zeta_{,i} - \delta_{ij}\zeta^{,p}\right)N_p\right],\\ h^{ik}h^{lj}N_{(i;j)}N_{(k;l)} &= a^{-4}e^{-4\zeta}\left[N_{(i,j)}\delta^{ik}\delta^{lj} - \left(\delta^{pk}\zeta^{,l} + \delta^{pl}\zeta^{,k} - \delta^{kl}\zeta^{,p}\right)N_p\right]\\ &\qquad \times\left[N_{(k,l)} - \left(\delta^r_k\zeta_{,l} + \delta^r_l\zeta_{,k} - \delta_{kl}\zeta^{,r}\right)N_r\right],\\ h^{ik}h^{lj}N_{(i;j)}N_{(k;l)} &= a^{-4}e^{-4\zeta}\delta^{ik}\delta^{lj}N_{(i,j)}N_{(k,l)}. \end{aligned} \tag{4.152}$$

We next turn our attention to E^2. For the quantity E we find

$$\begin{aligned}
E &= h^{ij}E_{ij},\\
&= a^{-2}e^{-2\zeta}\delta^{ij}\left[a^2e^{2\zeta}(H+\dot{\zeta})\delta_{ij} - N_{(i,j)} + \left(\delta^k_i\zeta_{,j} + \delta^k_j\zeta_{,i} - \delta_{ij}\zeta^{,k}\right)N_k\right],\\
&= 3(H+\dot{\zeta}) - a^{-2}e^{-2\zeta}\delta^{ij}N_{(i,j)} + a^{-2}e^{-2\zeta}\delta^{ij}\left(\delta^k_i\zeta_{,j} + \delta^k_j\zeta_{,i} - \delta_{ij}\zeta^{,k}\right)N_k,\\
E &= 3(H+\dot{\zeta}) - a^{-2}e^{-2\zeta}\delta^{ij}N_{(i,j)} - a^{-2}e^{-2\zeta}\zeta^{,i}N_i. \qquad (4.153)
\end{aligned}$$

For E^2 we have

$$\begin{aligned}
E^2 &= 9(H+\dot{\zeta})^2 - 6a^{-2}e^{-2\zeta}(H+\dot{\zeta})\delta^{ij}N_{(i,j)} - 6a^{-2}e^{-2\zeta}(H+\dot{\zeta})\zeta^{,i}N_i\\
&\quad + a^{-4}e^{-4\zeta}\delta^{ij}\delta^{kl}N_{(i,j)}N_{(k,l)} + 2a^{-4}e^{-4\zeta}\delta^{ij}N_{(i,j)}\zeta^{,k}N_k,\\
E^2 &= 9(H+\dot{\zeta})^2 - 6a^{-2}e^{-2\zeta}(H+\dot{\zeta})\left(\delta^{ij}N_{(i,j)} + \zeta^{,i}N_i\right)\\
&\quad + a^{-4}e^{-4\zeta}\delta^{ij}\delta^{kl}N_{(i,j)}N_{(k,l)}. \qquad (4.154)
\end{aligned}$$

Use (4.148) and the last equations in (4.151) and (4.152) in the equation for $E_{ij}E^{ij}$ given by the last of (4.147) and subtract from the resulting equation the expression for E^2 given above.

$$\begin{aligned}
E_{ij}E^{ij} - E^2 &= -6(H+\dot{\zeta})^2 + 4a^{-2}e^{-2\zeta}(H+\dot{\zeta})\left(\delta^{ij}N_{(i,j)} + \zeta^{,i}N_i\right)\\
&\quad + a^{-4}e^{-4\zeta}\left(\delta^{ik}\delta^{jl} - \delta^{ij}\delta^{kl}\right)N_{(i,j)}N_{(k,l)}. \qquad (4.155)
\end{aligned}$$

We need to multiply it by $\sqrt{h}N^{-1} = \sqrt{h}(1+\alpha)^{-1}$. Because $\alpha = \dot{\zeta}/H$, then

$$\begin{aligned}
\sqrt{h}N^{-1}(E_{ij}E^{ij} - E^2) &= -6a^3e^{3\zeta}H(H+\dot{\zeta}) + 4ae^{\zeta}H\left(\delta^{ij}N_{(i,j)} + \zeta^{,i}N_i\right)\\
&\quad + a^{-1}e^{-\zeta}(1-\alpha)\left(\delta^{ik}\delta^{jl} - \delta^{ij}\delta^{kl}\right)N_{(i,j)}N_{(k,l)},\\
\sqrt{h}N^{-1}(E_{ij}E^{ij} - E^2) &= -6a^3e^{3\zeta}H(H+\dot{\zeta}) + 4ae^{\zeta}H\left(\delta^{ij}N_{(i,j)} + \zeta^{,i}N_i\right)\\
&\quad + a^{-1}e^{-\zeta}\left(\delta^{ik}\delta^{jl} - \delta^{ij}\delta^{kl}\right)N_{(i,j)}N_{(k,l)}. \qquad (4.156)
\end{aligned}$$

Because $N_i = \psi^{(1)}_{,i}$ and the expression that we have is for $\nabla^2\psi^{(1)}$, then we

should perform integration by parts for the term $4ae^{\zeta}H\zeta^{,i}N_i$ in the first line.

$$\sqrt{h}N^{-1}(E_{ij}E^{ij}-E^2)\supset -6a^3e^{3\zeta}H(H+\dot{\zeta})+4ae^{\zeta}H\left(\delta^{ij}N_{(i,j)}-\partial^i N_i\right)$$
$$+a^{-1}e^{-\zeta}N^{-1}\left(\delta^{ik}\delta^{jl}-\delta^{ij}\delta^{kl}\right)N_{(i,j)}N_{(k,l)}. \quad (4.157)$$

Now, $\delta^{ij}N_{(i,j)}-\partial^i N_i=\delta^{ij}\psi^{(1)}_{,ij}-\partial^i\partial_i\psi^{(1)}=0$. We can thus, omit the second term in the right hand side.

$$\sqrt{h}N^{-1}(E_{ij}E^{ij}-E^2)\supset -6a^3e^{3\zeta}H(H+\dot{\zeta})+a^{-1}e^{-\zeta}N^{-1}\left(\delta^{ik}\delta^{jl}-\delta^{ij}\delta^{kl}\right)N_{(i,j)}N_{(k,l)}. \quad (4.158)$$

Since $N_{(i,j)}=\psi^{(1)}_{,ij}$, the second term in the right hand side can be written in terms of ψ as

$$a^{-1}e^{-\zeta}N^{-1}\partial_i\partial_j\psi^{(1)}\partial^i\partial^j\psi^{(1)}-a^{-1}e^{-\zeta}N^{-1}\partial^2\psi^{(1)}\partial^2\psi^{(1)}. \quad (4.159)$$

We perform integration by parts of the first term in the hope of canceling the second term.

$$\begin{aligned}
&e^{-\zeta}N^{-1}\partial_i\partial_j\psi^{(1)}\partial^i\partial^j\psi^{(1)}\\
&\quad\supset -\partial^i\left(e^{-\zeta}N^{-1}\partial_i\partial_j\psi^{(1)}\right)\partial^j\psi^{(1)},\\
&\quad=-\partial^i\left(e^{-\zeta}N^{-1}\right)\left(\partial_i\partial_j\psi^{(1)}\right)\partial_j\psi^{(1)}-e^{-\zeta}N^{-1}\partial^2\partial_j\psi^{(1)}\partial^j\psi^{(1)},\\
&\quad\supset -\partial^i\left(e^{-\zeta}N^{-1}\right)\left(\partial_i\partial_j\psi^{(1)}\right)\partial^j\psi^{(1)}+\partial_j\left(e^{-\zeta}N^{-1}\right)\partial^2\psi^{(1)}\partial^j\psi^{(1)}\\
&\qquad+e^{-\zeta}N^{-1}\partial^2\psi^{(1)}\partial^2\psi^{(1)},\\
&\quad=-\partial^i(e^{-\zeta}N^{-1})\left[(\partial_i\partial_j\psi^{(1)})\partial^j\psi^{(1)}-\partial^2\psi^{(1)}\partial_i\psi^{(1)}\right]+e^{-\zeta}N^{-1}\partial^2\psi^{(1)}\partial^2\psi^{(1)}.
\end{aligned} \quad (4.160)$$

The first term in the right hand side is third order in ζ while the second term exactly cancels the second term in (4.159). It follows that

$$\boxed{\sqrt{h}N^{-1}(E_{ij}E^{ij}-E^2)\supset -6a^3e^{3\zeta}H(H+\dot{\zeta}).} \quad (4.161)$$

It is now time to gather what we have derived and proceed with the substitution to obtain the second order action. We have from (4.139), (4.144), and (4.161)

$$\begin{aligned}
\sqrt{h}N\,{}^{(3)}R &\supset -2a\epsilon(\partial_i\zeta)^2,\\
2\sqrt{h}NP &\supset 2a^3e^{3\zeta}\left[3H^2(1+\alpha)+\alpha^2H^2\frac{\epsilon}{c_s^2}\right],\\
\sqrt{h}N^{-1}(E_{ij}E^{ij}-E^2) &\supset -6a^3e^{3\zeta}H(H+\dot\zeta).
\end{aligned} \tag{4.162}$$

The full expansion of these three expressions up to second order yields,

$$\begin{aligned}
\sqrt{h}N\,{}^{(3)}R &\supset -2a\epsilon(\partial_i\zeta)^2,\\
2\sqrt{h}NP &\supset 6a^3H^2+\left(18a^3H^2\zeta+6a^3H\dot\zeta\right)\\
&\quad+\left(27a^3H^2\zeta^2+18a^3H\zeta\dot\zeta+2a^3\frac{\epsilon}{c_s^2}\dot\zeta^2\right),\\
\sqrt{h}N^{-1}(E_{ij}E^{ij}-E^2) &\supset -6a^3H^2-\left(18a^3H^2\zeta+6a^3H\dot\zeta\right),\\
&\quad-\left(27a^3H^2\zeta^2+18a^3H\zeta\dot\zeta\right).
\end{aligned} \tag{4.163}$$

If we add the three expressions above and plug the sum into the action, we find $S^{(1)}=0$ as expected, and

Second-Order Action

$$S^{(2)}=\int \mathrm{d}t\,\mathrm{d}^3x\,\frac{a^2\epsilon}{c_s^2}\left(a\dot\zeta^2-\frac{c_s^2}{a}\zeta_{,i}\zeta^{,i}\right), \tag{4.164}$$

which is the sought-for second-order action.

We should add at this point that this simple form for the second-order action has been made possible by the intelligent choice of α namely, $\alpha\equiv N^{(1)}=\dot\zeta/H$. Recall in our calculation for α that it could not be derived explicitly, but could only be chosen for our convenience. Had we chose a different expression to $\dot\zeta/H$, we would have been not able to carry out integration by parts that eliminated some terms in the integrand. The choice of $N^{(1)}$ together with the clever use of integration by parts to eliminate some terms, left us with a simple second-order action.

And one more thing : suppose we followed an alternative path where we performed a full expansion of the Lagrangian such that we could pick up the zeroth-order, first-order, second-order, etc., group of terms. Then, we considered the second-order term and applied integration by parts. Would we be able to obtain the same result? To illustrate the point, consider the term $\sqrt{h}N\,{}^{(3)}R$ in the Lagrangian. It is given by

$$\sqrt{h}N\,{}^{(3)}R = -2ae^{\zeta}(1+\alpha)\left[2\nabla^2\zeta + (\partial_i\zeta)^2\right]; \qquad \alpha = \frac{\dot{\zeta}}{H}\,. \tag{4.165}$$

We can certainly expand this up to second order as

$$\sqrt{h}N\,{}^{(3)}R\Big|_{\mathcal{O}(2)} = -2\frac{a}{H}\left[2\zeta\nabla^2\zeta + 2\dot{\zeta}\nabla^2\zeta + H(\partial_i\zeta)^2\right]. \tag{4.166}$$

Can we put this in the form given by (4.139) namely,

$$\sqrt{h}N\,{}^{(3)}R \supset -2a\epsilon(\partial_i\zeta)^2 - 2a\epsilon\zeta(\partial_i\zeta)^2, \tag{4.167}$$

by way of using integration by parts? The answer is no (at least as far as our calculations are concerned). We would have some extra terms that cannot be removed by the other second-order group of terms. The key to establishing (4.139) is the realization that $(ae^{\zeta})^{\cdot} = e^{\zeta}(H+\dot{\zeta})$. Premature expansion and isolating those that are second-order can lead to complicated second-order action.

CHAPTER

5

Primordial Cosmological Perturbations

All that is gold does not glitter,
Not all those who wander are lost;
The old that is strong does not wither,
Deep roots are not reached by the frost

John Ronald Reuel Tolkien
The Fellowship of the Ring, 1954

5.1 Quantization of Perturbations
5.2 Superhorizon Modes
5.3 Two-Point Function
5.4 Tensor Perturbation

Primordial cosmological perturbations are the roots of the web of structures currently constituting the Universe. It is the origin of clusters of galaxies and essentially you and me. Back then, quantum perturbations were stretched beyond the Hubble horizon and enhanced by cosmic inflation before they froze. After the end of inflation, these perturbations went back to the Hubble sphere to seed structure formation. In this chapter, we dive deeper into the details of these perturbations. We derive their equations of motion to study their behavior in the subhorizon and superhorizon limits, and write down the working equations for the power spectra. The latter will be helpful in our calculations in the next chapters.

5.1 Quantization of Perturbations

We recall from the previous chapter that the action can be expanded with respect to the perturbation ζ as $S = S^{(0)} + S^{(1)} + S^{(2)} + S^{(3)} + \cdots$. In this expansion, $S^{(0)}$ corresponds to the background, $S^{(1)}$ vanishes due to the Hamiltonian constraints, $S^{(2)}$ serves as the free part corresponding to free fields, and $S^{(3)}$ contains the interaction terms. Since we are mainly interested (in this work) in the power spectrum corresponding to free fields, we do not pay attention to higher-order interaction terms. The decomposed action up to $S^{(2)}$ suffices for our purposes.

In order to calculate or at least setup the working equation for the power spectrum, one has to first derive the equations of motion and quantize the perturbations. This is what we do in this section. In the following section, we clarify the meaning of the terms *subhorizon* and *superhorizon* we have mentioned in the introduction above. As we shall see later, the power spectrum we are after is not simply for any modes but for frozen (constant) modes called the superhorizon modes. These modes are connected in time to the subhorizon modes. Such a connection is necessary to fully solve the equation of motion governing the perturbations. As such, a good understanding of perturbations requires a good understanding of the superhorizon and subhorizon modes. In the last two sections, we relate the power spectra to the two-point function of the scalar and tensor perturbations. The end results of these two sections are the working equations for the scalar and tensor power spectra.

Equation of Motion

The second-order action is given by (see **Sec. 4.5**)

$$S^{(2)} = \int \mathrm{d}t\, \mathrm{d}^3x\, \frac{a^2\epsilon}{c_s^2}\left(a\dot{\zeta}^2 - \frac{c_s^2}{a}\zeta_{,i}\zeta^{,i}\right). \tag{5.1}$$

This equation can be made more "compact" by introducing a variable

$$z \equiv \sqrt{\frac{2a^2\epsilon}{c_s^2}}, \tag{5.2}$$

and using the conformal time τ in place of the coordinate time t.

$$\mathrm{d}\tau \equiv \frac{\mathrm{d}t}{a}, \qquad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{\mathrm{d}\tau}{\mathrm{d}t}\frac{\mathrm{d}}{\mathrm{d}\tau} = \frac{1}{a}\frac{\mathrm{d}}{\mathrm{d}\tau}. \tag{5.3}$$

Then $\mathrm{d}^4x = \mathrm{d}t\,\mathrm{d}^3\mathbf{x} = a\,\mathrm{d}\tau\,\mathrm{d}^3\mathbf{x}$ and $\dot{\zeta}^2 = a^{-2}\zeta'^2$, where the prime indicates differentiation with respect to τ. It follows that the action can be written as

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}\tau\,\mathrm{d}^3\mathbf{x}\, z^2(\zeta'^2 - c_s^2\zeta_{,i}\zeta^{,i}). \tag{5.4}$$

The outlying variable z in the integrand can be "removed" by pairing it with ζ through the definition $v \equiv z\zeta$. Then,

$$\begin{aligned}
\zeta' &= \frac{v'}{z} - v\frac{z'}{z^2}, \\
z^2\zeta'^2 &= \left(v' - v\frac{z'}{z}\right)^2, \\
z^2\zeta'^2 &= v'^2 - 2vv'\frac{z'}{z} + v^2\left(\frac{z'}{z}\right)^2,
\end{aligned} \tag{5.5}$$

and the action can be rewritten as

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}\tau\,\mathrm{d}^3\mathbf{x}\left[v'^2 - 2vv'\frac{z'}{z} + v^2\left(\frac{z'}{z}\right)^2 - c_s^2 v_{,i}v^{,i}\right]. \tag{5.6}$$

We can perform integration by parts of the second term inside the pair of square brackets to possibly remove the third term and gain a shorter expression.

$$\begin{aligned}
-2vv'\frac{z'}{z} &= -(v^2)'\frac{z'}{z}, \\
&\supset v^2\left(\frac{z'}{z}\right)', \\
-2vv'\frac{z'}{z} &\supset v^2\frac{z''}{z} - v^2\frac{z'^2}{z^2}
\end{aligned} \tag{5.7}$$

Use this result in the expression for $S^{(2)}$.

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}\tau\, \mathrm{d}^3\mathbf{x}\, \left(v'^2 + v^2\frac{z''}{z} - c_s^2 v_{,i}v^{,i}\right). \tag{5.8}$$

The equation of motion for v follows from Euler-Lagrange equation involving the second-order Lagrangian $\mathcal{L}^{(2)}$ which is just (one half of) the integrand above.

$$\frac{\partial\mathcal{L}^{(2)}}{\partial v} - \frac{\partial}{\partial\tau}\left(\frac{\partial\mathcal{L}^{(2)}}{\partial v'}\right) - \frac{\partial}{\partial x^i}\left(\frac{\partial\mathcal{L}^{(2)}}{\partial v_{,i}}\right) = 0, \tag{5.9}$$

$$v\frac{z''}{z} - v'' - \frac{\partial}{\partial x^i}\left(-c_s^2 v^{,i}\right) = 0,$$

$$v'' - c_s^2\partial^i\partial_i v - v\frac{z''}{z} = 0. \tag{5.10}$$

Note that c_s^2 like the Hubble parameter, is only a function of time. This justifies the use of $\partial_i c_s^2 = 0$ in the second line above.

We can get rid of the spatial derivatives in the equation of motion above by Fourier transforming $v(\tau, \mathbf{x})$ to $v_\mathbf{k}(\tau)$ where

$$v_\mathbf{k}(\tau) = \int \mathrm{d}^3\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}}\, v(\tau, \mathbf{x}). \tag{5.11}$$

(This equation establishes our Fourier convention namely, we divide $d^3\mathbf{k}$ by $(2\pi)^3$ when transforming from $v_\mathbf{k}(\tau)$ to $v(\tau, \mathbf{x})$.) Then, noting that $k^i k_i = \mathbf{k}\cdot\mathbf{k} = k^2$, in $\mathbf{k}$-space,

Mukhanov-Sasaki Equation

$$\boxed{v_k'' + \left(k^2 c_s^2 - \frac{z''}{z}\right) v_k = 0.} \tag{5.12}$$

This differential equation commonly known as the **Mukhanov-Sasaki equation**, is our sought-for equation of motion. Being the *central working equation* of this work, we will be using it repetitively in our calculations. Observe that it resembles the form of a parametric oscillator with a corresponding potential

$$U_s \equiv \frac{z''}{z}. \tag{5.13}$$

Furthermore, we have written $v_{\mathbf{k}}$ as simply v_k because as is clear in the equation above, it depends only on the magnitude of $\mathbf{k}$.

Conditions on v_k and Quantization of v

In order to perform quantization we need to first promote $v(\tau, \mathbf{x})$ to an operator $\hat{v}(\tau, \mathbf{x})$. In terms of the mode functions $v_k(\tau)$ and the creation and annihilation operators $a^\dagger_{\mathbf{k}}$ and $a_{\mathbf{k}}$ respectively, it can be expressed as

Mode Expansion

$$\hat{v}(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left[v_k(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}} + v_k^*(\tau) e^{-i\mathbf{k}\cdot\mathbf{x}} a^\dagger_{\mathbf{k}} \right]. \tag{5.14}$$

The mode functions satisfy the Mukhanov-Sasaki equation. The conjugate momentum $\pi(\tau, \mathbf{x})$ corresponding to $v(\tau, \mathbf{x})$ follows from derivative of $\mathcal{L}^{(2)}$ as

$$\pi(\tau, \mathbf{x}) = \frac{\partial \mathcal{L}^{(2)}}{\partial v'} = v'(\tau, \mathbf{x}). \tag{5.15}$$

The mode expansion of the corresponding operator can be written as

$$\hat{\pi}(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left[v_k'(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}} + v_k^{*\prime}(\tau) e^{-i\mathbf{k}\cdot\mathbf{x}} a^\dagger_{\mathbf{k}} \right], \tag{5.16}$$

where $a_{\mathbf{k}}$ and $a^\dagger_{\mathbf{k}}$ are both time-independent.

Similar to that in Minkowski spacetime, we perform quantization by imposing the following canonical commutation relations on the creation and annihilation operators.[1]

Canonical Commutation Relation

$$[a_{\mathbf{k}}, a^\dagger_{\mathbf{l}}] = (2\pi)^3 \delta^3(\mathbf{k} - \mathbf{l}). \tag{5.17}$$

All other commutators involving the annihilation and creation operators vanish.

[1] One can also start here with the commutation relation involving $\hat{v}(\tau, \mathbf{x})$ and $\hat{\pi}(\tau, \mathbf{x})$. This requires however, a slightly longer calculation to reach the commutation relation for the creation and annihilation operators.

Consequently,

$$[\hat{v}(\tau,\mathbf{x}),\hat{\pi}(\tau,\mathbf{y})] = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{l}}{(2\pi)^3}\left\{v_k v_l^{*\prime} e^{i\mathbf{k}\cdot\mathbf{x}-i\mathbf{l}\cdot\mathbf{y}}[a_\mathbf{k},a_\mathbf{l}^\dagger] - v_k^* v_l' e^{-i\mathbf{k}\cdot\mathbf{x}+i\mathbf{l}\cdot\mathbf{y}}[a_\mathbf{l},a_\mathbf{k}^\dagger]\right\}$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{l}}{(2\pi)^3}\Big[v_k v_l^{*\prime} e^{i\mathbf{k}\cdot\mathbf{x}-i\mathbf{l}\cdot\mathbf{y}}(2\pi)^3\delta^3(\mathbf{k}-\mathbf{l}) - v_k^* v_l' e^{-i\mathbf{k}\cdot\mathbf{x}+i\mathbf{l}\cdot\mathbf{y}}(2\pi)^3\delta^3(\mathbf{k}-\mathbf{l})\Big]$$

$$[\hat{v}(\tau,\mathbf{x}),\hat{\pi}(\tau,\mathbf{y})] = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\left[v_k v_k^{*\prime} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} - v_k^* v_k' e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\right]. \tag{5.18}$$

For the second term inside the square brackets, we change the variable of integration from $\mathbf{k}\to-\mathbf{k}$. The mode $v_k\to v_k$ under the the change from $\mathbf{k}\to-\mathbf{k}$ because it only depends on the magnitude of $\mathbf{k}$. Then,

$$[\hat{v}(\tau,\mathbf{x}),\hat{\pi}(\tau,\mathbf{y})] = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\left(v_k v_k^{*\prime} - v_k^* v_k'\right)e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}. \tag{5.19}$$

The difference inside the pair of parentheses is the **Wronskian** of v_k. By virtue of the Mukhanov-Sasaki equation, we see that it is independent of time. We can then choose a constant normalization of the Wronskian such that the equal-time commutation relation between $\hat{v}(\tau,\mathbf{x})$ and $\hat{\pi}(\tau,\mathbf{x})$ is the same as that in quantum field theory in flat spacetime. For a homogeneous isotropic universe smoothly connected to a flat spacetime[2], the commutation relation is obviously that of the flat spacetime at that point in its evolution when it is effectively a flat spacetime. By continuation, either forward or backward in time, such commutation relation is preserved; otherwise, causality can be violated (see a more detailed argument presented in ref. [44]). Assuming that the universe we are considering has this structure, then we can take

Normalization of the Wronskian

$$\langle v_k, v_k^*\rangle \equiv v_k v_k^{*\prime} - v_k^* v_k' = i, \tag{5.20}$$

and the canonical commutation relation can be written as

$$[\hat{v}(\tau,\mathbf{x}),\hat{\pi}(\tau,\mathbf{y})] = i\delta^3(\mathbf{x}-\mathbf{y}). \tag{5.21}$$

[2] For instance, there is a point in its evolution where the variation of the scale factor is slow enough to approximate Minkowski spacetime.

The normalization of the Wronskian fixes one of the two boundary conditions necessary to fully solve the Mukhanov-Sasaki equation given by (5.12). The second boundary condition can be obtained by considering the very early time limit of the Mukhanov-Sasaki equation. Such a limit will become apparent when we express the quantity z''/z in terms of the conformal time. By definition $z^2 = 2a^2\epsilon/c_s^2$ and $\mathrm{d}\tau = \mathrm{d}t/a$. Then

$$\begin{aligned} z' &= a\dot{z}, \\ z'' &= a^2 H \dot{z} + a^2 \ddot{z}, \\ z'' &= a^2 H \frac{\mathrm{d}}{\mathrm{d}t}\sqrt{\frac{2a^2\epsilon}{c_s^2}} + a^2 \frac{\mathrm{d}^2}{\mathrm{d}t^2}\sqrt{\frac{2a^2\epsilon}{c_s^2}}. \end{aligned} \tag{5.22}$$

Using the definition of the Hubble and sound flow functions given by (4.16), we find

$$\frac{z''}{z} = (aH)^2 \left[2 - \epsilon_1 + \tfrac{3}{2}\,\epsilon_2 - \tfrac{1}{2}\,\epsilon_1\epsilon_2 + \tfrac{1}{4}\,\epsilon_2^2 + \tfrac{1}{2}\,\epsilon_2\epsilon_3 + \delta_1\,(3 - \epsilon_1 + \epsilon_2 + \delta_1 + \delta_2)\right]. \tag{5.23}$$

This untruncated solution will become useful in later chapters. Right now, we are mainly interested in the approximation $z''/z \approx 2(aH)^2$.

The factor aH is related to the conformal time as

$$\mathrm{d}\tau \equiv \frac{\mathrm{d}t}{a} = \frac{da}{a^2 H}. \tag{5.24}$$

We take the range of the conformal time as $(-\infty, 0]$ with $\tau = 0$ being the present time. As such,

$$\tau = \int \frac{\mathrm{d}a}{a^2 H} = -\frac{1}{aH} + \mathcal{O}(\epsilon). \tag{5.25}$$

In effect,

$$\frac{z''}{z} = \frac{2}{\tau^2}[1 + \mathcal{O}(\epsilon)], \tag{5.26}$$

and the Mukhanov-Sasaki equation becomes

$$\frac{d^2 v_k}{d\tau^2} + \left\{ k^2 c_s^2 - \frac{2}{\tau^2} \left[1 + \mathcal{O}(\epsilon) \right] \right\} v_k = 0. \tag{5.27}$$

The very early time corresponds to the limit as $\tau \to -\infty$. In this limit, the Mukhanov-Sasaki equation tends to

$$\frac{d^2 v_k}{d\tau^2} + k^2 v_k = 0, \tag{5.28}$$

where we have set $c_s^2 = 1$ for simplicity[3]. Alternatively, one can see that since $\tau \approx -1/aH$, during the very early times, the quantum fluctuations are well within the Hubble sphere with radius $1/(aH)$; i.e., $k/(aH) \gg 1$. Consequently, the governing equation of motion is simply that of a simple harmonic oscillator. The ground state of a simple harmonic oscillator is the vacuum in Minkowski space. We are then justified in choosing the lowest-energy state $|0\rangle$, annihilated by the action of $a_{\mathbf{k}}$ as the **Bunch-Davies vacuum** [45]—the Minkowski vacuum in the far past when all modes sit free and unconscious of gravity[4], well within the Hubble sphere.

The solution of the differential equation (5.27) can be written as

$$v_k = c_1 e^{-ik\tau} + c_2 e^{ik\tau}, \tag{5.29}$$

where c_1 and c_2 are constants. The normalization of the Wronskian gives us

$$\begin{aligned} i &= v_k v_k^{*\prime} - v_k^* v_k', \\ \frac{1}{k} &= (c_1 e^{-ik\tau} + c_2 e^{ik\tau})(c_1^* e^{ik\tau} - c_2^* e^{-ik\tau}) \\ &\quad - (c_1^* e^{ik\tau} + c_2^* e^{-ik\tau})(-c_1 e^{-ik\tau} + c_2 e^{ik\tau}), \\ \frac{1}{k} &= 2|c_1|^2 - 2|c_2|^2. \end{aligned} \tag{5.30}$$

[3] The calculation for $c_s^2 \neq 1$ is more complicated if c_s depends on time. However, the results below remain valid with k replaced by kc_s provided that c_s is slowly-varying at $\tau \to -\infty$ such that $\mathrm{d}^n c_s^2/\mathrm{d}t^n = 0$ for up to $n = 2$. This is what we assume in this work.

[4] More technically, the scale of the perturbations is much smaller than the scale of the gravitational field.

In order to determine the value of the two constants above, we need an additional condition. We recall that in flat spacetime, there is a unique vacuum corresponding to the lowest energy. For the case in hand, we apply the same condition for the energy of each mode characterized by the value of k corresponding to the Bunch-Davies vacuum. Such energy is an eigenvalue of the Hamiltonian that we proceed to calculate as follows. The Hamiltonian density in the (deep) subhorizon limit is given by (see (5.8) for the action $S^{(2)}$)

$$\begin{aligned}\mathcal{H} &= (\pi v' - \mathcal{L})\Big|_{\tau\simeq-\infty},\\ &= \left[\pi v' - \frac{1}{2}\left(v'^2 + v^2\frac{z''}{z} - v_{,i}v^{,i}\right)\right]_{\tau\simeq-\infty}\\ \mathcal{H} &= \frac{1}{2}(\pi^2 + v_{,i}v^{,i})\Big|_{\tau\simeq-\infty}. \end{aligned} \tag{5.31}$$

The Hamiltonian is then simply the integral of this over all space. We promote this to an operator and use the mode expansion for $\hat{v}(\tau,\mathbf{x})$ and $\hat{\pi}(\tau,\mathbf{x})$ given by (5.14) and (5.16) respectively. (Note that all expressions for $\hat{H}$ in the following calculation are evaluated at $\tau\simeq-\infty$.)

$$\begin{aligned}\hat{H} &= \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{l}}{(2\pi)^3}\Big\{\left(v'_k e^{i\mathbf{k}\cdot\mathbf{x}}a_\mathbf{k} + v^{*\prime}_k e^{-i\mathbf{k}\cdot\mathbf{x}}a^\dagger_\mathbf{k}\right)\left(v'_l e^{i\mathbf{l}\cdot\mathbf{x}}a_\mathbf{l} + v^{*\prime}_l e^{-i\mathbf{l}\cdot\mathbf{x}}a^\dagger_\mathbf{l}\right)\\ &\qquad - \mathbf{k}\cdot\mathbf{l}\left(v_k e^{i\mathbf{k}\cdot\mathbf{x}}a_\mathbf{k} - v^*_k e^{-i\mathbf{k}\cdot\mathbf{x}}a^\dagger_\mathbf{k}\right)\left(v_l e^{i\mathbf{l}\cdot\mathbf{x}}a_\mathbf{l} - v^*_l e^{-i\mathbf{l}\cdot\mathbf{x}}a^\dagger_\mathbf{l}\right)\Big\},\\ &= \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{l}}{(2\pi)^3}\Big\{v'_k v'_l e^{i(\mathbf{k}+\mathbf{l})\cdot\mathbf{x}}a_\mathbf{k}a_\mathbf{l} + v^{*\prime}_k v'_l e^{-i(\mathbf{k}-\mathbf{l})\cdot\mathbf{x}}a^\dagger_\mathbf{k}a_\mathbf{l}\\ &\qquad + v'_k v^{*\prime}_l e^{i(\mathbf{k}-\mathbf{l})\cdot\mathbf{x}}a_\mathbf{k}a^\dagger_\mathbf{l} + v^{*\prime}_k v^{*\prime}_l e^{-i(\mathbf{k}+\mathbf{l})\cdot\mathbf{x}}a^\dagger_\mathbf{k}a^\dagger_\mathbf{l} - \mathbf{k}\cdot\mathbf{l}\Big(v_k v_l e^{i(\mathbf{k}+\mathbf{l})\cdot\mathbf{x}}a_\mathbf{k}a_\mathbf{l}\\ &\qquad - v^*_k v_l e^{-i(\mathbf{k}-\mathbf{l})\cdot\mathbf{x}}a^\dagger_\mathbf{k}a_\mathbf{l} - v_k v^*_l e^{i(\mathbf{k}-\mathbf{l})\cdot\mathbf{x}}a_\mathbf{k}a^\dagger_\mathbf{l} + v^*_k v^*_l e^{-i(\mathbf{k}+\mathbf{l})\cdot x}a^\dagger_\mathbf{k}a^\dagger_\mathbf{l}\Big)\Big\},\\ &= \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\Big\{v'_k v'_k a_\mathbf{k}a_{-\mathbf{k}} + v^{*\prime}_k v'_k a^\dagger_\mathbf{k}a_\mathbf{k} + v'_k v^{*\prime}_k a_\mathbf{k}a^\dagger_\mathbf{k} + v^{*\prime}_k v^{*\prime}_k a^\dagger_\mathbf{k}a^\dagger_{-\mathbf{k}},\\ &\qquad + k^2\Big(v_k v_k a_\mathbf{k}a_{-\mathbf{k}} + v^*_k v_k a^\dagger_\mathbf{k}a_\mathbf{k} + v_k v^*_k a_\mathbf{k}a^\dagger_\mathbf{k} + v^*_k v^*_k a^\dagger_\mathbf{k}a^\dagger_{-\mathbf{k}}\Big)\Big\}\\ \hat{H} &= \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\Big\{\left(v^{*\prime}_k v'_k + k^2 v^*_k v_k\right)a^\dagger_\mathbf{k}a_\mathbf{k} + \left(v^{*\prime}_k v'_k + k^2 v^*_k v_k\right)a_\mathbf{k}a^\dagger_\mathbf{k}\end{aligned}$$

$$+ \left(v_k' v_k' + k^2 v_k v_k\right) a_{\mathbf{k}} a_{-\mathbf{k}} + \left(v_k^{*\prime} v_k^{*\prime} + k^2 v_k^* v_k^*\right) a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger \Big\} \tag{5.32}$$

The terms inside the pair of curly braces involving purely annihilation operators and purely creation operators do not contribute to the vacuum expectation value of the Hamiltonian. Using the commutation relations for $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ we find

$$\langle 0|\hat{H}|0\rangle = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left(v_k' v_k^{*\prime} + k^2 v_k v_k^*\right) + \text{const.} \tag{5.33}$$

For a given wavenumber we identify $E_k = v_k' v_k^{*\prime} + k^2 v_k v_k^*$ as the energy per cubic wavenumber. Then using the solution given by (5.29), we see that

$$\begin{aligned} E_k &= \left(c_1 e^{-ik\tau} + c_2 e^{ik\tau}\right)' \left(c_1^* e^{ik\tau} + c_2^* e^{-ik\tau}\right)' \\ &\quad + k^2 \left(c_1 e^{-ik\tau} + c_2 e^{ik\tau}\right) \left(c_1^* e^{ik\tau} + c_2^* e^{-ik\tau}\right), \\ E_k &= 2k^2(|c_1|^2 + |c_2|^2). \end{aligned} \tag{5.34}$$

In combination with the condition from the normalization of the Wronskian given by the last of (5.30), this can be rewritten as

$$E_k = 4k^2|c_2|^2 + k. \tag{5.35}$$

The energy obviously minimizes when $|c_2|^2 = 0$ with $E_k = k$. Consequently, we find

$$|c_1|^2 = \frac{1}{2k}. \tag{5.36}$$

Hence, the solution of the Mukhanov-Sasaki equation obeys the following condition.

$$\lim_{\tau \to -\infty} v_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{2k}}. \tag{5.37}$$

This initial condition as applied to solving the Mukhanov-Sasaki equation for v_k effectively selects the positive-frequency solution in the subhorizon limit. It is also worth noting that with this form of v_k, the Hamiltonian given by the

last of (5.32) is diagonal. In fact, we can also derive the above boxed equation for v_k by taking the Hamiltonian as diagonal as a consequence of the condition that the vacuum is an eigenstate of the Hamiltonian, and using the Wronskian given by (5.30).

During inflation, ϵ and its derivatives are nearly vanishing; the spacetime is nearly de Sitter. The de-Sitter limit of the Mukhanov-Sasaki equation is given by

de Sitter limit of the Mukhanov-Sasaki equation

$$\frac{d^2 v_k}{d\tau^2} + \left(k^2 - \frac{2}{\tau^2}\right) v_k = 0. \tag{5.38}$$

The solution of this differential equation takes the form

$$v_k(\tau) = c_1 e^{-ik\tau}\left(1 - \frac{i}{k\tau}\right) + c_2 e^{ik\tau}\left(1 + \frac{i}{k\tau}\right), \tag{5.39}$$

which is a generalization of the harmonic oscillator solution given by (5.29). Since it obeys the same conditions given by the normalization of the Wronskian (5.20) and the very early-time limit (5.37), the exact solution can be written as

de Sitter Solution

$$v_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{2k}}\left(1 - \frac{i}{k\tau}\right). \tag{5.40}$$

The solution for the case involving finite but non-vanishing slow-roll parameters branches from this equation. It serves as a consistency check for semi-analytical or numerical approaches to solving the Mukhanov-Sasaki equation.

5.2 Superhorizon Modes

In looking at perturbations in relation to inflation, one usually starts with these perturbations sitting inside the Hubble sphere. The Hubble sphere has a (comoving) Hubble radius of $1/(aH)$ as what we mentioned in **Chapter 2**. Inflation then stretches these perturbations very rapidly until they get out of the horizon. More specifically, a given mode is said to exit the horizon when its comoving wavelength becomes greater than (twice) $1/(aH)$. When its wave number becomes very small in comparison to the Hubble radius, i.e., $k/(aH) \ll$

1, the mode is termed as a **superhorizon mode** (see **Fig. 5.1**). As we shall see later in this section, this large-scale perturbation is constant (in time) subject to the condition that the perturbation is adiabatic in nature. When a mode becomes a superhorizon mode and freezes, it becomes classical. (The transition from quantum fluctuations to classical perturbation is quite a philosophically complicated issue because of the involvement of the still ill-defined notion of measurement in quantum physics, so aside from a short explanation below, we will not be delving into this topic much further). Upon re-entering the horizon at the end of inflation, the now classical perturbations seed the structure formation.

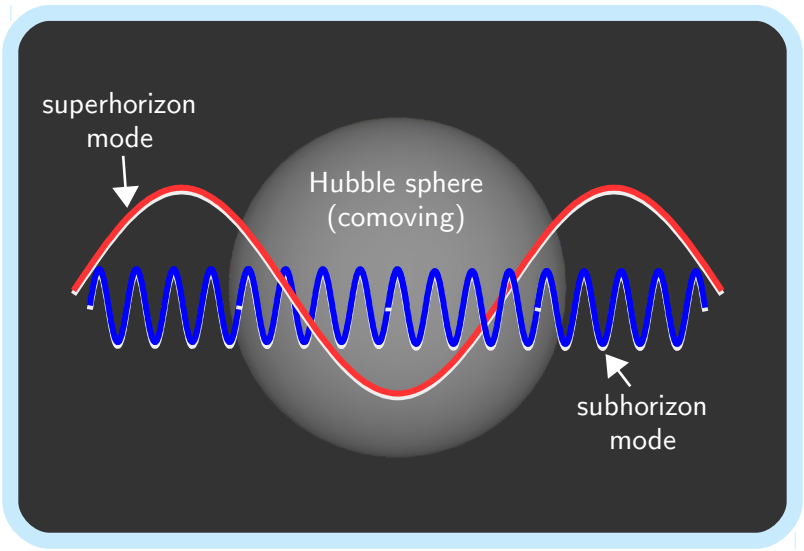


Figure 5.1: Superhorizon and Subhorizon modes. Superhorizon modes have (comoving) wavelengths far exceeding the (comoving) Hubble radius ($k \ll aH$) while subhorizon modes have (comoving) wavelengths much smaller than the (comoving) Hubble radius ($k \gg aH$).

Adiabatic Perturbation

The pressure associated with a given set of particles or fields is related to the energy density of that set of particles or field configuration by the equation

of state. Pressure perturbation is likewise related to the density perturbation. Intuitively, if p and ρ are the pressure and energy density respectively, then

definition of adiabatic perturbation

$$\delta p - \frac{dp}{d\rho}\delta\rho = 0. \tag{5.41}$$

When this relationship holds, the (density) perturbation is said to be **adiabatic**. The quantity $\delta p - (dp/d\rho)\delta\rho$ is of course, not necessarily vanishing. There is another kind of perturbation called the **isocurvature perturbation**; one in which (5.41) does not hold. All cosmological perturbations can be expressed as a sum of isocurvature and adiabatic perturbations.

The definition above can be quite problematic if the quantity $\delta p-(dp/d\rho)\delta\rho$ is not gauge-invariant. In such a case, one can choose a suitable coordinate system to change the nature of perturbation from one form to another! Let us show that it is invariant under the coordinate transformations given by (see **Section 4.2**),

$$\begin{aligned} t &\rightarrow t + \alpha \\ x^i &\rightarrow x^i + \beta^{,i}. \end{aligned} \tag{5.42}$$

We learned from **Section 4.2** that under these transformations, the density perturbation behaves as,

$$\delta\rho(t,\mathbf{x}) \rightarrow \delta\rho(t,\mathbf{x}) - \alpha\dot{\bar{\rho}}(t). \tag{5.43}$$

Following the same calculation as that for this equation, one can easily show that

$$\delta p \rightarrow \delta p - \alpha\dot{\bar{p}}. \tag{5.44}$$

Indeed, the transformation of the energy-momentum tensor tells us that (note : no implied sum over i)

$$\begin{aligned} T^i{}_i &= \frac{\partial x^i}{\partial x'^\mu}\frac{\partial x'^\nu}{\partial x^i}T'^\mu{}_\nu \\ &= \frac{\partial x^i}{\partial x'^0}\frac{\partial x'^0}{\partial x^i}T'^0{}_0 + \frac{\partial x^i}{\partial x'^0}\frac{\partial x'^j}{\partial x^i}T'^0{}_j + \frac{\partial x^i}{\partial x'^j}\frac{\partial x'^0}{\partial x^0}T'^j{}_0 + \frac{\partial x^i}{\partial x'^j}\frac{\partial x'^k}{\partial x^i}T'^j{}_k. \end{aligned} \tag{5.45}$$

The first three terms in the right hand side are all second-order in α and β; e.g., for the first term, the coefficient of $T'^0{}_0$ is $\dot{\beta}^{,i}\alpha_{,i}$. As such, we are left with

$$\begin{aligned} T^i{}_i &= \frac{\partial x^i}{\partial x'^j}\frac{\partial x'^k}{\partial x^i}T'^j{}_k \\ &= (\delta^i{}_j - \beta^{,i}{}_j)(\delta^k{}_i + \beta^{,k}{}_i)T'^{,j}{}_k \\ &= T'^i{}_i \\ &= \bar{p}'(t') + \delta p'(t', \mathbf{x}') \qquad (5.46) \\ p(t) + \delta p(t, \mathbf{x}) &= \bar{p}(t) + \alpha\dot{\bar{p}}(t) + \delta p'(t', \mathbf{x}') \\ \delta p' &= \delta p - \alpha\dot{\bar{p}}, \end{aligned}$$

which was to be shown.

With (5.42), (5.43), and (5.44) in hand, we can now see how the expression $\delta p - (dp/d\rho)\delta\rho$ transforms.

$$\begin{aligned} \delta p - \frac{\dot{\bar{p}}}{\dot{\bar{\rho}}}\delta\rho \;&\rightarrow\; \delta p - \dot{\bar{p}}\alpha - \frac{\dot{\bar{p}} + \alpha\ddot{\bar{p}}}{\dot{\bar{\rho}} + \alpha\ddot{\bar{\rho}}}(\delta\rho - \dot{\bar{\rho}}\alpha) \\ &= \delta p - \dot{\bar{p}}\alpha - \frac{\dot{\bar{p}} + \alpha\ddot{\bar{p}}}{\dot{\bar{\rho}}}(\delta\rho - \dot{\bar{\rho}}\alpha) \\ &= \delta p - \dot{\bar{p}}\alpha - \frac{\dot{\bar{p}}\delta\rho}{\dot{\bar{\rho}}} + \dot{\bar{p}}\alpha \end{aligned}$$

$$\delta p - \frac{\mathrm{d}p}{\mathrm{d}\rho}\delta\rho \;\rightarrow\; \delta p - \frac{\mathrm{d}p}{\mathrm{d}\rho}\delta\rho, \qquad (5.47)$$

This quantity used to define whether the perturbation is adiabatic or not, is **gauge-invariant**.

which was to be shown.

Perturbation Freezes

We wish to find an expression for the time derivative of the mode $\zeta_{\mathbf{k}}(t)$ and show that if the perturbation is adiabatic (cf. (5.41)) and $\zeta_{\mathbf{k}}(t)$ is a superhorizon mode, i.e., $k/(aH) \ll 1$, then the mode is constant. To do this, a suitable gauge has to be chosen for the calculation. We mentioned in **Chapter 4** that $\zeta(t, \mathbf{x})$ is

"gauge-invariant" so any choice of gauge will do good. We can certainly choose the comoving gauge (like what we always do,) where the inflaton fluctuation vanishes ($\delta\phi(x) = 0$) and the spatial metric h_{ij} in the ADM decomposition given by

$$ds^2 = -N^2 \mathrm{d}t^2 + h_{ij}(dx^i + N^i \mathrm{d}t)(\mathrm{d}x^j + N^j \mathrm{d}t), \tag{5.48}$$

can be expressed in terms of $\zeta(t, \mathbf{x})$ namely, $h_{ij} = a^2(t)e^{2\zeta(x)}\delta_{ij}$. Looking at (5.48) above however, tells us this is going to be a tough choice because of the term N^i "mixing" $\mathrm{d}x^i$ and $\mathrm{d}t$. We instead opt to use the much simpler **Newtonian gauge** [1] where the inflaton fluctuation is restored and the metric takes the form

Newtonian gauge

$$\mathrm{d}s^2 = -(1 + \Phi)\mathrm{d}t^2 + a^2(t)(1 - 2\Psi)\delta_{ij}\mathrm{d}x^i\mathrm{d}x^j. \tag{5.49}$$

As we may recall from **Section 4.2**, we have originally four scalars in the metric and two infinitesimally small scalars in the coordinate transformation. We used our freedom to choose these two small scalars to reduce the metric from having four to two scalar perturbations.

Our working equation is the conservation of the energy-momentum tensor.

$$T^{\mu}{}_{\nu;\mu} = T^{\mu}{}_{\nu,\mu} + \Gamma^{\mu}_{\alpha\mu}T^{\alpha}{}_{\nu} - \Gamma^{\alpha}_{\nu\mu}T^{\mu}{}_{\alpha} = 0 \tag{5.50}$$

The right hand side involves the Christoffel symbol $\Gamma^{\alpha}_{\mu\nu}$ containing Ψ that we can exchange with ζ through the definition given in **Section 4.2**:

$$\zeta(t, \mathbf{x}) \equiv -\Psi(t, \mathbf{x}) - \frac{H}{\dot{\bar{\rho}}(t)}\delta\rho(t, \mathbf{x}). \tag{5.51}$$

The Christoffel symbol is given by

$$\Gamma^{\alpha}_{\mu\nu} = \tfrac{1}{2}g^{\alpha\beta}\left(g_{\beta\mu,\nu} + g_{\nu\beta,\mu} - g_{\mu\nu,\beta}\right). \tag{5.52}$$

The components of the Christoffel symbol can be derived (or, use Maxima) from this equation and the equation for the metric in Newtonian gauge given

above.

$$\begin{aligned}
\Gamma^0_{00} &= \frac{\dot\Phi}{1+2\Phi} && : \quad \dot\Phi \\
\Gamma^i_{00} &= \frac{\Phi^{,i}}{a^2(1-2\Psi)} && : \quad \frac{ik^i}{a^2}\Phi \\
\Gamma^0_{0i} &= \frac{\Phi_{,i}}{1+2\Phi} && : \quad ik_i\Phi \\
\Gamma^i_{0j} &= \delta^i_j\frac{H-2H\Psi-\dot\Psi}{1-2\Psi} && : \quad \delta^i_j(H-\dot\Psi) \\
\Gamma^i_{jk} &= a^2(\delta^i_j\Psi_{,k}+\delta^i_k\Psi_{,j}-\delta^{il}\delta_{jk}\Psi_{,l}) && : \quad ia^2\Psi(\delta^i_j k_k+\delta^i_k k_j-\delta_{jk}k^i).
\end{aligned} \tag{5.53}$$

The terms in this second column are in Fourier space. We omitted the usual subscript **k** to not clutter our notation.

The terms following the equality symbol are in **x**-space while the terms after ':' are quantities in **k**-space. We have used the same symbol to not clutter our notation. (This is particularly important when we deal with the components of the energy-momentum tensor; for instance, we do not write the Fourier transform of $\delta T^i{}_j$ as $(\delta T^i{}_j)_{\mathbf{k}}$).

Consider the case where $\nu = 0$. Then,

$$\begin{aligned}
T^\mu{}_{0,\mu} &= T^0{}_{0,0} + T^i{}_{0,i} \\
\Gamma^\mu_{\alpha\mu}T^\alpha{}_0 &= \Gamma^0_{00}T^0{}_0 + \Gamma^i_{0i}T^0{}_0 + \Gamma^0_{j0}T^j{}_0 + \underbrace{\Gamma^i_{ji}T^j{}_0}_{\text{second order}} \\
\Gamma^\alpha_{0\mu}T^\mu{}_\alpha &= \Gamma^0_{00}T^0{}_0 + \Gamma^i_{00}T^0{}_i + \Gamma^0_{0j}T^j{}_0 + \underbrace{\Gamma^i_{0j}T^j{}_0}_{\text{second order}}
\end{aligned} \tag{5.54}$$

Using this in the conservation equation above, we find

$$T^0{}_{0,0} + T^i{}_{0,i} + \Gamma^i_{0i}T^0{}_0 - \Gamma^i_{0j}T^j{}_i = 0. \tag{5.55}$$

We extract from this equation another equation involving first-order quantities. In so doing, we note that $T^0{}_0 = -\bar\rho - \delta\rho$, where $\delta T^0{}_0 = -\delta\rho$, and use (5.53).

$$\begin{aligned}
(\delta T^0{}_0)^{\cdot} + ik_i\delta T^i{}_0 + 3H\delta T^0{}_0 + 3\dot\Psi\bar\rho - H\delta^i{}_j\delta T^j{}_i + 3\dot\Psi\delta^i{}_j T^i{}_j, &= 0 \\
-(\delta\rho)^{\cdot} + ik_i\delta T^i{}_0 - 3H\delta\rho + 3\dot\Psi\bar\rho - H\delta T^i{}_i + 3\dot\Psi p &= 0,
\end{aligned} \tag{5.56}$$

$$-(\delta\rho)^{\cdot} + ik_i\delta T^i{}_0 - 3H\delta\rho - H\delta T^i{}_i = -3(\bar{\rho}+\bar{p})\dot{\Psi}.$$

From the definition of ζ, we have

$$\Psi = \zeta - \frac{H}{\dot{\bar{\rho}}}\delta\rho \tag{5.57}$$

We know however, from **Chapter 1** that (continuity equation)

$$\dot{\bar{\rho}} = -3H(\bar{\rho}+\bar{p}). \tag{5.58}$$

In effect,

$$\begin{aligned}
-(\delta\rho)^{\cdot} + ik_i\delta T^i{}_0 - 3H\delta\rho - H\delta T^i{}_i &= -3(\rho+p)\left[\dot{\zeta} + \frac{(\delta\rho)^{\cdot}}{3(\bar{\rho}+\bar{p})} - \frac{(\delta\rho)(\dot{\bar{\rho}}+\dot{\bar{p}})}{3(\bar{\rho}+\bar{p})^2}\right], \\
ik_i\delta T^i{}_0 - H\delta T^i{}_i &= -3(\bar{\rho}+\bar{p})\dot{\zeta} + \frac{\dot{\bar{p}}\delta\rho}{\bar{\rho}+\bar{p}}, \\
ik_i\delta T^i{}_0 - 3H\delta p &= -3(\bar{\rho}+\bar{p})\dot{\zeta} + \frac{\dot{\bar{p}}\delta\rho}{\bar{\rho}+\bar{p}}.
\end{aligned} \tag{5.59}$$

In the last line, we have used $\delta T^i{}_i = 3\delta p$. The pressure fluctuation is *defined* as one third of the trace of $\delta T^i{}_j$.

We now solve for $\dot{\zeta}$.

$$\begin{aligned}
\dot{\zeta} &= \frac{1}{3(\bar{\rho}+\bar{p})}\left(\frac{\dot{\bar{p}}\delta\rho}{\bar{\rho}+\bar{p}} + 3H\delta p\right) - \frac{ik_i\delta T^i_0}{3(\bar{\rho}+\bar{p})}, \\
&= \frac{1}{3(\rho+p)^2}\left[\dot{\bar{p}}\delta\rho + 3H(\bar{\rho}+\bar{p})\delta p\right] - \frac{ik_i\delta T^i_0}{3(\bar{\rho}+\bar{p})}, \\
&= \frac{1}{3(\bar{\rho}+\bar{p})^2}\left(\dot{\bar{p}}\delta\rho - \dot{\bar{\rho}}\delta p\right) - \frac{ik_i\delta T^i_0}{3(\bar{\rho}+\bar{p})}, \\
\dot{\zeta} &= -\frac{\dot{\bar{\rho}}}{3(\bar{\rho}+\bar{p})^2}\left[\delta p - \frac{\partial p}{\partial\rho}\delta\rho\right] - \frac{ik_i\delta T^i_0}{3(\bar{\rho}+\bar{p})}.
\end{aligned} \tag{5.60}$$

For single-field inflation model described by the action given by

$$S = \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{-g}\,[R + 2P(\phi, X)], \tag{5.61}$$

the energy-momentum tensor is given by (see **Section 4.1**)

$$T^{\mu}{}_{\nu} = (\delta^{\mu}{}_{\nu}P + P_{,X}\,\phi^{,\mu}\,\phi_{,\nu}). \tag{5.62}$$

Note that although we do not cover perturbation in **Chapter 2**, the derivation of (5.62) does not necessitate that ϕ be merely a background field. For the components of $\delta T^{i}{}_{0}$ we have

$$\begin{aligned}
T^{i}{}_{0} &= P_{,X}g^{i\rho}\phi_{,\rho}\phi_{,0},\\
\delta T^{i}{}_{0} &= \underbrace{\delta P_{,X}g^{i\rho}\phi_{,\rho}\phi_{,0}}_{\text{second order}} + \underbrace{P_{,X}\delta g^{i\rho}\phi_{,\rho}\phi_{,0}}_{\text{second order}} + P_{,X}g^{i\rho}\delta\phi_{,\rho}\phi_{,0} + \underbrace{P_{,X}g^{i\rho}\phi_{,\rho}\delta\phi_{,0}}_{\text{second order}},\\
&= P_{,X}g^{i\rho}\delta\phi_{,\rho}\phi_{,0}\\
&= P_{,X}a^{-2}(1+2\Psi)\delta^{ij}(\delta\phi)_{,j}\dot{\bar{\phi}},\\
&= P_{,X}a^{-2}\delta^{ij}(\delta\phi)_{,j}\dot{\bar{\phi}},\\
\delta T^{i}{}_{0} &= P_{,X}a^{-2}ik^{i}(\delta\phi)\dot{\bar{\phi}},
\end{aligned} \tag{5.63}$$

where in the last line, we did the "hidden" Fourier transformation to extract the wave number k^i.

We use this result in the second term in the right hand side of the equation for $\dot{\zeta}$ given by last of (5.60).

$$\begin{aligned}
-\frac{ik_j\delta T^{j}_{0}}{3(\bar{\rho}+\bar{p})} &= -\frac{ik_ja^{-2}ik^{j}(\delta\phi)\,\dot{\bar{\phi}}P_{,X}}{3(\bar{\rho}+\bar{p})},\\
&= \frac{k^2P_{,X}\dot{\bar{\phi}}\,\delta\phi}{3a^2(\bar{\rho}+\bar{p})},\\
&= \frac{k^2}{a^2H^2}\frac{P_{,X}H^2\dot{\bar{\phi}}\,\delta\phi}{3a^2(\bar{\rho}+\bar{p})},\\
&= \frac{k^2}{a^2H^2}\frac{P_{,X}\bar{\rho}\dot{\bar{\phi}}\,\delta\phi}{3a^2(\bar{\rho}+\bar{p})},
\end{aligned}$$

$$-\frac{ik_j\delta T_0^j}{3(\bar{\rho}+\bar{p})} = \frac{k^2}{a^2H^2}\left(\frac{P_{,X}\dot{\bar{\phi}}\,\delta\phi}{1+\bar{p}/\bar{\rho}}\right). \tag{5.64}$$

This allows us to write the derivative of the primordial cosmological perturbation as

$$\dot{\zeta} = -\frac{\dot{\bar{\rho}}}{3(\bar{\rho}+\bar{p})^2}\left(\delta p - \frac{\partial p}{\partial\rho}\delta\rho\right) - \frac{k^2}{a^2H^2}\left(\frac{P_{,X}\dot{\bar{\phi}}\,\delta\phi}{1+\bar{p}/\bar{\rho}}\right). \tag{5.65}$$

Note that this equality pertains to the Fourier transform of $\zeta(\mathbf{x},t)$. For an adiabatic perturbation, the terms inside the first pair of parentheses vanish. Furthermore, if ζ is a superhorizon mode i.e., $k/(aH) \ll 1$, then the second term is also negligible. Hence, a superhorizon mode under the condition of adiabaticity, is constant. When ζ exits the horizon and further stretched by inflation so that its wavelength far exceeds the Hubble radius, it freezes. (For a thorough analysis of adiabatic solution of the field equations for cosmological perturbations and more general proofs of the constancy of ζ in the superhorizon limit, please refer to refs. [46, 47]).

Our argument seems to have a little flaw. One can argue that ζ being a superhorizon mode, is not a necessary condition for $\dot{\zeta}=0$ because the second term in the last equation above may also be negligible if $\dot{\bar{\phi}}$ is small during slow-roll inflation. This is actually misleading since (see **Sec. 4.1**),

$$\frac{\bar{\rho}}{\bar{\rho}+\bar{p}}P_{,X} = \frac{2XP_{,X}-P}{2X} \tag{5.66}$$

Considering that P can be expanded as $P = a_0 + a_1X + a_2X^2 + \cdots b_1\phi + b_2\phi^2 + \cdots +$ cross terms involving (ϕ, X), where $\{a_n, b_n\}$ are constants and $X = \frac{1}{2}\dot{\bar{\phi}}^2$, we see that in general, the term inside the second pair of parentheses in the expression for $\dot{\zeta}$ above is $\sim \delta\phi/\dot{\bar{\phi}}$. (This is easier to see in the canonical case). As such, the quotient inside the second pair of parentheses is not necessarily small. It is thus, the square of the small quantity (k/aH) that suppresses the second term.

Perturbation Becomes Classical

In **Sec. 5.1**, we quantized the perturbation $v(\tau, \mathbf{x}) \equiv z(\tau)\zeta(\tau, \mathbf{x})$. The resulting expression for $\hat{v}_{\mathbf{k}}(\tau)$ in the Heisenberg picture in terms of the annihilation and creation operators is given by

$$\hat{v}_{\mathbf{k}}(\tau) = \left[v_k(\tau) a_{\mathbf{k}} + v_k^*(\tau) a_{-\mathbf{k}}^\dagger \right]. \tag{5.67}$$

Here, the mode function $v_k(\tau)$ takes the form

$$v_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{2k}} \left(1 - \frac{i}{k\tau} \right), \tag{5.68}$$

in the de Sitter limit.

When $\zeta_{\mathbf{k}}$ is a subhorizon mode, $v_k(\tau)$ takes the form $v_k(\tau) \approx e^{-ik\tau}/\sqrt{2k}$. Its complex form tells us that after one measurement of $\hat{\zeta}_{\mathbf{k}}(\tau)$, the next measurement corresponding to $\hat{\zeta}_{\mathbf{k}}(\tau + \Delta\tau)$ will yield a different result unless $\Delta\tau \ll 1/k$. This is so because the state vector corresponding to $\hat{v}_{\mathbf{k}}(\tau)$ and $\hat{v}_{\mathbf{k}}(\tau + \Delta\tau)$ and of $\hat{\zeta}_{\mathbf{k}}(\tau)$ and $\hat{\zeta}_{\mathbf{k}}(\tau + \Delta\tau)$ are in general, different. When $\zeta_{\mathbf{k}}$ becomes a superhorizon mode, we see from the Mukhanov-Sasaki equation,

$$v_k'' - \frac{2}{\tau^2} v_k \approx 0, \tag{5.69}$$

that $v_k(\tau)$ takes the form

$$v_k(\tau) \;\approx\; -\frac{i}{k\tau\sqrt{2k}}, \tag{5.70}$$

because $\tau \approx -1/(aH)$ during inflation and $k/(aH) \ll 1$ for a superhorizon mode.[5] In other words, $v_k(\tau)$ becomes purely imaginary. The operator $\hat{v}_{\mathbf{k}}(\tau)$ then becomes

$$\hat{v}_{\mathbf{k}}(\tau) \approx \frac{-i}{k\tau\sqrt{2k}} (a_{\mathbf{k}} - a_{\mathbf{k}}^\dagger). \tag{5.71}$$

This complex form of the mode function tells us that the eigenvector remains

[5] Equation (5.70) did not come from an invalid comparison of the *real* number 1 and the *purely imaginary* number $-i/k\tau$ in (5.68); rather, we expanded the whole expression including the exponential function and take the limiting case where $|k\tau| \ll 1$.

the same with time. Furthermore, the fact that ζ_k (for $k \ll aH$,) is constant[6] implies that after one measurement of $\hat{\zeta}_{\mathbf{k}}(\tau)$, the next measurement corresponding to $\hat{\zeta}_{\mathbf{k}}(\tau + \Delta\tau)$ will yield the same result. It is in this sense that we say $\zeta_{\mathbf{k}}$ becomes classical when it becomes a superhorizon mode. [48] (So far, we have only considered the free part of the Hamiltonian. For an all-order derivation showing quantum-to-classical transition, refer to ref. [49])

5.3 Two-Point Function

The discussion in this section is based mainly on the lecture notes in ref. [50].

Two-point correlation function in x-space

Consider a homogeneous isotropic space. Associated with this space is a random field $f(\mathbf{x})$. We denote the probability of drawing $f(\mathbf{x})$ as $\mathcal{P}[f(\mathbf{x})]$. The correlation function of $f(\mathbf{x}_1)$ and $f(\mathbf{x}_2)$ is defined as

$$\langle f(\mathbf{x}_1) f(\mathbf{x}_2) \rangle = \int \mathcal{D}f \, \mathcal{P}[f] \, f(\mathbf{x}_1) f(\mathbf{x}_2). \tag{5.72}$$

Now, because space is homogeneous, the quantity $f(\mathbf{x}_1)$ is equally likely to be realized as $f(\mathbf{x}_1 + \mathbf{a})$, where $\mathbf{a}$ is an arbitrary constant vector. Mathematically,

$$\mathcal{P}[f(\mathbf{x}_1 + \mathbf{a})] = \mathcal{P}[f(\mathbf{x}_1)]. \tag{5.73}$$

As such, if we denote $\langle f(\mathbf{x}_1) f(\mathbf{x}_2) \rangle$ as $\mathcal{C}(\mathbf{x}_1, \mathbf{x}_2)$, we see that

$$\mathcal{C}(\mathbf{x}_1 + \mathbf{a}, \mathbf{x}_2 + \mathbf{a}) = \mathcal{C}(\mathbf{x}_1, \mathbf{x}_2). \tag{5.74}$$

The translation invariance of the correlation function stated above implies that it depends only on the difference $(\mathbf{x}_1 - \mathbf{x}_2)$.

$$\mathcal{C}(\mathbf{x}_1, \mathbf{x}_2) = \mathcal{C}(\mathbf{x}_1 - \mathbf{x}_2). \tag{5.75}$$

If the space over which we define $f(\mathbf{x})$ is isotropic, then $f(\mathbf{x})$ is equally likely to be realized as $f(\mathcal{O}\mathbf{x})$, where $\mathcal{O}$ is an orthogonal (real) rotation matrix.

[6] Since $\tau \approx -1/aH$, using the approximation for v_k given by (5.70), we find that the scale factor a is canceled in the quotient $v_k/z = \zeta_k$.

Mathematically,

$$\mathcal{P}[f(\mathcal{O}\mathbf{x})] = \mathcal{P}[f(\mathbf{x})]. \tag{5.76}$$

It follows that

$$\mathcal{C}(\mathcal{O}\mathbf{x}_1, \mathcal{O}\mathbf{x}_2) = \mathcal{C}(\mathbf{x}_1, \mathbf{x}_2). \tag{5.77}$$

But the space we are considering is also homogeneous.

$$\mathcal{C}(\mathcal{O}\mathbf{x}_1, \mathcal{O}\mathbf{x}_2) = \mathcal{C}(\mathcal{O}(\mathbf{x}_1 - \mathbf{x}_2)) = \mathcal{C}(\mathbf{x}_1 - \mathbf{x}_2). \tag{5.78}$$

It tells us that $\mathcal{C}(\mathbf{x}_1, \mathbf{x}_2)$ depends on $(\mathbf{x}_1 - \mathbf{x}_2)$ and that rotating $(\mathbf{x}_1 - \mathbf{x}_2)$ does not change the value of the correlation function. It is thus, independent of the direction of $(\mathbf{x}_1 - \mathbf{x}_2)$. Hence, homogeneity and isotropy of space imply

$$\boxed{\mathcal{C}(\mathbf{x}_1, \mathbf{x}_2) = \mathcal{C}(|\mathbf{x}_1 - \mathbf{x}_2|).} \tag{5.79}$$

Two-point correlation function in k-space

Let us look into the $\mathbf{k}$-space version of the $\mathbf{x}$-space relation given by (5.79). We denote the Fourier transform of $f(\mathbf{x})$ as $f(\mathbf{k})$ which for the most part, we simply write as $f_{\mathbf{k}}$.

$$f_{\mathbf{k}} = \int \mathrm{d}^3\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}). \tag{5.80}$$

Let us then calculate the correlation function of the two modes $f_{\mathbf{k}_1}$ and $f_{\mathbf{k}_2}$.

$$\begin{aligned}
\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2} \rangle &= \left\langle \int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1) \int \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_2\cdot\mathbf{x}_2} f(\mathbf{x}_2) \right\rangle, \\
&= \int \mathrm{d}^3\mathbf{x}_1\, \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1 - i\mathbf{k}_2\cdot\mathbf{x}_2} \langle f(\mathbf{x}_1) f(\mathbf{x}_2) \rangle, \\
&= \int \mathrm{d}^3\mathbf{x}_1\, \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1 - i\mathbf{k}_2\cdot\mathbf{x}_2} \langle f(\mathbf{x}_1 + \mathbf{a}) f(\mathbf{x}_2 + \mathbf{a}) \rangle, \\
\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2} \rangle &= \left\langle \int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1 + \mathbf{a}) \int \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_2\cdot\mathbf{x}_2} f(\mathbf{x}_2 + \mathbf{a}) \right\rangle.
\end{aligned} \tag{5.81}$$

The third line follows from the translation invariance of the correlation function. If we denote $\mathbf{x}_1 + \mathbf{a}$ by $\mathbf{x}_1'$ then

$$\int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1+\mathbf{a}) = e^{i\mathbf{k}_1\cdot\mathbf{a}} \int \mathrm{d}^3\mathbf{x}_1'\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1'} f(\mathbf{x}_1'),$$

$$\int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1+\mathbf{a}) = e^{i\mathbf{k}_1\cdot\mathbf{a}} \int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1). \tag{5.82}$$

It follows that the last of (5.81) can be written as

$$\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle = e^{i\mathbf{k}_1\cdot\mathbf{a}+i\mathbf{k}_2\cdot\mathbf{a}} \left\langle \int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1) \int \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_2} f(\mathbf{x}_2)\right\rangle,$$

$$\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle = e^{i\mathbf{k}_1\cdot\mathbf{a}+i\mathbf{k}_2\cdot\mathbf{a}} \langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle\,. \tag{5.83}$$

The exponential factor tells us that for the equality to hold, the two wave vectors should sum up to zero; i.e., $\mathbf{k}_1 + \mathbf{k}_2 = 0$. As such, we should be able to write the correlation function in $\mathbf{k}$-space as

$$\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle = \delta^3(\mathbf{k}_1+\mathbf{k}_2) F(\mathbf{k}_1). \tag{5.84}$$

The delta function constraint forces the function F to depend on either $\mathbf{k}_1$ only or $\mathbf{k}_2$ only.

Equation (5.84) can be further simplified by using rotational invariance of the correlation function. We follow effectively the same calculation as that of (5.81) in the following derivation.

$$\begin{aligned}
\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle &= \left\langle \int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathbf{x}_1) \int \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_2\cdot\mathbf{x}_2} f(\mathbf{x}_2)\right\rangle, \\
&= \int \mathrm{d}^3\mathbf{x}_1\, \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1 - i\mathbf{k}_2\cdot\mathbf{x}_2} \langle f(\mathbf{x}_1) f(\mathbf{x}_2)\rangle, \\
&= \int \mathrm{d}^3\mathbf{x}_1\, \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1 - i\mathbf{k}_2\cdot\mathbf{x}_2} \langle f(\mathcal{O}\mathbf{x}_1) f(\mathcal{O}\mathbf{x}_2)\rangle, \\
\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle &= \left\langle \int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathcal{O}\mathbf{x}_1) \int \mathrm{d}^3\mathbf{x}_2\, e^{-i\mathbf{k}_2\cdot\mathbf{x}_2} f(\mathcal{O}\mathbf{x}_2)\right\rangle.
\end{aligned} \tag{5.85}$$

If we denote $\mathcal{O}\mathbf{x}_1$ by $\mathbf{x}_1'$, we find

$$\mathbf{k}_1\cdot\mathbf{x}_1 = \mathbf{k}_1\cdot(\mathcal{O}^{-1}\mathbf{x}_1'); \qquad (O^{-1})_{ij} = \mathcal{O}_{ji}$$

$$\mathbf{k}_1 \cdot \mathbf{x}_1 = (\mathcal{O}\mathbf{k}_1) \cdot \mathbf{x}_1'. \tag{5.86}$$

Also, $\mathrm{d}^3\mathbf{x}_1' = \mathrm{d}^3\mathbf{x}_1$ because $\det(\mathcal{O}) = 1$. Then,

$$\int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathcal{O}\mathbf{x}_1) = \int \mathrm{d}^3\mathbf{x}_1'\, e^{-i(\mathcal{O}\mathbf{k}_1)\cdot\mathbf{x}_1'} f(\mathbf{x}_1'),$$

$$\int \mathrm{d}^3\mathbf{x}_1\, e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} f(\mathcal{O}\mathbf{x}_1) = f_{\mathcal{O}\mathbf{k}_1}\,, \tag{5.87}$$

and the last of (5.85) becomes

$$\begin{aligned}\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle &= \langle f_{\mathcal{O}\mathbf{k}_1} f_{\mathcal{O}\mathbf{k}_2}\rangle,\\ &= \delta^3(\mathcal{O}\mathbf{k}_1 + \mathcal{O}\mathbf{k}_2)F(\mathcal{O}\mathbf{k}_1),\\ \langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle &= \delta^3(\mathbf{k}_1 + \mathbf{k}_2)F(\mathcal{O}\mathbf{k}_1).\end{aligned} \tag{5.88}$$

The last line follows because $\det(\mathcal{O}) = 1$. If we compare (5.84) with the last equation above, we see that $F(\mathbf{k}_1) = F(\mathcal{O}\mathbf{k}_1)$. Rotating the vector $\mathbf{k}_1$ does not change the value of $F(\mathbf{k})$. It follows that F depends only on the magnitude of $\mathbf{k}$; i.e., $F = F(k)$.

Usually $F(k)$ is taken as $(2\pi)^3 P(k)$, where $P(k)$ is called the **power spectrum**. We thus write the correlation function of two modes $f_{\mathbf{k}_1}$ and $f_{\mathbf{k}_2}$ as

Definition of Power Spectrum

$$\boxed{\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle = (2\pi)^3 \delta^3(\mathbf{k}_1 + \mathbf{k}_2) P(k_1).} \tag{5.89}$$

Note that the form of the power spectrum given here does not assume any form of the probability distribution function $\mathcal{P}[f]$ except, that it is invariant under both translation and rotation. When $\mathcal{P}[f]$ is Gaussian, with the mean taken as zero ($\langle f_{\mathbf{k}}\rangle = 0$), the two-point correlation function completely specifies all the statistical properties of $f_{\mathbf{k}}$.

The Scalar Power Spectrum

The discussion in the previous two subsections readily extends to the quantum case where $f_{\mathbf{k}}$ in $\mathbf{k}$-space or $f(\mathbf{x})$ in $\mathbf{x}$-space, is replaced by a corresponding quantum field. Given two mode operators $\hat{\zeta}_{\mathbf{k}_1}$ and $\hat{\zeta}_{\mathbf{k}_2}$ in place of $f_{\mathbf{k}_1}$ and $f_{\mathbf{k}_2}$ respectively, in the boxed equation above for $\langle f_{\mathbf{k}_1} f_{\mathbf{k}_2}\rangle$, the homogeneity

and isotropy of space allow us to write the two-point function of these two operators as

$$\langle \hat{\zeta}_{\mathbf{k}_1} \hat{\zeta}_{\mathbf{k}_2} \rangle = (2\pi)^3 \delta^3(\mathbf{k}_1 + \mathbf{k}_2) P(k_1), \tag{5.90}$$

where $P(k_1)$ is the power spectrum.

In our treatment, $\zeta(\tau, \mathbf{x})$ is dimensionless. As such, ζ_k has a dimension of [length]^3. Since $\delta^3(\mathbf{k}_1 + \mathbf{k}_2)$ has a dimension of $1/k^3$ then the power spectrum has a dimension of [length]^3. It is often convenient to have a measure of spread/variation like the power spectrum that is dimensionless. We define the **dimensionless power spectrum** of $\hat{\zeta}_{\mathbf{k}}$ as

Dimensionless Power Spectrum

$$\Delta_s^2(k, \tau) \equiv \frac{k^3}{2\pi^2} P(k, \tau). \tag{5.91}$$

When no confusion may arise, we will simply call the dimensionless power spectrum as power spectrum.

The factor of $1/2\pi^2$ is for convenience. With such a factor in place, the two-point function of $\hat{\zeta}(\tau, \mathbf{x}_1)$ and $\hat{\zeta}(\tau, \mathbf{x}_2)$ can be conveniently written as

$$\langle \hat{\zeta}(\tau, \mathbf{x}_1) \hat{\zeta}(\tau, \mathbf{x}_2) \rangle = \int \frac{\mathrm{d}k}{k} \frac{\sin k|\mathbf{x}_1 - \mathbf{x}_2|}{k|\mathbf{x}_1 - \mathbf{x}_2|} \Delta_s^2(k, \tau), \tag{5.92}$$

without the extra factor involving π in the measure $\mathrm{d}k/k$. Indeed,

$$\begin{aligned}
\langle \hat{\zeta}(\tau, \mathbf{x}_1) \hat{\zeta}(\tau, \mathbf{x}_2) \rangle &= \int \frac{d^3\mathbf{k}_1}{(2\pi)^3} \frac{d^3\mathbf{k}_2}{(2\pi)^3} e^{i\mathbf{k}_1 \cdot \mathbf{x}_1 + i\mathbf{k}_2 \cdot \mathbf{x}_2} \langle \hat{\zeta}_{\mathbf{k}_1} \hat{\zeta}_{\mathbf{k}_2} \rangle, \\
&= \int \frac{d^3\mathbf{k}_1}{(2\pi)^3} \frac{d^3\mathbf{k}_2}{(2\pi)^3} e^{i\mathbf{k}_1 \cdot \mathbf{x}_1 + i\mathbf{k}_2 \cdot \mathbf{x}_2} (2\pi)^3 \delta^3(\mathbf{k}_1 + \mathbf{k}_2) P(k_1), \\
&= \int \frac{d^3\mathbf{k}_1}{(2\pi)^3} e^{i\mathbf{k}_1 \cdot (\mathbf{x}_1 - \mathbf{x}_2)} P(k_1), \\
&= \int \frac{k_1^2 dk_1 \sin\theta d\theta d\phi}{(2\pi)^3} e^{ik_1 |x_1 - x_2| \cos\theta} P(k_1), \\
&= \int \frac{k_1^2 dk_1 \sin\theta d\theta}{(2\pi)^2} e^{ik_1 |x_1 - x_2| \cos\theta} P(k_1),
\end{aligned}$$

$$= \int \frac{k_1^2 dk_1}{2\pi^2} \frac{\sin k_1|x_1 - x_2|}{k_1|x_1 - x_2|} P(k_1),$$

$$\langle \hat{\zeta}(\tau, \mathbf{x}_1)\hat{\zeta}(\tau, \mathbf{x}_2)\rangle = \int \frac{\mathrm{d}k}{k} \frac{\sin k|\mathbf{x}_1 - \mathbf{x}_2|}{k|\mathbf{x}_1 - \mathbf{x}_2|} \Delta_s^2(k, \tau). \tag{5.93}$$

The power spectrum can be expressed in terms of the mode functions $\zeta_k(\tau)$. We have

$$\begin{aligned}
\langle 0|\hat{\zeta}_{\mathbf{k}_1}\hat{\zeta}_{\mathbf{k}_2}|0\rangle &= \langle 0| \left(\zeta_{k_1} a_{\mathbf{k}_1} + \zeta_{k_1}^* a_{-\mathbf{k}_1}^\dagger\right) \left(\zeta_{k_2} a_{\mathbf{k}_2} + \zeta_{k_2}^* a_{-\mathbf{k}_2}^\dagger\right) |0\rangle, \\
&= \zeta_{k_1}\zeta_{k_2}^* \langle 0|a_{\mathbf{k}_1} a_{-\mathbf{k}_2}^\dagger|0\rangle, \\
&= \zeta_{k_1}\zeta_{k_2}^* \langle 0|[a_{\mathbf{k}_1}, a_{-\mathbf{k}_2}^\dagger]|0\rangle, \\
&= \zeta_{k_1}\zeta_{k_2}^* (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2), \\
\langle 0|\hat{\zeta}_{\mathbf{k}_1}\hat{\zeta}_{\mathbf{k}_2}|0\rangle &= |\zeta_{k_1}|^2 (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2).
\end{aligned} \tag{5.94}$$

It follows that

$$\Delta_s^2(k, \tau) = \frac{k^3}{2\pi^2} |\zeta_k(\tau)|^2 = \frac{k^3}{2\pi^2} \left|\frac{v_k(\tau)}{z}\right|^2. \tag{5.95}$$

This is our working equation for the power spectrum of $\hat{\zeta}_{\mathbf{k}}(\tau)$. Note that although the explicit time dependence is written out in the expression above, the power spectrum we are interested in is that of the (frozen) superhorizon modes. For most practical purposes, $\Delta_s^2(k)$ in inflationary cosmology (or at least in this work), is independent of time.

5.4 Tensor Perturbation

Up until now, we have been focusing on the scalar perturbation. The derivations leading to the power spectrum for the tensor perturbation follow the same way. One starts with the decomposition of the action with respect to γ_{ij} as $S = S^{(0)} + S^{(1)} + S^{(2)} + \cdots$. Then from $S^{(2)}$ we obtain the equation of motion. The equation of motion gives us the mode functions in terms of which the power spectrum can be written.

The second-order action for the tensor perturbation is given by [43]

$$S^{(2)} = \frac{1}{8}\int \mathrm{d}t\mathrm{d}^3\mathbf{x}\, a^3 \left[\dot{\gamma}_{ij}(x)\dot{\gamma}^{ij}(x) - \frac{1}{a^2}\gamma_{ij,l}(x)\gamma^{ij,l}(x)\right], \tag{5.96}$$

where the tensor perturbations γ_{ij} can be expanded as

$$\gamma_{ij}(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{s=\times,+} \epsilon^s_{ij}(\mathbf{k})\, h^s_k(t)\, e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{5.97}$$

with $(\epsilon^s)^i{}_i = k^i\epsilon^s_{ij} = 0$ in accord with the transverse-traceless condition for γ_{ij} and $\epsilon^s_{ij}(\mathbf{k})(\epsilon^{s'})^{ij}(\mathbf{k}) = 2\delta^{ss'}$. Unlike that of the scalar perturbation, the integrand in the action for tensor perturbations does not involve the slow-roll parameter ϵ and the speed of sound.

To derive the differential equation for the mode function needed to calculate the power spectrum, we first rewrite the action in terms of the conformal time.

$$S^{(2)} = \frac{1}{8}\int \mathrm{d}\tau\mathrm{d}^3\mathbf{x}\, a^2 \left(\gamma'_{ij}\gamma^{ij\prime} - \gamma_{ij,l}\gamma^{ij,l}\right). \tag{5.98}$$

Then, let $\tilde{\gamma}_{ij} \equiv a\gamma_{ij}$. In effect,

$$\begin{aligned} S^{(2)} &= \frac{1}{8}\int \mathrm{d}\tau\mathrm{d}^3\mathbf{x}\, a^2 \left[\frac{\tilde{\gamma}'_{ij}\tilde{\gamma}^{ij\prime}}{a^2} - \frac{(\tilde{\gamma}_{ij}\tilde{\gamma}^{ij})'}{a^2}\frac{a'}{a} + \frac{\tilde{\gamma}_{ij}\tilde{\gamma}^{ij}}{a^2}\frac{a'^2}{a^2} - \frac{\tilde{\gamma}_{ij,l}\tilde{\gamma}^{ij,l}}{a^2}\right], \\ &= \frac{1}{8}\int \mathrm{d}\tau\mathrm{d}^3\mathbf{x} \left[\tilde{\gamma}'_{ij}\tilde{\gamma}^{ij\prime} - (\tilde{\gamma}_{ij}\tilde{\gamma}^{ij})'\frac{a'}{a} + \tilde{\gamma}_{ij}\tilde{\gamma}^{ij}\frac{a'^2}{a^2} - \tilde{\gamma}_{ij,l}\tilde{\gamma}^{ij,l}\right], \\ S^{(2)} &= \frac{1}{8}\int \mathrm{d}\tau\mathrm{d}^3\mathbf{x} \left[\tilde{\gamma}'_{ij}\tilde{\gamma}^{ij\prime} + \tilde{\gamma}_{ij}\tilde{\gamma}^{ij}\frac{a''}{a} - \tilde{\gamma}_{ij,l}\tilde{\gamma}^{ij,l}\right]. \end{aligned} \tag{5.99}$$

The equation of motion for $\tilde{\gamma}_{ij}$ can be derived using the Euler-Lagrange equation. We have

$$\tilde{\gamma}''_{ij} - \tilde{\gamma}_{ij}\frac{a''}{a} - \partial^l\partial_l\tilde{\gamma}_{ij} = 0. \tag{5.100}$$

Substituting the mode expansion for γ_{ij} given above and denoting h^s_k by u^s_k/a, we find

$$\sum_{s=\pm}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\epsilon^s_{ij}(\mathbf{k})\left(u^{s\prime\prime}_k - u^s_k\frac{a''}{a} + k^2u^s_k\right) = 0,$$

Mukhanov-Sasaki Equation for Tensor Perturbations

$$u_k^{s\prime\prime} + \left(k^2 - \frac{a''}{a}\right) u_k^s = 0, \tag{5.101}$$

which is the Mukhanov-Sasaki equation for the tensor perturbations. This has the same form as that of the scalar perturbation with the correspondence u_k^s is to v_k and a is to z. Furthermore, the potential for scalar perturbation is $U_s = z''/z$ while here, it is $U_t = a''/a$.

The term a''/a can be written in terms of the Hubble radius $1/aH$ and the slow-roll parameter ϵ.

$$u_k^{s\prime\prime} + \left[k^2 - (aH)^2(2-\epsilon)\right] u_k^s = 0, \tag{5.102}$$

For subhorizon modes, $|k/aH| \gg 1$, it approaches the differential equation for a simple harmonic oscillator. For superhorizon modes, $|k/aH| \ll 1$, u_k tends to a. It implies that in the superhorizon limit, u_k/a approaches a constant value. Thus, like that of the scalar perturbation, tensor perturbations freeze at the superhorizon limit.

The tensor perturbation can be quantized[7] by promoting $\gamma_{ij}(x)$ to an operator $\hat{\gamma}_{ij}(x)$, with

$$\hat{\gamma}_{ij}(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{s=\times,+} \left[\epsilon_{ij}^s(\mathbf{k}) h_k^s(t) e^{i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}^s + \epsilon_{ij}^{s*}(\mathbf{k}) h_k^{s*}(t) e^{-i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}^{s\dagger}\right], \tag{5.103}$$

and imposing the canonical commutation relations on the annihilation and creation operators.

$$[a_{\mathbf{k}}^r, a_{\mathbf{l}}^{s\dagger}] = (2\pi)^3 \delta^3(\mathbf{k}-\mathbf{l})\delta^{rs}. \tag{5.104}$$

All other commutators of the creation and annihilation operators vanish.

With the mode expansion above, the (equal-time) two-point function of $\hat{\gamma}_{ij}(x)$ can be calculated as follows.

$\langle \hat{\gamma}_{ij}(\tau, \mathbf{x}_1) \hat{\gamma}^{ij}(\tau, \mathbf{x}_2) \rangle$

[7] Our treatment here is semi-classical in nature; we quantize the tensor perturbations within the framework of classical (curved) background.

$$
\begin{aligned}
&= \int \frac{\mathrm{d}^3\mathbf{k}_1}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{k}_2}{(2\pi)^3} \sum_{r,s=\times,+} \left\langle 0 \middle| \left\{ \epsilon^r_{ij}(\mathbf{k}_1) h^r_{k_1}(\tau) e^{i\mathbf{k}_1\cdot\mathbf{x}_1} a^r_{\mathbf{k}_1} + \epsilon^{r*}_{ij}(\mathbf{k}_1) h^{r*}_{k_1}(\tau) e^{-i\mathbf{k}_1\cdot\mathbf{x}_1} a^{r\dagger}_{\mathbf{k}_1} \right\} \right. \\
&\qquad \left. \times \left\{ (\epsilon^s)^{ij}(\mathbf{k}_2) h^s_{k_2}(\tau) e^{i\mathbf{k}_2\cdot\mathbf{x}_2} a^s_{\mathbf{k}_2} + (\epsilon^{s*})^{ij}(\mathbf{k}_2) h^{s*}_{k_2}(\tau) e^{-i\mathbf{k}_2\cdot\mathbf{x}_2} a^{s\dagger}_{\mathbf{k}_2} \right\} \middle| 0 \right\rangle, \\
&= \int \frac{\mathrm{d}^3\mathbf{k}_1}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{k}_2}{(2\pi)^3} \sum_{r,s=\times,+} \epsilon^r_{ij}(\mathbf{k}_1)(\epsilon^{s*})^{ij}(\mathbf{k}_2) h^r_{k_1}(\tau) h^{s*}_{k_2}(\tau) e^{i(\mathbf{k}_1\cdot\mathbf{x}_1 - \mathbf{k}_2\cdot\mathbf{x}_2)} \langle 0|[a^r_{\mathbf{k}_1}, a^{s\dagger}_{\mathbf{k}_2}]|0\rangle, \\
&= \int \frac{\mathrm{d}^3\mathbf{k}_1}{(2\pi)^3} \sum_{s=\times,+} \epsilon^s_{ij}(\mathbf{k}_1)(\epsilon^{s*})^{ij}(\mathbf{k}_1) h^s_{k_1}(\tau) h^{s*}_{k_1}(\tau) e^{i\mathbf{k}_1\cdot(\mathbf{x}_1-\mathbf{x}_2)}, \\
&= 2\sum_{s=\times,+} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} h^s_k(\tau) h^{s*}_k(\tau) e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}, \\
&= 2\sum_{s=\times,+} \int \frac{k^2 \mathrm{d}k \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi}{(2\pi)^3} \left|\frac{u^s_k}{a}\right|^2 e^{ik|\mathbf{x}_1-\mathbf{x}_2|\cos\theta}, \\
&= 2\sum_{s=\times,+} \int \frac{k^2 \mathrm{d}k \sin\theta\, \mathrm{d}\theta}{(2\pi)^2} \left|\frac{u^s_k}{a}\right|^2 e^{ik|\mathbf{x}_1-\mathbf{x}_2|\cos\theta}, \\
&= 4\sum_{s=\times,+} \int \frac{k^2 \mathrm{d}k}{(2\pi)^2} \frac{\sin k|\mathbf{x}_1-\mathbf{x}_2|}{k|\mathbf{x}_1-\mathbf{x}_2|} \left|\frac{u^s_k}{a}\right|^2, \\
&= \int \frac{\mathrm{d}k}{k} \frac{\sin k|\mathbf{x}_1-\mathbf{x}_2|}{k|\mathbf{x}_1-\mathbf{x}_2|} \left(\frac{k^3}{\pi^2} \sum_{s=\times,+} \left|\frac{u^s_k}{a}\right|^2\right). \qquad (5.105)
\end{aligned}
$$

We identify the term inside the pair of parentheses as the (dimensionless) power spectrum $\Delta^2_t(k,\tau)$. Assuming that the two polarization modes $(\times,+)$ contribute equally to the power spectrum, we may simply denote u^s_k by u_k and write

Tensor Power Spectrum

$$
\Delta^2_t(k,\tau) = \frac{2k^3}{\pi^2}\left|\frac{u_k(\tau)}{a}\right|^2. \qquad (5.106)
$$

Apart from the factor of $2k^3/\pi^2$ instead of $k^3/2\pi^2$ (cf. (5.95)), with u_k and a replaced by v_k and z respectively, this is essentially the same expression for the power spectrum of the scalar perturbation. Furthermore, note that although the time dependence is explicitly written out in the expression above, the power spectrum we are interested in is that of the superhorizon modes. In inflationary

cosmology (or at least in this work), for most practical purposes, the tensor and scalar power spectra are independent of time.

CHAPTER

6

Computation of the Power Spectra through the Uniform Approximation[51]

A well-made salad must have a certain uniformity; it should make perfect sense for those ingredients to share a bowl.

Yotam Ottolenghi

6.1 The Hankel-Function Approximation of the Power Spectrum

6.2 Uniform Approximation

6.3 Power Spectra in the Uniform Approximation

6.4 Second-Order Calculation of the Power Spectra

6.5 Logarithmic Divergences in the Power Spectra

Power spectrum is one of the most important physical quantities in inflationary cosmology. It corresponds to the dispersion of the CMB temperature fluctuation. From a theoretical perspective, it is imperative that we predict and explain the power spectrum based on sound mathematical and physical principles regarding the quantum origin of such fluctuation.

Leaning on the mathematical side, we examine one of the promising methods of calculation called the uniform approximation, used in the literature to calculate the power spectrum. This stems from the insight that such method might lead to unphysical result due to divergence. In relation to this, we wish to characterize the form of the possible divergence and determine if the resulting power spectrum would contain such a mathematical artifact.

6.1 The Hankel-Function Approximation of the Power Spectrum

In order to solve the power spectra of scalar and tensor perturbations, one must solve their corresponding Mukhanov-Sasaki equations. In most cases of practical and theoretical interests, the Mukhanov-Sasaki equation does not have an analytical solution; so we resort to numerical calculation or semi-analytical approximation. The latter can give us a better insight about the behavior of the solution (and the power spectrum) in relation to dependency on the quantities involved in the equation.

In this section, we wish to derive the power spectra of scalar and tensor perturbations using the method that we label as **Hankel-function approximation**. This method as we shall see later, is based on approximating the Mukhanov-Sasaki equation as a Bessel differential equation, the solutions of which can be written as a sum of Hankel functions. As a method in the list of semi-analytical approximation schemes, although the precision of the result with respect to the slow-roll parameters can be quite limited (typically, up to first order), it serves as a good starting point and a basis of comparison in some limiting cases of results based on more advanced methods.

Power Spectrum of the Scalar Perturbation

We proceed with the Mukhanov-Sasaki equation for scalar perturbation ζ_k. It reads (see **Sec. 5.1**)

$$v_k'' + (k^2 - U_s)v_k = 0, \tag{6.1}$$

where $\zeta_k = v_k/z$ and

$$U_s = (aH)^2 \left(2 - \epsilon_1 + \tfrac{3}{2}\,\epsilon_2 + \cdots\right), \tag{6.2}$$

Observe that we have retained only those terms first order in ϵ_1 inside the pair of parentheses indicative of our intention to calculate v_k up to first order in the slow-roll parameters, and have assumed that $c_s^2 = 1$.

In order to solve the Mukhanov-Sasaki equation, it is necessary to relate aH to the conformal time. The relationship can be derived using the differential

definition of τ given as $\mathrm{d}\tau \equiv \mathrm{d}t/a$, and the knowledge of its range; that is, $(-\infty, 0]$ (as what we impose). We can then use integration by parts to compute τ as[1]

$$\begin{aligned}
\tau &= \int \frac{\mathrm{d}a}{a^2 H}, \\
&= -\frac{1}{aH} + \int \frac{\mathrm{d}a}{a^2 H}\epsilon_1, \\
&= -\frac{1}{aH} - \frac{1}{aH}\epsilon_1 + \int \frac{\mathrm{d}a}{a^2 H}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\epsilon_1}{H}, \\
&= -\frac{1}{aH} - \frac{1}{aH}\epsilon_1 + \int \frac{\mathrm{d}a}{a^2 H}(\epsilon_1^2 + \epsilon_1\epsilon_2), \\
\tau &= -\frac{1}{aH} - \frac{1}{aH}\epsilon_1 - \frac{1}{aH}(\epsilon_1^2 + \epsilon_1\epsilon_2) + \int \frac{\mathrm{d}a}{a^2 H}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\epsilon_1^2 + \epsilon_1\epsilon_2}{H}. \qquad (6.3)
\end{aligned}$$

Each round of integration by parts brings a new set of terms one order higher than the previous one with respect to ϵ_1. The recursive process above can be continued arbitrarily to gain terms of the $\mathcal{O}(\epsilon^n)$, where $n = 0, 1, 2, \cdots$.

In fact, after few integrations, one may observe a pattern and establish the relation

Series Expansion of the Conformal Time

$$\tau = -\frac{1}{a}\sum_{n=0}^{\infty}\left(\frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \frac{1}{H}, \qquad (6.4)$$

through simple trial-and-error or more formally, induction; so we do not need to perform integration after all except for the preliminary steps to arrive at the equation above. The formula above effectively converted a relation based on integration to that based on the less cumbersome process of differentiation.

The expansion in the right hand side is a geometric series of operators called a **Neumann series** [52].

$$\tau = -\frac{1}{a}\left[1 + \left(\frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\right) + \left(\frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 + \cdots\right]\frac{1}{H},$$

[1] The expression for τ can be written as $\tau = -(1/aH)(1+\epsilon_1+\cdots)+C$, where C is a constant. At $\tau = -\infty$, the scale factor vanishes while H is finite and non-vanishing (otherwise, the curvature would diverge at infinite H). Hence, the constant of integration vanishes.

$$\tau = -\frac{1}{a}\left(1 - \frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\right)^{-1}\frac{1}{H} \tag{6.5}$$

This can be written as

$$\left(1 - \frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\right)(a\tau) = \frac{1}{H} \quad \Leftrightarrow \quad \mathrm{d}\tau = \frac{\mathrm{d}t}{a}, \tag{6.6}$$

justifying the boxed equation above for τ. We then see that even the integrations in the preliminary steps to establish the series expansion above for τ given by (6.5) may not be necessary at all.

In this section, we will not be needing an extremely precise expression for τ. We content ourselves with the truncated expression for the conformal time,

$$\tau = -\frac{1}{aH}(1 + \epsilon_1) + \cdots, \tag{6.7}$$

and likewise, for the Mukhanov-Sasaki equation,

$$v_k'' + \left[k^2 - \frac{2}{\tau^2}\left(1 + \frac{3}{2}\epsilon_1 + \frac{3}{4}\epsilon_2 + \cdots\right)\right]v_k = 0. \tag{6.8}$$

Our aim in this section is to solve this equation using a semi-analytical method based on the **Hankel-function approximation** commonly employed in the literature [6, 41, 48, 54]. In later sections, we will be needing the higher-order terms in investigating a different method of solving the Mukhanov-Sasaki equation namely, the **uniform approximation**.

Proceeding with the Hankel-function approximation, we aim to rewrite the Mukhanov-Sasaki equation in the form of a Bessel differential equation [53]. Let

$$\nu_s^2 - \tfrac{1}{4} \equiv 2 + 3\epsilon_1 + \tfrac{3}{2}\,\epsilon_2. \tag{6.9}$$

To first order in ϵ_1 we find

$$\nu_s = \tfrac{3}{2} + \epsilon_1 + \tfrac{1}{2}\,\epsilon_2. \tag{6.10}$$

In effect,

$$v_k'' + \left[k^2 - \frac{1}{\tau^2}\left(\nu_s^2 - \frac{1}{4}\right)\right]v_k = 0. \tag{6.11}$$

Let $x = -k\tau$ and $v_k = w_k\sqrt{x}$. Then

$$x^2\frac{\mathrm{d}^2 w_k}{\mathrm{d}x^2} + x\frac{\mathrm{d}w_k}{\mathrm{d}x} + (x^2 - \nu_s^2)w_k = 0, \tag{6.12}$$

which exactly resembles the Bessel differential equation for $w_k(x)$.

The solution of this differential equation can be written as a sum of two Hankel functions (also known as the Bessel functions of the third kind) as

$$w_k(x) = c_1 H_{\nu_s}^{(1)}(x) + c_2 H_{\nu_s}^{(2)}(x) \tag{6.13}$$

where, c_1 and c_2 are constants. This is under the provision that ν_s is a constant which is not the case in general, because ϵ_1 and ϵ_2 depend on time. However, note that the second term in their Taylor series expansion is always second order while the first term is first order; e.g., $\epsilon_1 = \epsilon_{1*} + \dot{\epsilon}_{1*}\Delta t + \cdots$, where '*' is an arbitrary point of evaluation (Below, we shall choose this as the time of horizon crossing). As such, the above solution is valid provided that it is restricted up to first order in the Hubble flow functions.

When $|x| \to \infty$ the Hankel functions behave as [55]

$$\begin{aligned} H_{\nu_s}^{(1)}(x) &\sim \sqrt{\frac{2}{\pi x}}\, e^{i\left(x - \frac{\pi}{2}\nu_s - \frac{\pi}{4}\right)}, \\ H_{\nu_s}^{(2)}(x) &\sim \sqrt{\frac{2}{\pi x}}\, e^{-i\left(x - \frac{\pi}{2}\nu_s - \frac{\pi}{4}\right)}. \end{aligned} \tag{6.14}$$

Because $x = -k\tau \approx k/aH$, such a limit corresponds to the subhorizon limit, $k/aH \gg 1$, given by (5.37),

$$\lim_{\tau\to-\infty} v_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{2k}}. \tag{6.15}$$

Since $v_k = w_k\sqrt{x}$ then

$$v_k(\tau) = \sqrt{x}\Big[c_1 H_{\nu_s}^{(1)}(x) + c_2 H_{\nu_s}^{(2)}(x)\Big]. \tag{6.16}$$

It follows that $c_2 = 0$ and we can write the solution of the Mukhanov-Sasaki equation as

$$v_k(\tau) = \frac{1}{2}\sqrt{\frac{\pi}{k}} e^{i\frac{\pi}{4}(2\nu_s+1)}\sqrt{x}H_{\nu_s}^{(1)}(x). \tag{6.17}$$

In the opposite extreme, $|x| \to 0$, and the Hankel function behaves as

$$H_{\nu}^{(1)}(x) \sim -\frac{i}{\pi}\Gamma(\nu_s)\left(\frac{x}{2}\right)^{-\nu_s}. \tag{6.18}$$

Such a limit corresponds to the superhorizon limit, $k/aH \ll 1$. We find

$$v_k(\tau) = -\frac{i}{\sqrt{\pi k}}\frac{2^{\nu_s}}{2}e^{i\frac{\pi}{4}(2\nu_s+1)}x^{\frac{1}{2}-\nu_s}\Gamma(\nu_s) \tag{6.19}$$

The power spectrum we are after involves the frozen superhorizon modes. Since ζ_k is constant at the superhorizon limit, we can evaluate it at any chosen value of $\tau \approx -1/aH$. It is customary to take $a_*H_* = k$ corresponding to the time of horizon crossing and this is what we follow here.

$$\Delta_s^2(k) = \frac{k^3}{2\pi^2}|\zeta_k|^2\Big|_{k=a_*H_*} = \frac{k^3}{2\pi^2}\left|\frac{v_k}{z}\right|_{k=a_*H_*} \tag{6.20}$$

We have

$$\left|\frac{v_{k*}}{z_*}\right|^2 = \frac{2^{2\nu_*}}{4\pi k}\frac{\Gamma^2(\nu_{s*})}{z_*^2}x_*^{1-2\nu_{s*}}. \tag{6.21}$$

For x_* we have the following calculations.

$$\begin{aligned}
1-2\nu_{s*} &= 1-2\Big(\tfrac{3}{2}+\epsilon_{1*}+\tfrac{1}{2}\epsilon_{2*}\Big),\\
1-2\nu_{s*} &= -2-2\epsilon_{1*}-\epsilon_{2*},\\
x_*^{1-2\nu_{s*}} &= \left[\frac{k}{a_*H_*}(1+\epsilon_{1*})\right]^{-2-2\epsilon_{1*}-\epsilon_{2*}},\\
&= (1-2\epsilon_{1*})(1+\epsilon_{1*})^{-2\epsilon_{1*}-\epsilon_{2*}},\\
x_*^{1-2\nu_{s*}} &= 1-2\epsilon_{1*}
\end{aligned} \tag{6.22}$$

For $\Gamma^2(\nu_{s*})$ we have

$$\begin{aligned}
\Gamma(\nu_{s*}) &= \Gamma(\tfrac{3}{2}+\epsilon_{1*}+\tfrac{1}{2}\epsilon_{2*}),\\
&= \Gamma(\tfrac{3}{2})+(\epsilon_{1*}+\tfrac{1}{2}\epsilon_{2*})\Gamma'(\tfrac{3}{2}),
\end{aligned}$$

$$\Gamma(\nu_{s*}) = \Gamma\left(\tfrac{3}{2}\right) + (\epsilon_{1*} + \tfrac{1}{2}\epsilon_{2*})\Gamma\left(\tfrac{3}{2}\right)(2 - \gamma - 2\ln 2),$$
$$\Gamma^2(\nu_{s*}) = \frac{\pi}{4}\Big[1 + (\epsilon_{1*} + \tfrac{1}{2}\epsilon_{2*})(2 - \gamma - \ln 2)\Big]^2,$$
$$\Gamma^2(\nu_{s*}) = \frac{\pi}{4}\Big[1 + (2\epsilon_{1*} + \epsilon_{2*})(2 - \gamma - 2\ln 2)\Big], \tag{6.23}$$

where $\gamma = 0.5772\ldots$, is the **Euler-Mascheroni constant**.

For $2^{2\nu_{s*}}$ we have

$$2^{2\nu_{s*}} = 2^{2\left(\frac{3}{2} + \epsilon_{1*} + \frac{1}{2}\epsilon_{2*}\right)},$$
$$= 8 \cdot 2^{2\epsilon_{1*} + \epsilon_{2*}},$$
$$2^{2\nu_{s*}} = 8\big[1 + (2\epsilon_{1*} + \epsilon_{2*})\ln 2\big] \tag{6.24}$$

The product of the three sub-results above can be simplified as

$$2^{2\nu_{s*}}\Gamma^2(\nu_{s*})x_*^{1-2\nu_*}$$
$$= 2\pi\big[1 + (2\epsilon_{1*} + \epsilon_{2*})\ln 2\big]\big[1 + (2\epsilon_{1*} + \epsilon_{2*})(2 - \gamma - 2\ln 2)\big](1 - 2\epsilon_{1*}),$$
$$= 2\pi\big[1 - 2\epsilon_{1*} + (2\epsilon_{1*} + \epsilon_{2*})(2 - \gamma - \ln 2)\big]. \tag{6.25}$$

Consequently,

$$\frac{k^3}{2\pi^2}\left|\frac{v_{k*}}{z_*}\right|^2 = \frac{k^2}{4\pi^2}\frac{1 - 2\epsilon_{1*} + (2\epsilon_{1*} + \epsilon_{2*})(2 - \gamma - \ln 2)}{z_*^2},$$

$$\boxed{\Delta_s^2(k) = \frac{H_*^2}{8\pi^2\epsilon_{1*}}(1 + \mu_{s*}),} \quad \begin{matrix}\text{Scalar}\\ \text{Power Spectrum}\end{matrix} \tag{6.26}$$

which our sought-for power spectrum. Here, $\mu_{s*} \equiv (2\epsilon_{1*} + \epsilon_{2*})(2 - \gamma - \ln 2) - 2\epsilon_{1*}$.

As what we have stated in the beginning of this section, the derivation leading to the expression for the power spectrum above assumes $c_s^2 = 1$. Had it not been the case, we would have written the Mukhanov-Sasaki equation as

$$v_k'' + \left[k^2 c_s^2 - \frac{1}{\tau^2}\left(\nu_s^2 - \frac{1}{4}\right)\right] v_k = 0, \tag{6.27}$$

where $\nu_s^2 - \frac{1}{4} = 2 + 3\epsilon_1 + \frac{3}{2}\epsilon_2 + 3\delta_1$. If we let $x = -kc_s\tau$ and $v_k = w_k\sqrt{x}$ then the differential equation above transforms to

$$x^2x'^2\frac{\mathrm{d}^2w_k}{\mathrm{d}x^2} + (x^2x'' + xx'^2)\frac{\mathrm{d}w_k}{\mathrm{d}x} + \left[x^2\left(\frac{1}{4\tau^2} - \frac{\nu_s^2}{\tau^2} + k^2c_s^2\right) - \frac{x'^2}{4} + \frac{xx''}{2}\right]w_k = 0.$$

This does *not* reduce exactly to the familiar Bessel differential equation.

Indeed, to first order in (ϵ_1, δ_1) we have

$$\begin{aligned} x' &= -k\dot{c}_s a\tau - kc_s, \\ &= kc_s(\tau aH)\delta_1 - kc_s, \\ x' &= -kc_s(1+\delta_1) + \cdots, \\ x'' &= -\frac{kc_s}{\tau}\delta_1 + \cdots. \end{aligned} \tag{6.28}$$

In effect,

$$\begin{aligned} x'^2 &= k^2c_s^2(1+2\delta_1), \\ x^2x'' + xx'^2 &= -x^2\frac{kc_s}{\tau}\delta_1 + xk^2c_s^2(1+2\delta_1), \\ x^2x'' + xx'^2 &= xk^2c_s^2(1+3\delta_1), \\ -\frac{x'^2}{4} + \frac{xx''}{2} &= -\frac{k^2c_s^2(1+2\delta_1)}{4} - \frac{xkc_s}{2\tau}\delta_1, \\ -\frac{x'^2}{4} + \frac{xx''}{2} &= -\frac{k^2c_s^2}{4}, \end{aligned} \tag{6.29}$$

and we can rewrite the last differential equation above as

$$x^2(1+2\delta_1)\frac{\mathrm{d}^2w_k}{\mathrm{d}x^2} + x(1+3\delta_1)\frac{\mathrm{d}w_k}{\mathrm{d}x} + (x^2 - \nu_s^2)w_k = 0. \tag{6.30}$$

It is tempting to solve the above equation through a perturbative method by letting $w_k = w_k^{(0)} + \delta_1 w_k^{(0)} + \cdots$. However, since ν_s involves both the Hubble and sound flow functions, it is not straightforward to decompose the differential equation into a sum of zeroth-order and first-order parts with respect to (ϵ_1, δ_1) while at the same time avoiding terms in the solution containing rational expressions involving (ϵ_1, δ_1). As such, when $\delta_1 \neq 0$, meaning that c_s depends

on time, the Hankel-function approximation does not seem to be a practical approach to solving the Mukhanov-Sasaki equation.

Power Spectrum of the Tensor Perturbations

The calculation of the power spectrum of the tensor perturbations follow essentially the same path. We start with the Mukhanov-Sasaki equation for the amplitude h_k, given by (5.102).

$$u_k^{s\prime\prime} + \left[k^2 - (aH)^2(2-\epsilon_1)\right] u_k^s = 0. \tag{6.31}$$

Then, since $\tau = -(aH)^{-1}(1+\epsilon_1+\cdots)$,

$$\begin{aligned} u_k^{s\prime\prime} + \left[k^2 - \frac{1}{\tau^2}(2+3\epsilon_1)\right] u_k^s &= 0, \\ u_k^{s\prime\prime} + \left[k^2 - \frac{1}{\tau^2}\left(\nu_t^2 - \frac{1}{4}\right)\right] u_k^s &= 0, \qquad \left(\nu_t = \tfrac{3}{2} + \epsilon_1\right) \end{aligned} \tag{6.32}$$

which is the same differential equation as that of the scalar perturbation that we have just solved. Accordingly, applying the condition

$$\lim_{\tau\to-\infty} u_k^s(\tau) = \frac{e^{-ik\tau}}{\sqrt{k}}, \tag{6.33}$$

we are led to the first of (6.26) with v_k replaced by u_k and z_* by a_*, and appropriate factors taken into account. We have

$$\frac{2k^3}{\pi^2}\left|\frac{u_{k*}}{a_*}\right|^2 = \frac{2k^2}{\pi^2}\frac{1-2\epsilon_{1*}+2\epsilon_{1*}(2-\gamma-\ln 2)}{a_*^2},$$

$$\boxed{\Delta_t^2(k) = \frac{2H_*^2}{\pi^2}(1+\mu_{t*}),} \qquad \text{Tensor Power Spectrum} \tag{6.34}$$

where $\mu_{t*} \equiv 2\epsilon_{1*}(1-\gamma-\ln 2)$. This is our sought-for expression for the tensor power spectrum to first order in the slow-roll parameter. Observe that unlike that of the scalar power spectrum, ϵ_* is absent in the denominator. The scalar power spectrum is thus, larger than the tensor power spectrum by a factor of

r called the **tensor-to-scalar ratio** given as

$$r \equiv \frac{\Delta_{t*}^2(k)}{\Delta_{s*}^2(k)} = 16\epsilon_{1*}. \tag{6.35}$$

6.2 Uniform Approximation

The discussion in the previous section highlights two of the limitations of the Hankel-function approach. First, the Hankel-function solution of the Mukhanov-Sasaki equation transformed to Bessel differential equation is only valid for constant $\nu^2 = \frac{9}{4} + 3\epsilon_1 + \frac{3}{2}\epsilon_2$. This limits the validity of the method up to first order in ϵ_1. Second, when the speed of sound is not constant, the Mukhanov-Sasaki equation cannot be exactly transformed to a Bessel differential equation. Furthermore, it is not straightforward to solve the resulting perturbed Bessel differential equation using the standard perturbative approach.

These limitations call for other semi-analytical approaches that may circumvent them. Several methods found in the literature include the **Wentzel-Kramers-Brillouin (WKB) method** [56, 57, 58], **Green's function method** [59, 60, 61], and **uniform approximation** [40, 51, 62, 63, 64, 65, 66, 67], among others. In this work, we focus on the uniform approximation as it applies to solving the power spectrum. We lay down its mathematical foundation and derive the working equation to solve the Mukhanov-Sasaki equation.

To shed light on the uniform approximation, following the discussion of Olver [63], we start with the intuitive idea of transforming a differential to another differential equation that may allow us to better approximate the solution. Consider a differential equation given by

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - f(x)y = 0. \tag{6.36}$$

Any second order differential equation may be written in this way through a suitable choice of new variables. Provided that $f(x)$ is sufficiently slowly-varying within the interval of interest on which we wish to find the solution, we may write

$$y(x) \approx c_1 e^{x\sqrt{f}} + c_2 e^{-x\sqrt{f}}, \tag{6.37}$$

where c_1 and c_2 are constants. Needless to say, the "approximation" becomes exact when $f(x) = \text{constant}$.

Now, let us introduce a new set of variables (Y, ξ).

$$y(x) = \left(\frac{\mathrm{d}x}{\mathrm{d}\xi}\right)^{\frac{1}{2}} Y(\xi) = x_\xi^{\frac{1}{2}} Y, \tag{6.38}$$

Here, the subscript ξ represents derivative with respect to ξ. It follows that

$$\begin{aligned}
\frac{\mathrm{d}y}{\mathrm{d}x} &= \frac{1}{x_\xi}\frac{\mathrm{d}}{\mathrm{d}\xi}\left(Y x_\xi^{\frac{1}{2}}\right), \\
&= \frac{\mathrm{d}Y}{\mathrm{d}\xi} x_\xi^{-\frac{1}{2}} + \frac{1}{2} Y x_\xi^{-\frac{3}{2}} x_{\xi\xi}, \\
\frac{\mathrm{d}y}{\mathrm{d}x} &= \frac{\mathrm{d}Y}{\mathrm{d}\xi} x_\xi^{-\frac{1}{2}} - Y\frac{\mathrm{d}}{\mathrm{d}\xi} x_\xi^{-\frac{1}{2}}, \\
\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} &= \frac{\mathrm{d}^2 Y}{\mathrm{d}\xi^2} x_\xi^{-\frac{3}{2}} - x_\xi^{-1} Y \frac{\mathrm{d}^2}{\mathrm{d}\xi^2} x_\xi^{-\frac{1}{2}},
\end{aligned} \tag{6.39}$$

and the original differential equation can be rewritten as

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}\xi^2} = \left(x_\xi^2 f + x_\xi^{\frac{1}{2}} \frac{\mathrm{d}^2}{\mathrm{d}\xi^2} x_\xi^{-\frac{1}{2}}\right) Y. \tag{6.40}$$

If we impose the condition $x_\xi^2 f(x) = 1$ then

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}\xi^2} = \left(1 - f^{-\frac{3}{4}} \frac{\mathrm{d}^2}{\mathrm{d}x^2} f^{-\frac{1}{4}}\right) Y. \tag{6.41}$$

The solution can then be approximated as

$$Y \approx c_1 e^{\xi} + c_2 e^{-\xi}. \tag{6.42}$$

Going back to the original variable y we find the so-called **Liouville-Green approximation** of the solution:

$$y(x) = f^{-\frac{1}{4}}\left(c_1 e^{\int \mathrm{d}x\sqrt{f}} + c_2 e^{-\int \mathrm{d}x\sqrt{f}}\right). \tag{6.43}$$



Example 1. Liouville-Green Approximation. Consider a differential equation given by

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} = (4x^2 - 2)y. \tag{6.44}$$

The function $y(x)$ satisfies the condition that as $x \to \infty$, $y \to 0$ and $y(1) = 1$. Find y using the Liouville-Green approximation and compare it with the exact solution and the exponential approximation given by (6.37).

Solution. We identify $f = 4x^2 - 2$. It follows that

$$\int \mathrm{d}x\sqrt{f} = \frac{x\sqrt{4x^2-2}}{2} - \frac{1}{2}\ln(2\sqrt{4x^2-2} + 4x), \tag{6.45}$$

and

$$e^{\int \mathrm{d}x\sqrt{f}} = \frac{1}{\sqrt{2}}\, e^{\frac{1}{2}(x\sqrt{4x^2-2})}\Big(\sqrt{4x^2-2} + 2x\Big)^{-\frac{1}{2}}, \tag{6.46}$$

and we can write the LG approximation as

$$y(x) = \frac{c_1}{\sqrt{2}f^{\frac{1}{4}}} e^{\frac{1}{2}x\sqrt{4x^2-2}}\Big(\sqrt{4x^2-2} + 2x\Big)^{-\frac{1}{2}} + \frac{\sqrt{2}c_2}{f^{\frac{1}{4}}} e^{-\frac{1}{2}x\sqrt{4x^2-2}}\Big(\sqrt{4x^2-2} + 2x\Big)^{\frac{1}{2}}$$

For very large x, the first term in the right hand side diverges, so we take $c_1 = 0$. The constant c_2 is easily obtained as follows.

$$y(x) = \sqrt{2}c_2 e^{-\frac{1}{2}x\sqrt{4x^2-2}}\Big(\sqrt{4x^2-2} + 2x\Big)^{\frac{1}{2}}\Big(4x^2-2\Big)^{-\frac{1}{4}},$$

$$y(1) = \sqrt{2}c_2 e^{-\frac{1}{2}\sqrt{2}}\Big(\sqrt{2}+2\Big)^{\frac{1}{2}} 2^{-\frac{1}{4}},$$

$$\sqrt{2}c_2 = \frac{2^{\frac{1}{4}} e^{\frac{1}{\sqrt{2}}}}{(\sqrt{2}+2)^{\frac{1}{2}}} \approx 1.30528\ldots .$$

We may then write the solution in the LG approximation as

$$y(x) \approx 1.30528 e^{-\frac{1}{2}x\sqrt{4x^2-2}} \frac{\Big(\sqrt{4x^2-2} + 2x\Big)^{\frac{1}{2}}}{\Big(4x^2-2\Big)^{\frac{1}{4}}}. \tag{6.47}$$

For very large x, it tends to e^{-x^2}, which is the form of the exact solution; in particular, $y = e^{1-x^2}$.

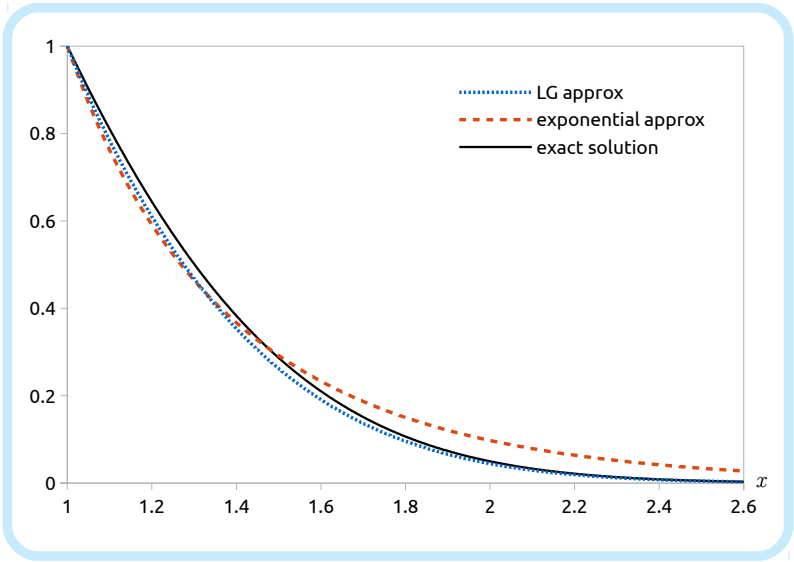


Figure 6.1: LG Approximation. Comparison of the LG approximation with the exact solution and the exponential approximation.

The exponential approximation given by (6.37) can be written as $y(x) \approx c_1 e^{\sqrt{4x^2-1}} + c_2 e^{-\sqrt{4x^2-1}}$. Using the boundary conditions, we find

$$y(x) \approx e^{\sqrt{2}-\sqrt{4x^2-2}}. \tag{6.48}$$

For very large x, it tends to $\sim e^{-2x}$ in contrast to that of the LG approximation. We thus expect it to deviate from the exact solution and that of the LG approximation for sufficiently large x. In fact, as can be seen in **Fig. 6.1**, even for small values of x, the latter gives a better approximation except at the small region about $x \approx 1.5$.

The differential equation above involves $f(x) = 4x^2 - 2$ that is simple enough for the approximating solution to closely follow the exact solution. In particular,

this simple form of f leads to a solution with a uniform behavior; that is, exponentially decaying for $|x| \to \infty$. There are differential equations in physics where the solution exhibits a different behavior depending on the range of values of the independent variable being considered. Consider for instance, a one-dimensional tunneling problem in quantum mechanics where the particle of interest has an energy less than the rectangular barrier height. Outside of the barrier, the particle wavefunction is sinusoidal while inside the barrier, it is exponentially decaying. In this case, the usual approach is to segment the x-axis into several regions and perform solution matching at the boundaries of the regions to gain the complete solution.

The solution of the Mukhanov-Sasaki equation exhibits a similar behavior depending on the value of the conformal time $\tau \approx -1/aH$. For superhorizon modes, $k \ll aH$, $v_k \sim z$ corresponding to constant ζ_k, while for subhorizon modes, $k \gg aH$, v_k is sinusoidal. In principle, one can do a sort of solution matching similar to that of the tunneling problem we have mentioned above. Alternatively, we may rewrite the Mukhanov-Sasaki equation following a procedure similar to that of the LG approximation, to gain an approximating differential equation whose *single* analytic solution can capture the characteristics of the exact solution at both regions of τ corresponding to the subhorizon and superhorizon modes. Such a single analytic solution that converges in all directions or regions is said to *uniformly approximate* the exact solution. The method of deriving the solution is called the **uniform approximation**.

6.3 Power Spectra in the Uniform Approximation[2]

Scalar Power Spectrum in the Uniform Approximation

The point at which the solution of a differential equation changes its behavior (say, from oscillatory to exponentially decaying) is called the **turning point**. We are fortunate enough that the Mukhanov-Sasaki equation has only one turning point. This may allow us to easily pick a function that may correctly "mimic" the behavior of the exact solution. To find such a function, we recall from (6.11)

[2] We follow here the logic behind uniform approximation as applied to inflation in refs. [40, 65, 64]. The basic mathematical foundation of this method is discussed in ref. [63].

that we can write the Mukhanov-Sasaki equation as

$$v_k'' + \left[\left(k^2c_s^2 - \frac{\nu_s^2}{\tau^2}\right) + \frac{1}{4\tau^2}\right]v_k = 0,$$

$$v_k'' - \Big[f(\tau) + g(\tau)\Big]v_k = 0, \tag{6.49}$$

where

$$f(\tau) = -k^2c_s^2 + \frac{\nu_s^2}{\tau^2}, \qquad g(\tau) = -\frac{1}{4\tau^2}, \qquad \text{and} \qquad \nu_s^2 \equiv \frac{1}{4} + \tau^2 U_s(\tau). \tag{6.50}$$

We could have just let the sum $f + g$ be simply f, as in the LG approximation above. But there is often a merit with this decomposition; it can result to a better approximation of the solution.

We introduce new variables ξ and V through the assignments [63, 64, 65]

$$\xi\xi'^2 = f(\tau) \quad \text{and} \quad v_k = \frac{V}{\sqrt{\xi'}}. \tag{6.51}$$

(Note that we have chosen to write V without the subscript k for brevity.) The differential equation in terms of V and ξ can then be calculated as follows.

$$\begin{aligned}
v_k &= V\left(\frac{f}{\xi}\right)^{-\frac{1}{4}} = V\tilde{f}^{-\frac{1}{4}}; \quad \tilde{f} \equiv \frac{f}{\xi},\\
v_k' &= V_\xi \tilde{f}^{\frac{1}{4}} + V(\tilde{f}^{-\frac{1}{4}})',\\
v_k'' &= V_{\xi\xi}\tilde{f}^{\frac{3}{4}} + \frac{1}{4}V_\xi \tilde{f}^{-\frac{3}{4}}\tilde{f}' + V_\xi \tilde{f}^{\frac{1}{2}}(\tilde{f}^{-\frac{1}{4}})' + V(\tilde{f}^{-\frac{1}{4}})'',\\
v_k'' &= V_{\xi\xi}\tilde{f}^{\frac{3}{4}} + V(\tilde{f}^{-\frac{1}{4}})''.
\end{aligned} \tag{6.52}$$

Adding $-(f + g)v_k$ we find

$$V_{\xi\xi}\tilde{f}^{\frac{3}{4}} + V(\tilde{f}^{-\frac{1}{4}})'' - Vf\tilde{f}^{-\frac{1}{4}} - Vg\tilde{f}^{-\frac{1}{4}} = 0,$$

$$V_{\xi\xi} - \left[\xi - \tilde{f}^{-\frac{3}{4}}(\tilde{f}^{-\frac{1}{4}})'' + \frac{g}{\tilde{f}}\right]V = 0,$$

$$\boxed{V_{\xi\xi} - [\xi + \psi(\xi)]V = 0,} \tag{6.53}$$

where

$$\psi(\xi) = -\tilde{f}^{-\frac{3}{4}}(\tilde{f}^{-\frac{1}{4}})'' + \frac{g}{\tilde{f}},$$

$$\psi(\xi) = \frac{\xi}{16f^3}(4ff'' - 5f'^2) + \frac{5}{16\xi^2} + \xi\frac{g}{f}. \tag{6.54}$$

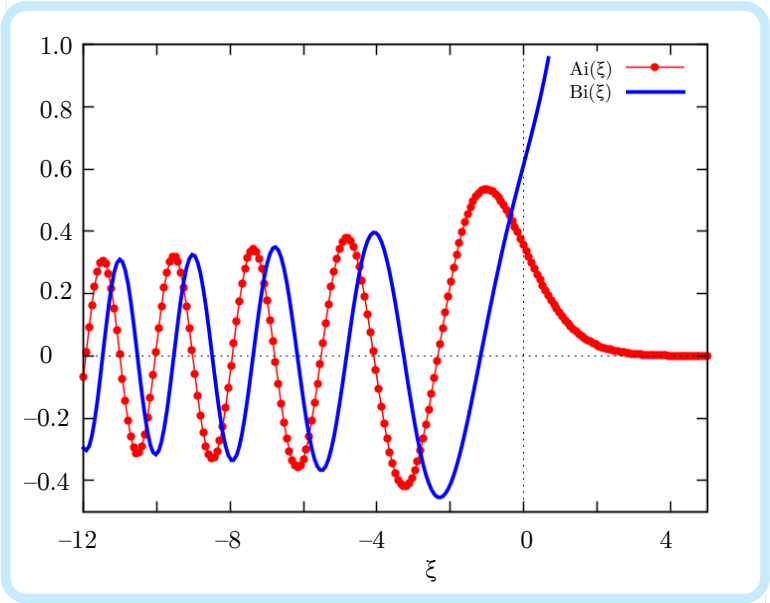


Figure 6.2: Graphs of Airy functions. Note the turning point at $\xi = 0$. The function $\mathrm{Ai}(\xi)$ transitions from oscillatory to exponentially decaying function while $\mathrm{Bi}(\xi)$ becomes exponentially increasing. [code]

For small enough $\psi(\xi)$ the transformed differential equation above reduces to Airy differential equation,

$$\frac{\mathrm{d}^2V}{\mathrm{d}\xi^2} - \xi V = 0, \tag{6.55}$$

the solution of which can be written as a sum of two Airy functions $\mathrm{Ai}(\xi)$ and $\mathrm{Bi}(\xi)$.

$$V(\xi) \approx c_1\mathrm{Ai}(\xi) + c_2\mathrm{Bi}(\xi). \tag{6.56}$$

These two functions have a single turning point (at $\xi = 0$) corresponding to that of the solution of the original Mukhanov-Sasaki equation we start with. Both functions are oscillatory for $\xi < 0$. Beyond this, $\mathrm{Ai}(\xi)$ is exponentially decaying while $\mathrm{Bi}(\xi)$ is exponentially increasing (see **Fig. 6.2**).

From the assignment given by the first of (6.51) we can write a more explicit relation between ξ and f.

$$\xi\xi'^2 = f \quad \Rightarrow \quad \xi' = \pm\left(\frac{f}{\xi}\right)^{\frac{1}{2}} \tag{6.57}$$

The first equation above tells us that ξ and f have the same sign. Furthermore, the turning point $\xi = 0$ corresponds to $f(\tau_\star) = 0$. Given this turning point at $\tau = \tau_\star$, the form of f tells us that for $\tau > \tau_\star$ the function $f(\tau) > 0$. We can then write

$$\int_0^\xi \mathrm{d}\tilde{\xi}\,\tilde{\xi}^{\frac{1}{2}} = \pm\int_{\tau_\star}^{\tau} \mathrm{d}\tilde{\tau}\sqrt{f(\tilde{\tau})}, \tag{6.58}$$

and remove the minus sign because it will result to contradiction.

$$\frac{2}{3}\xi^{\frac{3}{2}} = \int_{\tau_\star}^{\tau} \mathrm{d}\tilde{\tau}\sqrt{f(\tilde{\tau})}. \tag{6.59}$$

For $\tau < \tau_\star$, the function $f(\tau) < 0$ and we can solve for ξ as follows.

$$\begin{aligned}
\xi' &= \pm\left(\frac{-f}{-\xi}\right)^{\frac{1}{2}}, \\
\int_\xi^0 \mathrm{d}\tilde{\xi}\sqrt{-\tilde{\xi}} &= \pm\int_\tau^{\tau_\star} \mathrm{d}\tilde{\tau}\sqrt{-f(\tilde{\tau})}, \\
\frac{2}{3}(-\xi)^{\frac{3}{2}} &= \pm\int_\tau^{\tau_\star} \mathrm{d}\tilde{\tau}\sqrt{-f(\tilde{\tau})}.
\end{aligned} \tag{6.60}$$

The left hand side is positive and apart from the $\pm$ sign, the integral in the right hand side is positive; so we choose the positive sign.

$$\frac{2}{3}(-\xi)^{\frac{3}{2}} = \int_\tau^{\tau_\star} \mathrm{d}\tilde{\tau}\sqrt{-f(\tilde{\tau})}. \tag{6.61}$$

We rewrite our two results above relating ξ and f for a quick reference.

$$\boxed{\begin{aligned} \frac{2}{3}\xi^{\frac{3}{2}} &= \int_{\tau_\star}^{\tau} \mathrm{d}\tilde{\tau}\sqrt{f(\tilde{\tau})}, \qquad \tau > \tau_\star \\ \frac{2}{3}(-\xi)^{\frac{3}{2}} &= \int_{\tau}^{\tau_\star} \mathrm{d}\tilde{\tau}\sqrt{-f(\tilde{\tau})}, \quad \tau < \tau_\star \end{aligned}} \tag{6.62}$$

Since $f(\tau) = \nu^2/\tau^2 - k^2c_s^2$, the first integral above covers the extremal case of superhorizon modes while the second one covers the extremal case of subhorizon modes.

Let us now try to derive the uniform approximation for v_k. Since $v_k = V/\sqrt{\xi'}$ and $\xi\xi'^2 = f$ then

$$\begin{aligned} v_k &\approx \left(\frac{\xi}{f}\right)^{\frac{1}{4}} V(\xi), \\ v_k &\approx \left(\frac{\xi}{f}\right)^{\frac{1}{4}} \left[c_1\mathrm{Ai}(\xi) + c_2\mathrm{Bi}(\xi)\right]. \end{aligned} \tag{6.63}$$

For very large $-x \in \mathbb{R}$, the Airy functions behave as [55]

$$\mathrm{Ai}(-x) \sim \frac{\sin\left(\frac{2}{3}x^{\frac{3}{2}} + \frac{\pi}{4}\right)}{\sqrt{\pi}x^{\frac{1}{4}}}, \qquad \mathrm{Bi}(-x) \sim \frac{\cos\left(\frac{2}{3}x^{\frac{3}{2}} + \frac{\pi}{4}\right)}{\sqrt{\pi}x^{\frac{1}{4}}} \tag{6.64}$$

This asymptotic behavior includes the limit $\tau \to -\infty$ corresponding to the subhorizon modes satisfying the condition $|kc_s\tau| \gg 1$. We have

$$\begin{aligned} \lim_{\tau\to-\infty} v_k &\approx \lim_{\tau\to-\infty} \left(\frac{-\xi}{-f}\right)^{\frac{1}{4}} \left[c_1 \frac{\sin\left(\frac{2}{3}(-\xi)^{\frac{3}{2}} + \frac{\pi}{4}\right)}{\sqrt{\pi}(-\xi)^{\frac{1}{4}}} + c_2 \frac{\cos\left(\frac{2}{3}(-\xi)^{\frac{3}{2}} + \frac{\pi}{4}\right)}{\sqrt{\pi}(-\xi)^{\frac{1}{4}}}\right], \\ &= \lim_{\tau\to-\infty} \frac{1}{(-f)^{\frac{1}{4}}\sqrt{\pi}} \left\{ \left(\frac{c_1}{2i} + \frac{c_2}{2}\right) \exp\left[i\left(\frac{2}{3}(-\xi)^{\frac{3}{2}} + \frac{\pi}{4}\right)\right] \right. \\ &\qquad \left. + \left(-\frac{c_1}{2i} + \frac{c_2}{2}\right) \exp\left[-i\left(\frac{2}{3}(-\xi)^{\frac{3}{2}} + \frac{\pi}{4}\right)\right]\right\}, \\ \lim_{\tau\to-\infty} v_k &\approx \lim_{\tau\to-\infty} \frac{1}{2\sqrt{\pi}\sqrt{kc_s}} \left\{ (c_2 - ic_1)\, e^{i\frac{\pi}{4}} \exp\left(i\frac{2}{3}(-\xi)^{\frac{3}{2}}\right) \right. \end{aligned}$$

$$+ \left(c_2 + ic_1\right) e^{-i\frac{\pi}{4}} \exp\left(-i\frac{2}{3}(-\xi)^{\frac{3}{2}}\right)\Big\}. \tag{6.65}$$

We have the condition that

$$\lim_{\tau\to-\infty} v_k = \frac{e^{-ikc_s\tau}}{\sqrt{2kc_s}}. \tag{6.66}$$

It follows from the second of (6.62) that

$$\begin{aligned}
\lim_{\tau\to-\infty} v_k &\approx \lim_{\tau\to-\infty} \frac{e^{i\frac{\pi}{4}}}{2\sqrt{\pi kc_s}}\Big\{ \left(c_2 - ic_1\right) \exp\left(i\frac{2}{3}(-\xi)^{\frac{3}{2}}\right)\Big\}, \\
\lim_{\tau\to-\infty} v_k &\approx \lim_{\tau\to-\infty} \frac{e^{i\frac{\pi}{4}} c_3}{2\sqrt{\pi kc_s}}\Big\{ \left(c_2 - ic_1\right) e^{-ikc_s\tau}\Big\},
\end{aligned} \tag{6.67}$$

where c_3 is some constant phase factor corresponding to the upper bound of integration $\tau = \tau_\star$ in the second of (6.62). Comparing the last equation above with the condition for $\lim_{\tau\to-\infty} v_k$, we find

$$c_2 - ic_1 = \frac{\sqrt{2\pi}e^{-i\frac{\pi}{4}}}{c_3}. \tag{6.68}$$

Having found this, we can now write down the full solution for $\tau < \tau_\star$. Since we are interested with the superhorizon-mode solution let us trace back from the last of (6.65) involving exponentials to that involving the Airy functions.

$$\begin{aligned}
v_k \quad &: \quad \frac{c_2 - ic_1}{2\sqrt{\pi}\sqrt{kc_s}} e^{i\frac{\pi}{4}} \exp\left(i\frac{2}{3}(-\xi)^{\frac{3}{2}}\right), \\
&: \quad \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}\sqrt{kc_s}}\left[i\sin\left(\frac{2}{3}(-\xi)^{\frac{3}{2}} + \frac{\pi}{4}\right) + \cos\left(\frac{2}{3}(-\xi)^{\frac{3}{2}} + \frac{\pi}{4}\right)\right], \\
&: \quad \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}(-f)^{\frac{1}{4}}}\left[i\sqrt{\pi}(-\xi)^{\frac{1}{4}}\mathrm{Ai}(\xi) + \sqrt{\pi}(-\xi)^{\frac{1}{4}}\mathrm{Bi}(\xi)\right], \\
v_k \quad &: \quad \sqrt{\frac{\pi}{2}}\left(\frac{\xi}{f}\right)^{\frac{1}{4}} e^{-i\frac{\pi}{4}}\left[i\,\mathrm{Ai}(\xi) + \mathrm{Bi}(\xi)\right].
\end{aligned} \tag{6.69}$$

This form of $v_k(\tau)$ allows us to easily "connect" the superhorizon-mode solution corresponding to $\tau \to 0$ and the subhorizon mode solution corresponding to $\tau \to -\infty$.

The superhorizon limit corresponds to large ξ. For very large $x \in \mathbb{R}$, the Airy functions behave as [55]

$$\mathrm{Ai}(x) \sim \frac{e^{-\frac{2}{3}x^{\frac{3}{2}}}}{2\sqrt{\pi}x^{\frac{1}{4}}} \quad \text{and} \quad \mathrm{Bi}(x) \sim \frac{e^{\frac{2}{3}x^{\frac{3}{2}}}}{\sqrt{\pi}x^{\frac{1}{4}}}\,. \tag{6.70}$$

We find that the component involving $\mathrm{Ai}(\xi)$ is unnecessary in the calculation of the power spectrum because it is exponentially decaying.

$$\lim_{\tau\to 0} v_k \approx \lim_{\tau\to 0}\left(\frac{\xi}{f}\right)^{\frac{1}{4}} c_2\,\mathrm{Bi}(\xi). \tag{6.71}$$

Using the last of (6.69) and calculating the limit, we get

$$\begin{aligned}
\lim_{\tau\to 0} v_k &\approx \lim_{\tau\to 0} e^{-i\frac{\pi}{4}}\sqrt{\frac{\pi}{2}}\left(\frac{\xi}{f}\right)^{\frac{1}{4}}\mathrm{Bi}(\xi),\\
&= \lim_{\tau\to 0}\frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}f^{\frac{1}{4}}}\exp\left(\frac{2}{3}\xi^{\frac{3}{2}}\right),\\
&= \lim_{\tau\to 0}\frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}}\left(-\frac{\tau}{\nu_s}\right)^{\frac{1}{2}}\exp\left(\int_{\tau_\star}^{\tau}\mathrm{d}\tilde{\tau}\sqrt{f(\tilde{\tau})}\right),\\
\lim_{\tau\to 0} v_k &\approx \lim_{\tau\to 0}\frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}}\left(-\frac{\tau}{\nu_s}\right)^{\frac{1}{2}}\exp\left(\int_{\tau_\star}^{\tau}\mathrm{d}\tilde{\tau}\sqrt{-k^2c_s^2+\frac{\nu_s^2}{\tilde{\tau}^2}}\right).
\end{aligned} \tag{6.72}$$

It is now straightforward to derive the working equation for the power spectrum from here. By virtue of (5.95) we have [40]

$$\Delta_s^2(k) = \lim_{\tau\to 0}\frac{k^3}{2\pi^2}\left|\frac{v_k(\tau)}{z}\right|^2; \qquad z^2 = \frac{2a^2\epsilon_1}{c_s^2},$$

$$\boxed{\Delta_s^2(k) = -\lim_{\tau\to 0}\frac{k^3}{8\pi^2}\frac{\tau c_s^2}{a^2\nu_s\epsilon_1}e^{2\Psi_s},} \tag{6.73}$$

Scalar Power Spectrum in the Uniform Approximation

where

$$\Psi_s \equiv \int_{\tau_\star}^{\tau}\mathrm{d}\tilde{\tau}f_s^{\frac{1}{2}}(\tilde{\tau}) \equiv \int_{\tau_\star}^{\tau}\mathrm{d}\tilde{\tau}\sqrt{\frac{\nu_s^2}{\tilde{\tau}^2}-k^2c_s^2}. \tag{6.74}$$

Tensor Power Spectrum in the Uniform Approximation

We setup the working equation for the tensor power spectrum using effectively the same pathway as that of the scalar power spectrum. In so doing, having the same form, we need only to take note of the slight differences in the corresponding pair of equations for tensor and scalar perturbations. We have for the tensor power spectrum (see (5.106)),

$$\Delta_t^2(k) = \lim_{\tau\to 0} \frac{2k^3}{\pi^2} \left|\frac{u_k(\tau)}{a}\right|^2 \quad \text{instead of} \quad \Delta_s^2(k) = \lim_{\tau\to 0} \frac{k^3}{2\pi^2} \left|\frac{v_k(\tau)}{z}\right|^2,$$

and the condition given by (6.33),

$$\lim_{\tau\to -\infty} u_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{k}}, \tag{6.75}$$

instead of that given by (6.66),

$$\lim_{\tau\to -\infty} v_k = \frac{e^{-ikc_s\tau}}{\sqrt{2kc_s}}, \tag{6.76}$$

to be used in the uniform approximation. Note that $c_s^2 = 1$ and the factor $\sqrt{2}$ is missing in the subhorizon limit for tensor perturbations.

It follows that instead of (6.72) we have (ignoring the constant phase factor)

$$\lim_{\tau\to 0} u_k \approx \lim_{\tau\to 0} \left(-\frac{\tau}{\nu_t}\right)^{\frac{1}{2}} \exp\left(\int_{\tau_\star}^{\tau} \mathrm{d}\tilde{\tau} \sqrt{-k^2 + \frac{\nu_t^2}{\tilde{\tau}^2}}\right), \tag{6.77}$$

with

$$\nu_t^2 = \frac{1}{4} + \tau^2 U_t = \frac{1}{4} + \tau^2 \frac{a''}{a}. \tag{6.78}$$

We then find our sought-for working equation for the tensor power spectrum in the uniform approximation as

Tensor Power Spectrum in the Uniform Approximation

$$\Delta_t^2(k) = -\lim_{\tau\to 0} \frac{2k^3}{\pi^2} \frac{\tau}{a^2\nu_t} e^{2\Psi_t}, \tag{6.79}$$

where

$$\psi_t \equiv \int_{\tau_\star}^{\tau} \mathrm{d}\tilde{\tau} g_t^{\frac{1}{2}}(\tilde{\tau}) \equiv \int_{\tau_\star}^{\tau} \mathrm{d}\tilde{\tau} \sqrt{\frac{\nu_t^2}{\tilde{\tau}^2} - k^2}. \tag{6.80}$$

6.4 Second-Order Calculation of the Power Spectra

Expansion of ϵ_n, δ_n, c_s^2, a^2, and ν

In this section, we wish to calculate the power spectra up to second order in the Hubble and sound flow functions evaluated at the turning point. Proceeding with that of the scalar perturbations, we see that our working equation in the uniform approximation given by (6.73),

$$\Delta_s^2(k) = -\lim_{\tau\to 0} \frac{k^3}{8\pi^2} \frac{\tau c_s^2}{a^2 \nu_s \epsilon_1} e^{2\Psi_s}, \tag{6.81}$$

requires us to take the limit as $\tau \to 0$ of the expression in the right hand side. As such, in order to solve for the scalar power spectrum, we need to express c_s^2, a^2, ν_s, and ϵ_1 in terms of τ and carry out the integration for Ψ_s.

Conformal time. In the following, we follow the logic of ref. [40] in the recursive computation of the above-mentioned quantities in terms of conformal time and the Hubble and sound flow parameters. Crucial in this calculation is the availability of the expansion of the conformal time with respect to (ϵ_n, δ_n). As we shall see, since τ can be expressed in terms of (ϵ_n, δ_n) to arbitrary order, c_s^2, a^2, ν_s, and ϵ_1 can be written in terms of $(\epsilon_{n*}, \delta_{n*})$ to any order we want. For our purposes in this section, it is only sufficient to write down τ up to few orders following the series expansion given by (6.4)[3].

$$\tau = -\frac{1}{a} \sum_{n=0}^{\infty} \left(\frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \frac{1}{H} = \sum_{n=0}^{\infty} \tau_n \tag{6.82}$$

[3] In ref. [40], the calculation for τ was done through recursive integration by parts. Here, we use the simple formula we derived in **Sec. 6.1**

We find

$$\begin{aligned}
\bar{\tau}_0 &= 1,\\
\bar{\tau}_1 &= \epsilon_1,\\
\bar{\tau}_2 &= \epsilon_1^2 + \epsilon_1\epsilon_2,\\
\bar{\tau}_3 &= \epsilon_1^3 + 3\epsilon_1^2\epsilon_2 + \epsilon_1\epsilon_2^2 + \epsilon_1\epsilon_2\epsilon_3,\\
\bar{\tau}_4 &= \epsilon_1^4 + 6\epsilon_1^3\epsilon_2 + 7\epsilon_1^2\epsilon_2^2 + \epsilon_1\epsilon_2^3 + 4\epsilon_1^2\epsilon_2\epsilon_3 + 3\epsilon_1\epsilon_2^2\epsilon_3 + \epsilon_1\epsilon_2\epsilon_3^2 + \epsilon_1\epsilon_2\epsilon_3\epsilon_4,\\
&\vdots
\end{aligned} \tag{6.83}$$

where $\bar{\tau}_n = -(aH)\tau_n \sim \mathcal{O}(\epsilon^n)$. Note that the number of terms for $\bar{\tau}_n$ grows as 2^{n-1} because of the recursive way ϵ_n is defined as in (4.16); that is, $\dot{\epsilon}_n \equiv H\epsilon_n\epsilon_{n+1}$. For this reason, carrying out the calculation of the power spectrum beyond the first order manually becomes unwieldy. We opt to use a computer algebra system (e.g., Maxima [69], Maple [69], and Mathematica [70]) to make our calculations more manageable.

Hubble flow functions. Let us now proceed with ϵ_1. By definition, $\dot{\epsilon}_1 = H\epsilon_1\epsilon_2 \Leftrightarrow \epsilon_1' = (aH)\epsilon_1\epsilon_2$. Then

$$\begin{aligned}
\frac{\mathrm{d}\epsilon_1}{\mathrm{d}\tau} &= -\frac{1}{\tau}\epsilon_1\epsilon_2 + \mathcal{O}(\epsilon^3),\\
\epsilon_1 - \epsilon_{1\star} &= -\int_{\tau_\star}^{\tau}\frac{\mathrm{d}\tilde{\tau}}{\tilde{\tau}}\epsilon_1\epsilon_2 + \mathcal{O}(\epsilon^3),\\
\epsilon_1 &= \epsilon_{1\star} - \epsilon_{1\star}\epsilon_{2\star}L + \mathcal{O}(\epsilon_\star^3),
\end{aligned} \tag{6.84}$$

where $L \equiv \ln(\tau/\tau_\star)$. Likewise, $\epsilon_2 = \epsilon_{2\star} + \epsilon_{2\star}\epsilon_{3\star}L + \mathcal{O}(\epsilon_\star^3)$. We can go beyond the second order by using the Taylor series expansion of ϵ_1 with respect to the number of e-folds N,

$$\epsilon_1 = \epsilon_{1\star} + \left.\frac{\mathrm{d}\epsilon_1}{\mathrm{d}N}\right|_\star (\Delta N) + \frac{1}{2!}\left.\frac{\mathrm{d}^2\epsilon_1}{\mathrm{d}N^2}\right|_\star (\Delta N)^2 + \cdots, \tag{6.85}$$

where $\Delta N = N - N_\star$. Note that because $\mathrm{d}N \equiv \mathrm{d}\ln a$ then using our preliminary result for ϵ_1 and ϵ_2 above we can calculate ΔN as

$$N - N_\star = \int_{a_\star}^{a}\frac{\mathrm{d}\tilde{a}}{\tilde{a}} = -\int_{\tau_\star}^{\tau}\frac{\mathrm{d}\tilde{\tau}}{\tilde{\tau}}(1 + \epsilon_1 + \epsilon_1^2 + \epsilon_1\epsilon_2 + \cdots),$$

$$= -\int_{\tau_\star}^{\tau} \frac{\mathrm{d}\tilde{\tau}}{\tilde{\tau}}[1+\epsilon_{1\star}-\epsilon_{1\star}\epsilon_{2\star}L+\epsilon_{1\star}^2+\epsilon_{1\star}\epsilon_{2\star}+\mathcal{O}(\epsilon_\star^3)],$$

$$\Delta N = -(1+\epsilon_{1\star}+\epsilon_{1\star}^2+\epsilon_{1\star}\epsilon_{2\star})L+\tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}L^2+\mathcal{O}(\epsilon_\star^3). \tag{6.86}$$

Observe that the quantity ΔN is at least $\mathcal{O}(\epsilon_\star^0)$. Furthermore, $\mathrm{d}^n\epsilon_1/\mathrm{d}N^n \sim \mathcal{O}(\epsilon^{n+1})$. As such, to find ϵ_1 up to third order, we need only to consider the Taylor series expansion above up to the term involving the second order derivative (i.e., $\mathrm{d}\epsilon_1^2/\mathrm{d}N^2$) and ΔN up to first order.

Substituting the last expression above for ΔN in the Taylor series expansion for ϵ_1 we find

$$\epsilon_1 = \epsilon_{1\star}\Big\{1-\epsilon_{2\star}L-\big[\epsilon_{1\star}\epsilon_{2\star}L-\tfrac{1}{2}\,(\epsilon_{2\star}^2+\epsilon_{2\star}\epsilon_{3\star})L^2\big]+\mathcal{O}(\epsilon_\star^3)\Big\}. \tag{6.87}$$

Similarly,

$$\epsilon_2 = \epsilon_{2\star}\Big\{1-\epsilon_{3\star}L-\big[\epsilon_{1\star}\epsilon_{3\star}L-\tfrac{1}{2}\,(\epsilon_{3\star}^2+\epsilon_{3\star}\epsilon_{4\star})L^2\big]+\mathcal{O}(\epsilon_\star^3)\Big\}. \tag{6.88}$$

In general, to find ϵ_1 up to n^{th} order, we need only to consider the Taylor series expansion up to the term involving $(n-1)^{\text{th}}$ derivative and ΔN up to $(n-2)^{\text{th}}$ order. This leads us to a recursive calculation of the Hubble flow functions involving the alternating computation of the Hubble flow functions and ΔN. The result of the calculation for the Hubble flow functions are being fed into the calculation of ΔN which in turn, is used to get higher order expression for the Hubble flow functions. This recursive calculation up to arbitrary order is possible because we can express τ up to any order with respect to the Hubble flow functions. Along the way in the recursive calculation, we can compute ΔN in terms of the Hubble flow parameters and L due to its relation with τ namely, $\mathrm{d}N = (aH)\mathrm{d}\tau$; the increment in order by which we can compute ΔN is only limited by the order of the previous result for the Hubble flow functions.

Speed of Sound. The speed of sound can also be computed in an ascending order using the Taylor series expansion with respect to N. This time however, we need to consider not only the Hubble flow function but also the sound flow functions.

$$c_s^2 = c_{s\star}^2 + \left.\frac{\mathrm{d}c_s^2}{\mathrm{d}N}\right|_\star (\Delta N) + \frac{1}{2!}\left.\frac{\mathrm{d}^2c_s^2}{\mathrm{d}N^2}\right|_\star (\Delta N)^2 + \cdots \tag{6.89}$$

From the second of (4.16) defining the Hubble flow functions and the second of

(4.17) defining δ_0,

$$\delta_{n+1} \equiv \frac{\mathrm{d}\ln\delta_n}{\mathrm{d}N}, \qquad \delta_0 \equiv \frac{c_{s,i}}{c_s}, \tag{6.90}$$

we can relate c_s and its derivative with δ_n.

$$\delta_1 = \frac{\mathrm{d}\ln\delta_0}{\mathrm{d}N} = -\frac{\mathrm{d}\ln c_s}{\mathrm{d}N} = -\frac{1}{2c_s^2}\frac{\mathrm{d}c_s^2}{\mathrm{d}N} \tag{6.91}$$

It follows that

$$\frac{\mathrm{d}c_s^2}{\mathrm{d}N} = -2c_s^2\delta_1 \quad \text{and} \quad \frac{\mathrm{d}^2c_s^2}{\mathrm{d}N^2} = c_s^2(4\delta_1^2 - 2\delta_1\delta_2). \tag{6.92}$$

Substitution in the Taylor series expansion for c_s^2 gives us

$$\begin{aligned} c_s^2 &= c_{s\star}^2\Big[1 - 2\delta_{1\star}(\Delta N) + 2(\delta_{1\star}^2 - \delta_{1\star}\delta_{2\star})(\Delta N)^2 + \cdots\Big], \\ c_s^2 &= c_{s\star}^2\Big\{1 + 2\delta_{1\star}L + \big[2\epsilon_{1\star}\delta_{1\star}L + (2\delta_{1\star}^2 - \delta_{1\star}\delta_{2\star})L^2\big] + \mathcal{O}\big((\epsilon_\star,\delta_\star)^3\big)\Big\}. \end{aligned} \tag{6.93}$$

Scale Factor. The next quantity that we wish to express in terms of τ and the Hubble flow parameters is the (square of the) scale factor. This time we are not going to employ its series expansion with respect to N but use its explicit relation with ΔN. From the definition $\mathrm{d}N \equiv \mathrm{d}\ln a$ we can write the scale factor as $a = a_\star e^{\Delta N}$. Then

$$\begin{aligned} a &= a_\star \exp\Big(-L - (\epsilon_{1\star} + \epsilon_{1\star}^2 + \epsilon_{1\star}\epsilon_{2\star})L + \tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}L^2 + \mathcal{O}(\epsilon_\star^3)\Big), \\ &= \frac{a_\star\tau_\star}{\tau}\exp\Big(-(\epsilon_{1\star} + \epsilon_{1\star}^2 + \epsilon_{1\star}\epsilon_{2\star})L + \tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}L^2 + \mathcal{O}(\epsilon_\star^3)\Big), \\ a^2 &= \frac{1}{(H_\star\tau)^2}\Big\{1 + 2(\epsilon_{1\star} - \epsilon_{1\star}L) + \big[3\epsilon_{1\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star} - (6\epsilon_{1\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star})L, \\ &\qquad + (2\epsilon_{1\star}^2 + \epsilon_{1\star}\epsilon_{2\star})L^2\big] + \mathcal{O}\big((\epsilon_\star,\delta_\star)^3\big)\Big\}, \end{aligned} \tag{6.94}$$

where in the last equality we have used the equation for the conformal time.

Index Function. Finally, we consider the **index function** ν which are of two types namely, ν_s and ν_t. By definition,

$$\nu_s^2 \equiv \frac{1}{4} + \tau^2 U_s(\tau) \quad \text{and} \quad \nu_t^2 \equiv \frac{1}{4} + \tau^2 U_t(\tau), \tag{6.95}$$

where from (5.23) and (6.31),

$$U_s = (aH)^2 \left[2 - \epsilon_1 + \tfrac{3}{2}\,\epsilon_2 - \tfrac{1}{2}\,\epsilon_1\epsilon_2 + \tfrac{1}{4}\,\epsilon_2^2 + \tfrac{1}{2}\,\epsilon_2\epsilon_3 + \delta_1\,(3 - \epsilon_1 + \epsilon_2 + \delta_1 + \delta_2)\right],$$
$$U_t = (aH)^2(2 - \epsilon_1). \tag{6.96}$$

Because $\tau = -(aH)^{-1}(1+\epsilon_1+\cdots)$, the conformal time cancels in the equations for the potentials; ν is expressible solely in terms of the Hubble and sound flow *functions* (ϵ_n, δ_n). We can express ν in terms of the Hubble and sound flow *parameters* $(\epsilon_{n\star}, \delta_{n\star})$ and conformal time by performing Taylor series expansion with respect to N and then substituting from the equation for ΔN in the resulting expression. Alternatively, we can simply use the equations for (ϵ_n, δ_n) in the equation for ν. For this second approach, we need the expressions for $\{\epsilon_n\}$ given by (6.87) and (6.88), and that for $\{\delta_n\}$ that we can derive using essentially the same logic as that for $\{\epsilon_n\}$.

$$\delta_1 = \delta_{1\star} - \delta_{1\star}\delta_{2\star}L + \mathcal{O}\big((\epsilon_\star, \delta_\star)^3\big),$$
$$\delta_2 = \delta_{2\star} - \delta_{2\star}\delta_{3\star}L + \mathcal{O}\big((\epsilon_\star, \delta_\star)^3\big). \tag{6.97}$$

Needless to say, the two approaches above for deriving the index function yield the same result (as we have verified by direct calculation).

$$\nu_s = \tfrac{3}{2} + (\epsilon_{1\star} + \tfrac{1}{2}\,\epsilon_{2\star} + \delta_{1\star}) + \Big[\epsilon_{1\star}^2 + \epsilon_{1\star}\delta_{1\star} + \tfrac{11}{6}\,\epsilon_{1\star}\epsilon_{2\star} + \tfrac{1}{6}\,\epsilon_{2\star}\epsilon_{3\star} + \tfrac{1}{3}\,\delta_{1\star}\delta_{2\star}$$
$$- \Big(\epsilon_{1\star}\epsilon_{2\star} + \tfrac{1}{2}\,\epsilon_{2\star}\epsilon_{3\star} + \delta_{1\star}\delta_{2\star}\Big)L\Big] + \mathcal{O}\Big((\epsilon_\star, \delta_\star)^3\Big),$$
$$\nu_t = \tfrac{3}{2} + \epsilon_{1\star} + \Big(\epsilon_{1\star}^2 + \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star} - \epsilon_{1\star}\epsilon_{2\star}L\Big) + \mathcal{O}(\epsilon_\star^3). \tag{6.98}$$

The Power Spectra up to Second-Order

All the relevant expansions for the literal coefficients of the exponential function in the working equations for the power spectra given by (6.73) and (6.79) are now in place. Now, we have to mind the exponential function; in particular, we need to expand the argument Ψ and perform integration. For the scalar

perturbation we have

$$f_s^{\frac{1}{2}} = f_s^{\frac{1}{2}}\Big|_{c_{s\star},\nu_{s\star}} + \frac{\partial f_s^{\frac{1}{2}}}{\partial \nu_s}\Big|_{c_{s\star},\nu_{s\star}} (\Delta\nu_s) + \frac{\partial f_s^{\frac{1}{2}}}{\partial c_s^2}\Big|_{c_{s\star},\nu_{s\star}} (\Delta c_s^2) + \frac{1}{2!}\frac{\partial^2 f_s^{\frac{1}{2}}}{\partial (c_s^2)^2}\Big|_{c_{s\star},\nu_{s\star}} (\Delta c_s^2)^2 + \cdots , \tag{6.99}$$

where $\Delta\nu_s = \nu_s - \nu_{s\star}$ and $\Delta c_s^2 = c_s^2 - c_{s\star}^2$. Note that $\Delta\nu_s$ is second order while Δc_s^2 is first order. As such, the set of terms in the right hand side before the dots is just sufficient to calculate the power spectrum up to second order.

Now, since $f_s = \nu_s^2/\tau^2 - k^2 c_s^2$ then more explicitly,

$$\begin{aligned} f_s^{\frac{1}{2}} = &-\frac{\nu_{s\star}}{\tau}\Big(1 - \frac{k^2 c_{s\star}^2 \tau^2}{\nu_{s\star}^2}\Big)^{\frac{1}{2}} + \frac{k^2\tau}{2\nu_{s\star}}\Big(1 - \frac{k^2 c_{s\star}^2\tau^2}{\nu_{s\star}^2}\Big)^{-\frac{1}{2}} (\Delta c_s^2) \\ &- \frac{1}{\tau}\Big(1 - \frac{k^2 c_{s\star}^2\tau^2}{\nu_\star^2}\Big)^{-\frac{1}{2}} (\Delta\nu_s) + \frac{k^4\tau^3}{8\nu_\star^3}\Big(1 - \frac{k^2 c_{s\star}^2\tau^2}{\nu_\star^2}\Big)^{-\frac{3}{2}} (\Delta c_s^2)^2 + \cdots . \end{aligned} \tag{6.100}$$

Using this in the equation for Ψ_s we find

$$\begin{aligned} \Psi_s = &-\nu_{s\star}\int_1^w \frac{\mathrm{d}u}{u}(1-u^2)^{\frac{1}{2}} + \frac{\nu_{s\star}}{2}\int_1^w \frac{\mathrm{d}u\, u}{(1-u^2)^{\frac{1}{2}}}(\Delta s) \\ &- \int_1^w \frac{\mathrm{d}u}{u(1-u^2)^{\frac{1}{2}}}(\Delta\nu_s) + \frac{\nu_{s\star}}{8}\int_1^w \frac{\mathrm{d}u\, u^3}{(1-u^2)^{\frac{3}{2}}}(\Delta s)^2 + \cdots , \end{aligned} \tag{6.101}$$

where

$$u \equiv -\frac{kc_{s\star}\tilde{\tau}}{\nu_{s\star}}, \qquad w \equiv -\frac{kc_{s\star}\tau}{\nu_{s\star}}, \quad \text{and} \quad \Delta s \equiv \frac{c_s^2 - c_{s\star}^2}{c_{s\star}^2} \tag{6.102}$$

and Δs, $(\Delta s)^2$, and $\Delta\nu_s$ to relevant orders can be written as

$$\begin{aligned} \Delta s &= 2\delta_{1\star}L + 2\epsilon_{1\star}\delta_{1\star}L + (2\delta_{1\star}^2 - \delta_{1\star}\delta_{2\star})L^2 + \mathcal{O}\Big((\epsilon_\star,\delta_\star)^3\Big), \\ (\Delta s)^2 &= 4\delta_{1\star}^2 L^2 + \mathcal{O}\Big((\epsilon_\star,\delta_\star)^3\Big), \\ \Delta\nu_s &= -\epsilon_{1\star}\epsilon_{2\star}L - \tfrac{1}{2}\,\epsilon_{2\star}\epsilon_{3\star}L - \delta_{1\star}\delta_{2\star}L + \mathcal{O}\Big((\epsilon_\star,\delta_\star)^3\Big). \end{aligned} \tag{6.103}$$

From these equations, we find that the relevant integrals needed to evaluate Ψ_s involve $L = \ln(\tau/\tau_\star) = \ln u$ up to second power. Here are the results of

integration.

$$
\begin{aligned}
A_0 &= \int_1^w \mathrm{d}u\, \frac{(1-u^2)^{\frac{1}{2}}}{u} = 1 - \ln 2 + \ln w, \\
B_1 &= \int_1^w \mathrm{d}u\, \frac{u \ln u}{(1-u^2)^{\frac{1}{2}}} = 1 - \ln 2, \\
B_2 &= \int_1^w \mathrm{d}u\, \frac{u \ln^2 u}{(1-u^2)^{\frac{1}{2}}} = -2 - \ln^2 2 + 2 \ln 2 + \frac{\pi^2}{12}, \\
C_1 &= \int_1^w \mathrm{d}u\, \frac{\ln u}{u(1-u^2)^{\frac{1}{2}}} = \frac{\pi^2}{24} - \frac{1}{2} \ln^2 2 + \frac{1}{2} \ln^2 w, \\
C_2 &= \int_1^w \mathrm{d}u\, \frac{\ln^2 u}{u(1-u^2)^{\frac{1}{2}}} = -\frac{1}{2}\zeta(3) + \frac{\pi^2}{12} \ln 2 - \frac{1}{3} \ln^3 2 + \frac{1}{3} \ln^3 w, \\
D_2 &= \int_1^w \mathrm{d}u\, \frac{u^3 \ln^2 u}{(1-u^2)^{\frac{3}{2}}} = 2 + 2 \ln^2 2 - 2 \ln 2 - \frac{\pi^2}{6}.
\end{aligned}
\tag{6.104}
$$

The labels A, B, ..., D correspond respectively, to the visible four integrals in the equation for Ψ_s above. The subscript of each letter corresponds to the power of the logarithmic function in the integrand. Note that the limit as $w \to 0$ is implicit in the expressions above.

It would be instructive to outline how to carry out the integrals above. The form of the integrands are deceptively simple yet the calculation can be lengthy even with the help of CAS; this is particularly true as the power of the logarithmic function increases. Here, we outline the calculation of C_2 as a representative example; the rest can be calculated using effectively the same approach. We have

$$
C_2 = \int_1^w \mathrm{d}u\, \frac{\ln^2 u}{u(1-u^2)^{\frac{1}{2}}} = -\frac{1}{2}\zeta(3) + \frac{\pi^2}{12} \ln 2 - \frac{1}{3} \ln^3 2 + \frac{1}{3} \ln^3 w. \tag{6.105}
$$

The first step is to perform a suitable transformation to reduce the integrand

to an expression that can be managed by an integrator[4]. Let

$$u = \sqrt{1-(1-x)^2} \quad \Rightarrow \quad \mathrm{d}u = \frac{1-x}{\sqrt{2x-x^2}}\mathrm{d}x. \tag{6.106}$$

Notice that u and x have a one-to-one correspondence. Furthermore, $u = (1,0)$ corresponds to $x = (1,0)$. With the above transformation, C_2 can be rewritten as

$$C_2 = \int_1^{u=w} \mathrm{d}x\, \frac{\ln^2 x(2-x)}{4x(2-x)} = \int_1^{u=w} \mathrm{d}x \left[\frac{\ln^2 x}{4x(2-x)} + \frac{\ln x\, \ln(2-x)}{2x(2-x)} + \frac{\ln^2(2-x)}{4x(2-x)}\right].$$

This evaluates to

$$\begin{aligned} C_2 = \Bigg[&-\frac{1}{2}\mathrm{Li}_3\left(1-\frac{x}{2}\right) + \frac{1}{2}\mathrm{Li}_3\frac{x}{2} + \frac{1}{2}\mathrm{Li}_2\left(1-\frac{x}{2}\right)\ln(2-x) - \frac{1}{2}\mathrm{Li}_2\frac{x}{2}\,\ln x \\ &- \frac{1}{24}\ln^3(2-x) + \frac{\ln^3 x}{24} + \frac{1}{8}\ln x\,\ln^2(2-x) - \frac{1}{24}\ln 64\,\ln^2(2-x) \\ &- \frac{1}{8}\ln^2 x\,\ln(2-x) + \frac{1}{24}\ln 64\,\ln^2 x\Bigg]_1^{u=w}, \end{aligned} \tag{6.107}$$

where $\mathrm{Li}(x)$ is the **polylogarithm function** given by

$$\mathrm{Li}_s(x) \equiv \sum_{n=1}^{\infty}\frac{x^n}{n^s} = x + \frac{x^2}{2^s} + \frac{x^3}{3^s} = -\frac{1}{(n-2)!}\int_0^1 \mathrm{d}t\,\frac{\ln(1-tx)}{t}\ln^{s-2}\frac{1}{t}. \tag{6.108}$$

For $x = 1$ it reduces to the **Riemann zeta function**. Some special values useful in our calculation are given below:

$$\begin{aligned} &\mathrm{Li}_2\left(\tfrac{1}{2}\right) = \tfrac{1}{12}\pi^2 - \tfrac{1}{2}\ln^2 2, \quad \mathrm{Li}_3\left(\tfrac{1}{2}\right) = \tfrac{1}{6}\ln^3 2 - \tfrac{1}{12}\pi^2\ln 2 + \tfrac{7}{8}\zeta(3), \\ &\mathrm{Li}_2(1) = \tfrac{1}{6}\pi^2, \qquad \mathrm{Li}_3(1) = \zeta(3). \end{aligned} \tag{6.109}$$

The integral evaluated at $u = 1$ is vanishing while that in the limit as

[4] In our case, we use the online Mathematica integrator for the integration and Maple for the simplification. For the type of integrals we tried, Mathematica significantly outperformed Maple.

$u = w \to 0$ diverges.

$$C_2 = -\frac{1}{2}\zeta(3) + \tfrac{1}{12}\,\pi^2 \ln 2 - \tfrac{7}{24}\,\ln^3 2 + \tfrac{1}{8}\,\ln^2 2\,\ln x + \tfrac{1}{8}\,\ln 2\,\ln^2 x + \tfrac{1}{24}\,\ln^3 x$$

Note that in calculating the limit as $u = w \to 0$ we do not simply take the limit as $x \to 0$ even though $u = 0$ corresponds to $x = 0$; the ways these two variables approach zero are slightly different. We have from the definition above of x,

$$x = 1 - \sqrt{1 - u^2}. \tag{6.110}$$

As such,

$$\begin{aligned}
\ln x &= \ln(1 - \sqrt{1 - w^2}) = 2\ln w - \ln 2,\\
\ln^2 x &= 4\ln^2 w - 4\ln 2\,\ln w + \ln^2 2,\\
\ln^3 x &= 8\ln^3 w - 12\ln 2\,\ln^2 w + 6\ln^2 2\,\ln w - \ln^3 2.
\end{aligned} \tag{6.111}$$

Upon performing substitution in the last expression for C_2 above, all those terms involving $\ln^2 w$ and $\ln^3 w$ cancel and we get the desired expression for C_2.

$$C_2 = \int_1^w \mathrm{d}u\,\frac{\ln^2 u}{u(1-u^2)^{\frac{1}{2}}} = -\frac{1}{2}\zeta(3) + \frac{\pi^2}{12}\ln 2 - \frac{1}{3}\ln^3 2 + \frac{1}{3}\ln^3 w. \tag{6.112}$$

Observe the presence of the logarithmically divergent term $\ln w$ (raised to the third power) in the right hand of the equation for C_2. Variants of such term differing only in power of $\ln w$ are also present in the equation for A_0 and C_1. In order to have a sensible power spectrum then, the logarithmically divergent terms in e^{Ψ_s} in the working equation for $\Delta_s^2(k)$ should exactly cancel those coming from the literal coefficients of e^{Ψ_s}. As it turns out, upon performing substitution from our results for a^2, ϵ_1, c_s^2, and ν_s, and for e^{Ψ_s}, the resulting power spectrum is finite.

$$\Delta_s^2(k) = \frac{H_\star^2 c_0}{8\pi^2 \epsilon_{1\star} c_{s\star}}\left[\bar{\Delta}_s^{2(0)} + \bar{\Delta}_s^{2(1)} + \bar{\Delta}_s^{2(2)}\right], \tag{6.113}$$

where where $c_0 = 18e^{-3} \approx 0.896$ and

$$\bar{\Delta}_s^{2(0)} = 1,$$

$$\bar{\Delta}_s^{2(1)} = -(\tfrac{8}{3} - 2\ln 2)\epsilon_{1\star} - (\tfrac{1}{3} - \ln 2)\epsilon_{2\star} + (\tfrac{7}{3} - \ln 2)\delta_{1\star}, \tag{6.114}$$

$$\begin{aligned}\bar{\Delta}_s^{2(2)} = {} & (\tfrac{13}{9} - \tfrac{10}{3}\ln 2 + 2\ln^2 2)\epsilon_{1\star}^2 - (\tfrac{25}{9} - \tfrac{1}{12}\pi^2 - \tfrac{1}{3}\ln 2 - \ln^2 2)\epsilon_{1\star}\epsilon_{2\star} \\ & - (\tfrac{1}{18} + \tfrac{1}{3}\ln 2 - \tfrac{1}{2}\ln^2 2)\epsilon_{2\star}^2 - (\tfrac{1}{9} - \tfrac{1}{24}\pi^2 - \tfrac{1}{3}\ln 2 + \tfrac{1}{2}\ln^2 2)\epsilon_{2\star}\epsilon_{3\star} \\ & - (\tfrac{25}{9} - \tfrac{13}{3}\ln 2 + 2\ln^2 2)\epsilon_{1\star}\delta_{1\star} - (\tfrac{2}{9} - \tfrac{5}{3}\ln 2 + \ln^2 2)\epsilon_{2\star}\delta_{1\star} \\ & + (\tfrac{23}{18} - \tfrac{4}{3}\ln 2 + \tfrac{1}{2}\ln^2 2)\delta_{1\star}^2 + (\tfrac{25}{9} - \tfrac{1}{24}\pi^2 - \tfrac{7}{3}\ln 2 + \tfrac{1}{2}\ln^2 2)\delta_{1\star}\delta_{2\star}.\end{aligned}$$

This is the same expression derived in ref. [40]. The authors noted that the "exact cancellation... [of the logarithmically divergent terms] ... constitute a consistency check of the method." Following this line of thinking, one should expect the same to hold for tensor perturbation. As we have verified, using the equations above for a^2 and ν_t, and for e^{Ψ_t},

$$\Delta_t^2(k) = \frac{2H_\star^2 c_0}{\pi^2}\Big[\bar{\Delta}_t^{2(0)} + \bar{\Delta}_t^{2(1)} + \bar{\Delta}_t^{2(2)}\Big], \tag{6.115}$$

where

$$\begin{aligned}\bar{\Delta}_t^{2(0)} &= 1 \\ \bar{\Delta}_t^{2(1)} &= (-\tfrac{8}{3} + 2\ln 2)\epsilon_{1\star} \\ \bar{\Delta}_t^{2(2)} &= (\tfrac{13}{9} - \tfrac{10}{3}\ln 2 + 2\ln^2 2)\epsilon_{1\star}^2 - (\tfrac{26}{9} - \tfrac{1}{12}\pi^2 - \tfrac{8}{3}\ln 2 + \ln^2 2)\epsilon_{1\star}\epsilon_{2\star},\end{aligned} \tag{6.116}$$

in agreement with ref. [40].

6.5 Logarithmic Divergences in the Power Spectra

The striking balance of logarithmically divergent terms for up to second order calculation of the power spectra is a compelling evidence that the calculation demonstrated above can be carried out to all orders in the Hubble and sound flow parameters. One should not worry about the logarithmic terms in the intermediate steps since taking the limit at the end of the calculation yields a finite result. This is particularly gratifying since once we have the certainty that we can go up to any order in $(\epsilon_\star, \delta_\star)$ then we can mind improving the result

in the uniform approximation and yield an approximation precise enough to be compared with experimental results now and in the future. So far, the working equation for the power spectra that we have given by (6.73) and (6.79), are only an approximation to leading order in the uniform approximation. These have yielded an obvious imperfection in the value of $c_0 = 18e^{-3} \approx 0.896$— a little bit off from the expected value of unity—and in the coefficients of $\epsilon_\star$, $\epsilon_{2\star}$, etc. It is then a matter of simply going beyond the leading order in the uniform approximation, we might think, that we can rectify these numerical errors.

Nevertheless, the astonishing cancellation of logarithmically divergent terms however physically desirable it may be, should be placed under close scrutiny before we can proceed to the computation beyond the leading order in the uniform approximation. For sure, if we carefully follow the derivation of the working equations for the power spectra to leading order in the uniform approximation given by (6.73) and (6.79),

$$\Delta_s^2(k) = -\lim_{\tau\to 0}\frac{k^3}{8\pi^2}\frac{\tau c_s^2}{a^2\nu_s\epsilon_1}e^{2\Psi_s},$$
$$\Delta_t^2(k) = -\lim_{\tau\to 0}\frac{2k^3}{\pi^2}\frac{\tau}{a^2\nu_t}e^{2\Psi_t}, \tag{6.117}$$

we find nothing suspicious so as to render the result divergent. If there is anything immediately unusual in these equations, it is the danger that taking the limit as $\tau \to 0$ would yield zero and not a divergent expression. We immediately find however, using the available expressions for a^2, ν, and other functions involved in the approximation for $\Delta^2(k)$ that indeed, the result does not vanish (unless we have a trivial scenario where $a_\star = 0$.).



Example 2. The Power Spectrum is Nontrivial. Show that the working equation for the scalar power spectrum given by the first of (6.117) does not yield a trivial result in the zeroth order approximation in $(\epsilon_\star, \delta_\star)$.

Solution. To zeroth order we have

$$c_s^2 = c_{s\star}^2, \quad a^2 = \frac{1}{H_\star^2\tau^2}, \quad \nu_s = \frac{3}{2}, \quad \epsilon_1 = \epsilon_{1\star}, \tag{6.118}$$

and $kc_{s\star} = -\nu_{s\star}\tau_\star$. Then

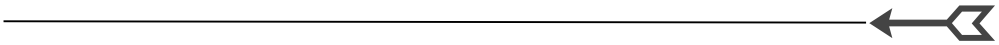
$$-\left(\frac{k^3}{8\pi^2}\frac{\tau c_s^2}{a^2\nu_s\epsilon_1}\right)^{(0)} = \frac{1}{8\pi^2}\left(\frac{9}{4}\right)\frac{H_\star^2}{\epsilon_{1\star}c_{s\star}}\left(\frac{\tau}{\tau_\star}\right)^3. \tag{6.119}$$

On the other hand,

$$\begin{aligned}\left(e^{2\Psi_s}\right)^{(0)} &= \exp\left(-\nu_{s\star}\int_1^w \frac{\mathrm{d}u}{u}(1-u^2)^{\frac{1}{2}}\right),\\ &= \exp\left(-3+3\ln 2-3\ln\frac{\tau}{\tau_\star}\right),\\ \left(e^{2\Psi_s}\right)^{(0)} &= 8e^{-3}\left(\frac{\tau_\star}{\tau}\right)^3\end{aligned} \tag{6.120}$$

Multiplying the two sub-results above cancels the factor $\tau^3/\tau_\star^3$ thus, yielding a nontrivial zeroth order power spectrum given by

$$\Delta_s^{2(0)} = \frac{H_\star^2 c_0}{8\pi^2\epsilon_{1\star}c_{s\star}}. \tag{6.121}$$



What can arouse our curiosity are not the working equations per se but the way we implement them; in particular, we use a series expansion of the Hubble and sound flow functions (and other functions such as a^2, ν, etc.,) that involve logarithmically divergent terms in the limit as $\tau \to 0$. For instance, from (6.87) we have

$$\epsilon_1 = \epsilon_{1\star}\Big\{1-\epsilon_{2\star}L-\left[\epsilon_{1\star}\epsilon_{2\star}L-\tfrac{1}{2}\left(\epsilon_{2\star}^2+\epsilon_{2\star}\epsilon_{3\star}\right)L^2\right]+\mathcal{O}(\epsilon_\star^3)\Big\}. \tag{6.122}$$

Needless to say, the necessary requirement for this series to converge is to have an ever decreasing term going down the line of the series expansion. For $\tau_\star < \tau \ll 0$, this is evidently the case as the sequence of terms constituting the series involves terms higher and higher order in $\epsilon_\star$. But when we consider the limit $\tau \to 0$, the quantity L diverges and the series for ϵ_1 diverges too. This is unphysical as during inflation, ϵ_1 goes from near zero to unity marking the end of inflation.

This insight is compelling enough to doubt the perfect cancellation of logarithmic divergences to all orders in $(\epsilon_\star, \delta_\star)$. In this section, we extend the calculation of the power spectra beyond the second order using exactly the same scheme as that in the preceding sections and determine at what order in $(\epsilon_\star, \delta_\star)$ such an exact cancellation would probably fail. To proceed, we need to extend the expressions for the terms involved in the literal coefficient of $e^{2\Psi}$ in the working equation for $\Delta^2(k)$ namely, ϵ_n, δ_n, c_s^2, a^2, and ν, up to an order sufficient to calculate the power spectrum up to third order. We have the following results.[5]

$$\begin{aligned}
\epsilon_1 = \epsilon_{1\star}\big\{1 - \epsilon_{2\star}L - \big[\epsilon_{1\star}\epsilon_{2\star}L - \tfrac{1}{2}(\epsilon_{2\star}^2 + \epsilon_{2\star}\epsilon_{3\star})L^2\big] \\
- \big[(\epsilon_{1\star}^2\epsilon_{2\star} + \epsilon_{1\star}\epsilon_{2\star}^2)L - (\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \tfrac{3}{2}\,\epsilon_{1\star}\epsilon_{2\star}^2)L^2 \\
+ \tfrac{1}{6}(\epsilon_{2\star}^3 + 3\epsilon_{2\star}^2\epsilon_{3\star} + \epsilon_{2\star}\epsilon_{3\star}^2 + \epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star})L^3\big] + \mathcal{O}(\epsilon_\star^4)\big\},
\end{aligned}$$

$$\begin{aligned}
\epsilon_2 = \epsilon_{2\star}\big\{1 - \epsilon_{3\star}L - \big[\epsilon_{1\star}\epsilon_{3\star}L - \tfrac{1}{2}(\epsilon_{3\star}^2 + \epsilon_{3\star}\epsilon_{4\star})L^2\big] \\
- \big[(\epsilon_{1\star}^2\epsilon_{3\star} + \epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star})L - (\tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \epsilon_{1\star}\epsilon_{3\star}^2 + \epsilon_{1\star}\epsilon_{3\star}\epsilon_{4\star})L^2 \\
+ \tfrac{1}{6}(\epsilon_{3\star}^3 + 3\epsilon_{3\star}^2\epsilon_{4\star} + \epsilon_{3\star}\epsilon_{4\star}^2 + \epsilon_{3\star}\epsilon_{4\star}\epsilon_{5\star})L^3\big] + \mathcal{O}(\epsilon_\star^4)\big\},
\end{aligned}$$

$$\delta_1 = \delta_{1\star}\big\{1 - \delta_{2\star}L - \tfrac{1}{2}\left[2\epsilon_{1\star}\delta_{2\star}L - (\delta_{2\star}^2 + \delta_{2\star}\delta_{3\star})L^2\right] + \mathcal{O}\big((\epsilon_\star, \delta_\star)^3\big)\big\}$$

$$\delta_2 = \delta_{2\star}\big\{1 - \delta_{3\star}L - \tfrac{1}{2}\left[2\epsilon_{1\star}\delta_{3\star}L - (\delta_{3\star}^2 + \delta_{3\star}\delta_{4\star})L^2\right] + \mathcal{O}\big((\epsilon_\star, \delta_\star)^3\big)\big\},$$

$$\begin{aligned}
c_s^2 = c_{s\star}^2\Big\{1 + 2\delta_{1\star}L + \big[2\epsilon_{1\star}\delta_{1\star}L + (2\delta_{1\star}^2 - \delta_{1\star}\delta_{2\star})L^2\big] \\
+ 2(\epsilon_{1\star}^2\delta_{1\star} + \epsilon_{1\star}\epsilon_{2\star}\delta_{1\star})L - (\epsilon_{1\star}\epsilon_{2\star}\delta_{1\star} + 2\epsilon_{1\star}\delta_{1\star}\delta_{2\star} - 4\epsilon_{1\star}\delta_{1\star}^2)L^2 \\
+ \tfrac{1}{3}\,(4\delta_{1\star}^3 - 6\delta_{1\star}^2\delta_{2\star} + \delta_{1\star}\delta_{2\star}^2 + \delta_{1\star}\delta_{2\star}\delta_{3\star})L^3 + \mathcal{O}\big((\epsilon_\star, \delta_\star)^4\big)\Big\},
\end{aligned}$$

$$\begin{aligned}
a^2 = \frac{1}{(H_\star\eta)^2}\Big\{1 + 2\big[\epsilon_{1\star} - \epsilon_{1\star}L\big] + \big[3\epsilon_{1\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star} - (6\epsilon_{1\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star})L \\
+ (2\epsilon_{1\star}^2 + \epsilon_{1\star}\epsilon_{2\star})L^2\big] + \big[4\epsilon_{1\star}^3 + 8\epsilon_{1\star}^2\epsilon_{2\star} + 2\epsilon_{1\star}\epsilon_{2\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} \\
- (12\epsilon_{1\star}^3 + 14\epsilon_{1\star}^2\epsilon_{2\star} + 2\epsilon_{1\star}\epsilon_{2\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star})L
\end{aligned}$$

[5] See the Maple codes in the Appendix that we used to calculate these results and the power spectra.

$$
\begin{aligned}
&+ \left(8\epsilon_{1\star}^3 + 9\epsilon_{1\star}^2\epsilon_{2\star} + \epsilon_{1\star}\epsilon_{2\star}^2 + \epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}\right)L^2 \\
&- \tfrac{1}{3}\left(4\epsilon_{1\star}^3 + 6\epsilon_{1\star}^2\epsilon_{2\star} + \epsilon_{1\star}\epsilon_{2\star}^2 + \epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}\right)L^3\big] + \mathcal{O}\big((\epsilon_\star,\delta_\star)^4\big)\Big\},
\end{aligned}
$$

$$
\begin{aligned}
\nu_s = \tfrac{3}{2} &+ \big[\epsilon_{1\star} + \tfrac{1}{2}\,\epsilon_{2\star} + \delta_{1\star}\big] + \big[\epsilon_{1\star}^2 + \epsilon_{1\star}\delta_{1\star} + \tfrac{11}{6}\,\epsilon_{1\star}\epsilon_{2\star} + \tfrac{1}{6}\,\epsilon_{2\star}\epsilon_{3\star} + \tfrac{1}{3}\,\delta_{1\star}\delta_{2\star} \\
&- \left(\epsilon_{1\star}\epsilon_{2\star} + \tfrac{1}{2}\,\epsilon_{2\star}\epsilon_{3\star} + \delta_{1\star}\delta_{2\star}\right)L\big] + \big[\epsilon_{1\star}^3 + \tfrac{77}{18}\,\epsilon_{1\star}^2\epsilon_{2\star} + \tfrac{17}{9}\,\epsilon_{1\star}\epsilon_{2\star}^2 \\
&+ \tfrac{14}{9}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} - \tfrac{1}{18}\,\epsilon_{2\star}^2\epsilon_{3\star} + \epsilon_{1\star}^2\delta_{1\star} + \tfrac{10}{9}\,\epsilon_{1\star}\epsilon_{2\star}\delta_{1\star} - \tfrac{1}{9}\,\epsilon_{2\star}\epsilon_{3\star}\delta_{1\star} \\
&+ \tfrac{4}{9}\,\epsilon_{1\star}\delta_{1\star}\delta_{2\star} - \tfrac{1}{9}\,\epsilon_{2\star}\delta_{1\star}\delta_{2\star} - \tfrac{2}{9}\,\delta_{1\star}^2\delta_{2\star} - \big(3\epsilon_{1\star}^2\epsilon_{2\star} + \tfrac{11}{6}\,\epsilon_{1\star}\epsilon_{2\star}^2 \\
&+ \tfrac{7}{3}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \tfrac{1}{6}\,\epsilon_{2\star}\epsilon_{3\star}^2 + \tfrac{1}{6}\,\epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star} + \epsilon_{1\star}\epsilon_{2\star}\delta_{1\star} + 2\epsilon_{1\star}\delta_{1\star}\delta_{2\star} \\
&+ \tfrac{1}{3}\,\delta_{1\star}\delta_{2\star}^2 + \tfrac{1}{3}\,\delta_{1\star}\delta_{2\star}\delta_{3\star}\big)L + \big(\tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}^2 + \tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \tfrac{1}{4}\,\epsilon_{2\star}\epsilon_{3\star}^2 \\
&+ \tfrac{1}{4}\,\epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star} + \tfrac{1}{2}\,\delta_{1\star}\delta_{2\star}^2 + \tfrac{1}{2}\,\delta_{1\star}\delta_{2\star}\delta_{3\star}\big)L^2\big] + \mathcal{O}\big((\epsilon_\star,\delta_\star)^4\big),
\end{aligned}
$$

$$
\begin{aligned}
\nu_t = \tfrac{3}{2} &+ \epsilon_{1\star} + \big[\epsilon_{1\star}^2 + \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star} - \epsilon_{1\star}\epsilon_{2\star}L\big] + \big[\epsilon_{1\star}^3 + \tfrac{34}{9}\,\epsilon_{1\star}^2\epsilon_{2\star} + \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star}^2 \\
&+ \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} - \big(3\epsilon_{1\star}^2\epsilon_{2\star} + \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star}^2 + \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}\big)L \\
&+ \big(\tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}^2 + \tfrac{1}{2}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}\big)L^2\big] + \mathcal{O}\big((\epsilon_\star,\delta_\star)^4\big).
\end{aligned}
\tag{6.123}
$$

It is worth emphasizing the obvious observation that all possible divergences in the expressions above for ϵ_n, δ_n, c_s^2, a^2, and ν are logarithmic in nature. For the power spectrum to converge, all divergences in $e^{2\Psi}$ should therefore all be of the same nature. To check this, we have to expand Ψ using the expression for f as before but this time aiming for at least the third order power spectrum. For the scalar perturbations we have[6]

$$
\begin{aligned}
\Psi_s = &-\nu_{s\star}\int_1^w \frac{\mathrm{d}u}{u}(1-u^2)^{\frac{1}{2}} + \frac{\nu_{s\star}}{2}\int_1^w \frac{\mathrm{d}u\,u}{(1-u^2)^{\frac{1}{2}}}(\Delta s) \\
&- \int_1^w \frac{\mathrm{d}u}{u(1-u^2)^{\frac{1}{2}}}(\Delta\nu_s) + \frac{\nu_{s\star}}{8}\int_1^w \frac{\mathrm{d}u\,u^3}{(1-u^2)^{\frac{3}{2}}}(\Delta s)^2 \\
&- \frac{1}{2}\int_1^w \frac{\mathrm{d}u\,u}{(1-u^2)^{\frac{3}{2}}}(\Delta s)(\Delta\nu_s) + \frac{\nu_{s\star}}{16}\int_1^w \frac{\mathrm{d}u\,u^5}{(1-u)^{\frac{5}{2}}}(\Delta s)^3 + \cdots,
\end{aligned}
\tag{6.124}
$$

where terms represented by the dots in the right hand side are at least fourth

[6] The expression for Ψ_t apart from some constant factors, is effectively a subset of this.

order in $(\epsilon_\star, \delta_\star)$. Since both Δs and $\Delta\nu_s$ involve powers of $L = \ln u$, all integrals above are of the form

$$\int_1^w \mathrm{d}u\, u^p (1-u^2)^q \ln^r u, \tag{6.125}$$

where $p, q, r \in \mathbb{Z}$. The integration of the first term in the right hand side of the equation for Ψ_s above yields a logarithmically divergent term $\ln w$. For the remaining terms, we classify them as follows: those involving

(a) $(\Delta s)^n$ only,

(b) $(\Delta\nu_s)^n (\Delta s)^p$, and

(c) $(\Delta\nu_s)^n$ only,

where $n, p \geq 1$.

The integrals involving $(\Delta s)^n$ only have the form

$$\int_1^w \mathrm{d}u\, \frac{u^{2n-1} \ln^m u}{(1-u^2)^{n-\frac{1}{2}}}, \qquad (1 \leq n \leq m). \tag{6.126}$$

The integrand is continuous on $(0, 1)$. For the bounds of integration, the factor u^{2n-1} in the numerator ensures that the limit as $u \to 0^+$ of the integrand vanishes while the logarithmic factor ensures that the limit as $u \to 1^-$ also vanishes. Thus, all integrals involving $(\Delta s)^n$ only are convergent. Following essentially the same logic, we find that all integrals involving $(\Delta\nu_s)^n (\Delta s)^p$ for $n, p \geq 1$, converge. For integrals involving $(\Delta\nu_s)^n$ only we have

$$\int_1^w \mathrm{d}u \left[\frac{c_1 \ln^m u}{u(1-u^2)^{n-\frac{1}{2}}} + \frac{c_2 \ln^m u}{u(1-u^2)^{n-\frac{3}{2}}} + \cdots \right], \qquad (1 \leq n \leq m) \tag{6.127}$$

where c_i's are constants. The number of terms inside the pair of square brackets for a given value of m depends on whether n is even or odd. For odd and even values of n we have $(n+1)/2$ and $(n+2)/2$ terms respectively. Each term is continuous on $(0, 1)$ and the limit as $u \to 1^-$ exists. However, the limit as $u \to 0^+$ diverges. This leads to a logarithmically divergent integral; e.g.,

$$\int_1^w \frac{\mathrm{d}u\, \ln^m u}{u(1-u^2)^{n-\frac{1}{2}}} = \frac{(\ln w)^{m+1}}{m+1} + \text{const.}, \tag{6.128}$$

where it is implicit that we take the limit as $w \to 0^+$. Hence, apart from the first integral in (6.124), all divergences in Ψ_s stem only from those terms involving $(\Delta\nu_s)^n$. Moreover, all divergences in Ψ_s are logarithmic in nature.

Had it been the case that some divergences in Ψ_s deviated from logarithmic nature, there could be no way by which our approximation for the power spectrum could converge because those in the literal coefficient of $e^{2\Psi_s}$ are all logarithmic in nature. This characterization of divergences allows us to continue our calculation in the hope that exact cancellation could occur. For all the visible integrals in the expression for Ψ_s above we find[7]

$$
\begin{aligned}
A_0 &= \int_1^w \mathrm{d}u\, \frac{(1-u^2)^{\frac{1}{2}}}{u} = 1 - \ln 2 + \ln w, \\
B_1 &= \int_1^w \mathrm{d}u\, \frac{u\, \ln u}{(1-u^2)^{\frac{1}{2}}} = 1 - \ln 2, \\
B_2 &= \int_1^w \mathrm{d}u\, \frac{u\, \ln^2 u}{(1-u^2)^{\frac{1}{2}}} = -2 - \ln^2 2 + 2\ln 2 + \frac{\pi^2}{12}, \\
B_3 &= \int_1^w \mathrm{d}u\, \frac{u\, \ln^3 u}{(1-u^2)^{\frac{1}{2}}} = -\frac{3}{2}\zeta(3) - 6\ln 2 + 6 + \frac{\pi^2}{4}\ln 2 + 3\ln^2 2 - \ln^3 2 - \frac{\pi^2}{4}, \\
C_1 &= \int_1^w \mathrm{d}u\, \frac{\ln u}{u\,(1-u^2)^{\frac{1}{2}}} = \frac{\pi^2}{24} - \frac{1}{2}\ln^2 2 + \frac{1}{2}\ln^2 w, \\
C_2 &= \int_1^w \mathrm{d}u\, \frac{\ln^2 u}{u\,(1-u^2)^{\frac{1}{2}}} = -\frac{1}{2}\zeta(3) + \frac{\pi^2}{12}\ln 2 - \frac{1}{3}\ln^3 2 + \frac{1}{3}\ln^3 w, \qquad (6.129) \\
D_2 &= \int_1^w \mathrm{d}u\, \frac{u^3\, \ln^2 u}{(1-u^2)^{\frac{3}{2}}} = 2 + 2\ln^2 2 - 2\ln 2 - \frac{\pi^2}{6}, \\
D_3 &= \int_1^w \mathrm{d}u\, \frac{u^3\, \ln^3 u}{(1-u^2)^{\frac{3}{2}}} = 3\zeta(3) - 6 - 3\ln^2 2 + 6\ln 2 - \frac{\pi^2}{2}\ln 2 + 2\ln^3 2 + \frac{\pi^2}{4}, \\
E_2 &= \int_1^w \mathrm{d}u\, \frac{u\, \ln^2 u}{(1-u^2)^{\frac{3}{2}}} = -\frac{\pi^2}{12} + \ln^2 2,
\end{aligned}
$$

[7] The calculation of these innocent-looking integrals can be laborious as alluded to in the previous section for the simple case of C_2. In **Appendix B** we demonstrate how to calculate a more complex integral namely, F_3, using Computer Algebra System and some simple tricks.

$$F_3 = \int_1^w \mathrm{d}u\, \frac{u^5 \ln^3 u}{(1-u^2)^{\frac{5}{2}}} = -4\zeta(3) + 6 + 2\ln^2 2 - \frac{8}{3}\ln^3 2 + \frac{2\pi^2}{3}\ln 2 - 6\ln 2 - \frac{\pi^2}{6}.$$

Using this together with (6.123) for a^2, ϵ_1, etc., in the working equation for $\Delta_s^2(k)$ we find

$$\Delta_s^2(k) = \frac{H_\star^2 c_0}{8\pi^2 \epsilon_{1\star} c_{s\star}} [\bar{\Delta}_s^{2(0)} + \bar{\Delta}_s^{2(1)} + \bar{\Delta}_s^{2(2)} + \bar{\Delta}_s^{2(3)}], \tag{6.130}$$

where $\bar{\Delta}_s^{2(0)}$, $\bar{\Delta}_s^{2(1)}$, and $\bar{\Delta}_s^{2(2)}$ are given by (6.114) and

$$\begin{aligned}
\bar{\Delta}_s^{2(3)} = {} & \left(\tfrac{4}{9} - \tfrac{4}{9}\ln 2 - \tfrac{4}{3}\ln^2 2 + \tfrac{4}{3}\ln^3 2\right)\epsilon_{1\star}^3 \\
& + \left(\tfrac{2}{3} + \tfrac{1}{36}\pi^2 + \tfrac{1}{6}\pi^2 \ln 2 - 6\ln 2 + 3\ln^2 2\right)\epsilon_{1\star}^2 \epsilon_{2\star} \\
& - \left(\tfrac{23}{9} - \tfrac{1}{8}\pi^2 - \tfrac{1}{2}\zeta(3) + \tfrac{1}{3}\ln 2 - \tfrac{1}{6}\ln^2 2 - \tfrac{1}{3}\ln^3 2\right)\epsilon_{1\star}\epsilon_{2\star}^2 \\
& + \left(\tfrac{1}{18} - \tfrac{1}{18}\ln 2 - \tfrac{1}{6}\ln^2 2 + \tfrac{1}{6}\ln^3 2\right)\epsilon_{2\star}^3 \\
& - \left(\tfrac{26}{9} - \tfrac{1}{12}\pi^2 - \tfrac{1}{2}\zeta(3) - 2\ln 2 + \tfrac{1}{3}\ln^2 2 + \tfrac{2}{3}\ln^3 2\right)\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} \\
& - \left(\tfrac{1}{72}\pi^2 - \tfrac{1}{24}\pi^2 \ln 2 + \tfrac{1}{3}\ln 2 + \tfrac{1}{2}\ln^3 2 - \tfrac{1}{2}\ln^2 2\right)\epsilon_{2\star}^2 \epsilon_{3\star} \\
& + \left(\tfrac{1}{72}\pi^2 + \tfrac{1}{4}\zeta(3) - \tfrac{1}{24}\pi^2 \ln 2 - \tfrac{1}{6}\ln^2 2 + \tfrac{1}{6}\ln^3 2\right)\epsilon_{2\star}\epsilon_{3\star}^2 \\
& + \left(\tfrac{1}{72}\pi^2 + \tfrac{1}{4}\zeta(3) - \tfrac{1}{24}\pi^2 \ln 2 - \tfrac{1}{6}\ln^2 2 + \tfrac{1}{6}\ln^3 2\right)\epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star} \\
& - \left(\tfrac{2}{3} - 2\ln^2 2 - \tfrac{2}{3}\ln 2 + 2\ln^3 2\right)\epsilon_{1\star}^2 \delta_{1\star} \\
& - \left(\tfrac{2}{3} + \tfrac{1}{72}\pi^2 - \tfrac{10}{3}\ln 2 + \tfrac{1}{12}\pi^2 \ln 2 + \tfrac{1}{2}\ln^2 2 + \ln^3 2\right)\epsilon_{1\star}\epsilon_{2\star}\delta_{1\star} \\
& - \left(\tfrac{1}{6} - \tfrac{1}{6}\ln 2 - \tfrac{1}{2}\ln^2 2 + \tfrac{1}{2}\ln^3 2\right)\epsilon_{2\star}^2 \delta_{1\star} \\
& + \left(\ln^3 2 - \ln^2 2 + \tfrac{1}{3} - \tfrac{1}{3}\ln 2\right)\epsilon_{1\star}\delta_{1\star}^2 + \left(\tfrac{1}{6} - \tfrac{1}{6}\ln 2 - \tfrac{1}{2}\ln^2 2 + \tfrac{1}{2}\ln^3 2\right)\epsilon_{2\star}\delta_{1\star}^2 \\
& + \left(\tfrac{1}{72}\pi^2 + \tfrac{1}{3}\ln 2 - \tfrac{1}{24}\pi^2 \ln 2 - \tfrac{1}{2}\ln^2 2 + \tfrac{1}{2}\ln^3 2\right)\epsilon_{2\star}\epsilon_{3\star}\delta_{1\star} \\
& - \left(\tfrac{1}{18} - \tfrac{1}{18}\ln 2 - \tfrac{1}{6}\ln^2 2 + \tfrac{1}{6}\ln^3 2\right)\delta_{1\star}^3
\end{aligned} \tag{6.131}$$

$$
\begin{aligned}
&- \Big(\tfrac{1}{18}\,\pi^2 - \tfrac{14}{3}\,\ln 2 + \tfrac{1}{12}\,\pi^2 \ln 2 + 4\ln^2 2 - \ln^3 2\Big)\epsilon_{1\star}\delta_{1\star}\delta_{2\star} \\
&- \Big(\tfrac{1}{36}\,\pi^2 - \tfrac{7}{3}\,\ln 2 + \tfrac{1}{24}\,\pi^2 \ln 2 + 2\ln^2 2 - \tfrac{1}{2}\,\ln^3 2\Big)\epsilon_{2\star}\delta_{1\star}\delta_{2\star} \\
&+ \Big(\tfrac{1}{36}\,\pi^2 - \tfrac{7}{3}\,\ln 2 + \tfrac{1}{24}\,\pi^2 \ln 2 + 2\ln^2 2 - \tfrac{1}{2}\,\ln^3 2\Big)\delta_{1\star}^2\delta_{2\star} \\
&+ \Big(3 - \tfrac{7}{72}\,\pi^2 - \tfrac{1}{4}\,\zeta(3) - 3\ln 2 + \tfrac{1}{24}\,\pi^2 \ln 2 + \tfrac{7}{6}\,\ln^2 2 - \tfrac{1}{6}\,\ln^3 2\Big)\delta_{1\star}\delta_{2\star}^2 \\
&+ \Big(3 - \tfrac{7}{72}\,\pi^2 - \tfrac{1}{4}\,\zeta(3) - 3\ln 2 + \tfrac{1}{24}\,\pi^2 \ln 2 + \tfrac{7}{6}\,\ln^2 2 - \tfrac{1}{6}\,\ln^3 2\Big)\delta_{1\star}\delta_{2\star}\delta_{3\star} \\
&+ \tfrac{1}{9}\Big(2\epsilon_{1\star}\epsilon_{2\star}^2 + 2\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \epsilon_{2\star}\epsilon_{3\star}^2 + \epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star} + 2\delta_{1\star}\delta_{2\star}^2 + 2\delta_{1\star}\delta_{2\star}\delta_{3\star}\Big)\ln w.
\end{aligned}
$$

Here we find that our calculation fails; although the third order power spectrum is for the most part finite, the last set of terms above diverges.

$$
\bar{\Delta}_s^{2(3)} \supset \big(\tfrac{2}{9}\epsilon_{1\star}\epsilon_{2\star}^2 + \tfrac{2}{9}\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \tfrac{1}{9}\epsilon_{2\star}\epsilon_{3\star}^2 + \tfrac{1}{9}\epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star} + \tfrac{2}{9}\delta_{1\star}\delta_{2\star}^2 + \tfrac{2}{9}\delta_{1\star}\delta_{2\star}\delta_{3\star}\big)\ln w. \tag{6.132}
$$

Further note that setting the speed of sound to $c_s^2 = \text{const.}$, does not help it. Since this result is carried in the calculation of higher order terms and logarithmic divergences involved in terms of different orders in $\mathcal{O}(\epsilon_\star, \delta_\star)$ cannot cancel each other, the approximation for the scalar power spectrum in the limit as $\tau \to 0^+$, is logarithmically divergent.

Following essentially the same route, we find for the tensor power spectrum that

$$
\Delta_t^2(k) = \frac{2H_\star^2 c_0}{\pi^2}\Big[\bar{\Delta}_t^{2(0)} + \bar{\Delta}_t^{2(1)} + \bar{\Delta}_t^{2(2)} + \bar{\Delta}_t^{2(3)}\Big], \tag{6.133}
$$

where $\bar{\Delta}_t^{2(0)}$, $\bar{\Delta}_t^{2(1)}$, and $\bar{\Delta}_t^{2(2)}$ are given by (6.116) and

$$
\begin{aligned}
\bar{P}_t^{(3)} = &\Big(\tfrac{4}{9} - \tfrac{4}{9}\,\ln 2 - \tfrac{4}{3}\,\ln^2 2 + \tfrac{4}{3}\,\ln^3 2\Big)\epsilon_{1\star}^3 \\
&+ \Big(\tfrac{1}{36}\,\pi^2 - \tfrac{16}{3}\,\ln 2 + \tfrac{1}{6}\,\pi^2 \ln 2 + 5\ln^2 2 - 2\ln^3 2\Big)\epsilon_{1\star}^2\epsilon_{2\star} \\
&- \Big(\tfrac{26}{9} - \tfrac{1}{9}\,\pi^2 - \tfrac{1}{2}\,\zeta(3) - \tfrac{8}{3}\,\ln 2 + \tfrac{1}{12}\,\pi^2 \ln 2 + \tfrac{4}{3}\,\ln^2 2 - \tfrac{1}{3}\,\ln^3 2\Big)\epsilon_{1\star}\epsilon_{2\star}^2 \\
&- \Big(\tfrac{26}{9} - \tfrac{1}{9}\,\pi^2 - \tfrac{1}{2}\,\zeta(3) - \tfrac{8}{3}\,\ln 2 + \tfrac{1}{12}\,\pi^2 \ln 2 + \tfrac{4}{3}\,\ln^2 2 - \tfrac{1}{3}\,\ln^3 2\Big)\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}
\end{aligned}
$$

$$+ \frac{2}{9}\left(\epsilon_{1\star}\epsilon_{2\star}^2 + \epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}\right)\ln w. \tag{6.134}$$

Similar to that of the scalar power spectrum, the logarithmic divergences survive in the third order part of the power spectrum.

It would not be unreasonable if the first response to the pair of physically useless results above is doubt. Although we have put forward some reservations above about the expansion of ϵ_n involving $\ln w$, the striking balance in the zeroth, first, and second order calculations yielding finite results have given us some hope to yield the same in the third order calculation. As systematic our calculation might be, some errors might have been committed. As such, it would be better to probe further and see where in our calculation the logarithmic divergences failed to cancel. For this task, we consider only the divergences in the scalar power spectrum; that of the tensor perturbations follow essentially the same path.

For the following calculations, we follow a slightly different path—we place all expansions (of a^2, ϵ_1, ν_s, etc.) as an argument of an exponential function. By doing this, we would not be needing to expand the exponential function $e^{2\Psi_s}$ using the Taylor series; rather, the test for cancellation should happen "inside" the exponential function. To proceed, note that we can write the conformal time as $\eta = -(1+\alpha)/(aH)$ where $\alpha = \epsilon_1 + \epsilon_1^2 + \epsilon_1\epsilon_2 + \cdots$. As such, $\mathrm{d}a/a = -(\mathrm{d}\tau/\tau)(1+\alpha)$ and we find

$$\begin{aligned}
\frac{a}{a_\star} &= \exp\left(-\int_{\tau_\star}^{\tau}\frac{\mathrm{d}\tilde{\tau}}{\tau}(1+\alpha)\right),\\
a^2 &= a_\star^2\frac{\tau_\star^2}{\tau^2}\exp\left(-2\int_{\tau_\star}^{\tau}\frac{\mathrm{d}\tilde{\tau}}{\tilde{\tau}}\alpha\right),\\
a^2 &= \frac{(1+\alpha_\star)^2}{(H_\star\tau)^2}\exp\left(-2\int_{\tau_\star}^{\tau}\frac{\mathrm{d}\tilde{\tau}}{\tilde{\tau}}\alpha\right).
\end{aligned} \tag{6.135}$$

For ϵ_1 we have by definition $\dot{\epsilon}_1 = H\epsilon_1\epsilon_2$. Then

$$\begin{aligned}
\frac{\mathrm{d}\epsilon_1}{\epsilon_1} &= H\epsilon_2\,\mathrm{d}t = aH\epsilon_2\,\mathrm{d}\tau,\\
\epsilon_1 &= \epsilon_{1\star}\exp\left(-\int_{\tau_\star}^{\tau}\frac{\mathrm{d}\tau}{\tau}\epsilon_2(1+\alpha)\right).
\end{aligned} \tag{6.136}$$

For ν_s we decompose it as $\nu_s = \nu_{s\star} + \Delta\nu_s$. Then

$$\frac{1}{\nu_s} = \frac{1}{\nu_{s\star}}\left(1 - \frac{\Delta\nu_s}{\nu_{s\star}} + \cdots\right),$$
$$\frac{1}{\nu_s} = \frac{1}{\nu_{s\star}} \exp\left(-\frac{\Delta\nu_s}{\nu_{s\star}}\right). \tag{6.137}$$

Because $\Delta\nu \sim \mathcal{O}((\epsilon_\star, \delta_\star)^2)$, the last equation above holds up to third order.

Using the last four results above in the working equation for the power spectrum given by the first of (6.117), we find

$$\Delta_s^2(k) = \mathcal{N}(\eta) \exp\left\{\int_{\eta_*}^{\eta} \frac{\mathrm{d}\tau}{\tau}\Big[\alpha(2 + \epsilon_2 + 2\delta_1) + \epsilon_2 + 2\delta_1\Big] - \frac{\Delta\nu}{\nu_*} + 2\Psi_s\right\}, \tag{6.138}$$

where

$$\mathcal{N}(\tau) \equiv -\frac{k^3}{4\pi^2} \frac{H_\star^2 c_{s\star}^2}{\epsilon_{1\star}\nu_{s\star}(1+\alpha_\star)^2}\tau^3. \tag{6.139}$$

All possible sources of divergences are now lumped together as argument of the exponential function. Considering that our problem involves only those third order terms involving $\ln w$ and not $\{\ln^2 w, \ln^3 w, \cdots\}$ (as they are canceled along the way,) we focus only on the former. The third argument namely, $2\Psi_s$, contains the integrals listed in (6.129) to be substituted to the expression for Ψ_s given by (6.124). As we have argued above, those involving $(\Delta\nu_s)^2$ only are the sole contributor of logarithmic divergences aside from the first term in the right hand side of (6.124). However, $(\Delta\nu_s) \sim L$ at least, so the corresponding integral is at least $\sim \ln^2 w$. It follows that the first integral in (6.124) is the sole contributor of possible logarithmically divergent terms involving $\ln w$ (to the first power). We have

$$\begin{aligned} 2\Psi_s \supset -\Big(&2\epsilon_{1\star}^3 + \tfrac{28}{9}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \tfrac{34}{9}\,\epsilon_{1\star}\epsilon_{2\star}^2 + \tfrac{77}{9}\,\epsilon_{1\star}^2\epsilon_{2\star} \\ &- \tfrac{1}{9}\,\epsilon_{2\star}^2\epsilon_{3\star} + 2\epsilon_{1\star}^2\delta_{1\star} + \tfrac{8}{9}\,\epsilon_{1\star}\delta_{1\star}\delta_{2\star} + \tfrac{20}{9}\,\epsilon_{1\star}\epsilon_{2\star}\delta_{1\star} \\ &- \tfrac{2}{9}\,\epsilon_{2\star}\delta_{1\star}\delta_{2\star} - \tfrac{2}{9}\,\epsilon_{2\star}\epsilon_{3\star}\delta_{1\star} - \tfrac{4}{9}\,\delta_{1\star}^2\delta_{2\star}\Big)\ln w. \end{aligned} \tag{6.140}$$

The second argument of the exponential function in (6.138) also contributes

third order terms involving $\ln w$.

$$-\frac{\Delta\nu_s}{\nu_{s\star}} \supset \Big(\tfrac{14}{9}\,\epsilon_{1\star}^2\epsilon_{2\star} + \epsilon_{1\star}\epsilon_{2\star}^2 + \tfrac{4}{3}\,\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} - \tfrac{1}{9}\,\epsilon_{2\star}^2\epsilon_{3\star} + \tfrac{2}{9}\,\epsilon_{1\star}\epsilon_{2\star}\delta_{1\star} + \tfrac{8}{9}\,\epsilon_{1\star}\delta_{1\star}\delta_{2\star} - \tfrac{2}{9}\,\epsilon_{2\star}\epsilon_{3\star}\delta_{1\star} - \tfrac{2}{9}\,\epsilon_{2\star}\delta_{1\star}\delta_{2\star} - \tfrac{4}{9}\,\delta_{1\star}^2\delta_{2\star} + \tfrac{1}{9}\,\epsilon_{2\star}\epsilon_{3\star}^2 + \tfrac{1}{9}\,\epsilon_{2\star}\epsilon_{3\star}\epsilon_{4\star} + \tfrac{2}{9}\,\delta_{1\star}\delta_{2\star}\delta_{3\star} + \tfrac{2}{9}\,\delta_{1\star}\delta_{2\star}^2\Big)\ln w \tag{6.141}$$

Already at this point, we observe that the last four terms inside the pair of parentheses constitute four out of six divergent terms in (6.132) and there is no way they could be canceled by those from $2\Psi_s$. We are then compelled to look at the first argument of the exponential function in (6.138). The integrand reads

$$\begin{aligned}
&\alpha(2+\epsilon_2+2\delta_1)+\epsilon_2+2\delta_1\\
&\quad=(2\epsilon_1+\epsilon_2+2\delta_1)+(3\epsilon_1\epsilon_2+2\epsilon_1^2+2\epsilon_1\delta_1)\\
&\qquad+(2\epsilon_1\epsilon_2\epsilon_3+3\epsilon_1\epsilon_2^2+7\epsilon_1^2\epsilon_2+2\epsilon_1^3+2\epsilon_1\epsilon_2\delta_1+2\epsilon_1^2\delta_1).
\end{aligned}\tag{6.142}$$

We can draw from the first line in the right hand side after integration, terms involving $\{\ln^2 w, \ln^3 w, \cdots\}$ so they are not our concern here. Considering the second line however, does not help in canceling the underlined terms in (6.141).

$$2\epsilon_1\epsilon_2\epsilon_3+3\epsilon_1\epsilon_2^2+7\epsilon_1^2\epsilon_2+2\epsilon_1^3+2\epsilon_1\epsilon_2\delta_1+2\epsilon_1^2\delta_1$$

$$\Downarrow$$

$$\big(2\epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}+3\epsilon_{1\star}\epsilon_{2\star}^2+7\epsilon_{1\star}^2\epsilon_{2\star}+2\epsilon_{1\star}^3+2\epsilon_{1\star}\epsilon_{2\star}\delta_{1\star}+2\epsilon_{1\star}^2\delta_{1\star}\big)\ln w. \tag{6.143}$$

We thus find that four out of six logarithmically divergent terms in (6.132) come from $\Delta\nu/\nu_{s\star}$. The other two are contributed by the integral and the term $2\Psi_s$ in the argument of the exponential function in (6.138).

The foregoing settles the existence of logarithmic divergence in the our calculation following [40]. Consequently, the result for the power spectra including those finite zeroth, first, and second order parts may be seen as not resting on solid mathematical ground. With the working equations for $\Delta_s^2(k)$ and $\Delta_t^2(k)$ established from sound mathematical principles, it is only the expansion scheme containing logarithmically divergent terms (from the very beginning) that may shoulder the blame for the error. It would then be good to find another expan-

sion scheme that would not contain mathematically problematic terms.

One "alternative" scheme was considered in refs. [71, 72]. In such a scheme, one has the conformal time as the variable of expansion. Consider for instance, ϵ_1.

$$\epsilon_1 = \epsilon_{1\star} + \left.\frac{\mathrm{d}\epsilon_1}{\mathrm{d}\tau}\right|_\star (\tau - \tau_\star) + \frac{1}{2!}\left.\frac{\mathrm{d}^2\epsilon_1}{\mathrm{d}\tau^2}\right|_\star (\tau - \tau_\star)^2 + \cdots . \tag{6.144}$$

However, in agreement with ref. [71] this is not a good expansion because higher order derivative terms contain terms lower order in the Hubble and sound flow parameters.

$$\begin{aligned}
\epsilon'_{1\star} &= (a_\star H_\star)\epsilon_{1\star}\epsilon_{2\star}, \\
\epsilon''_{1\star} &= (a_\star H_\star)^2(\epsilon_{1\star}\epsilon_{2\star} - \epsilon_{1\star}^2\epsilon_{2\star} + \epsilon_{1\star}\epsilon_{2\star}^2 + \epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star}), \\
\epsilon'''_{1\star} &= 2(a_\star H_\star)^3(\epsilon_{1\star}\epsilon_{2\star} - \epsilon_{1\star}^2\epsilon_{2\star} + \epsilon_{1\star}\epsilon_{2\star}^2 + \epsilon_{1\star}\epsilon_{2\star}\epsilon_{3\star} + \cdots).
\end{aligned} \tag{6.145}$$

Consequently, ignoring those higher order terms results to loss of precision.

If we choose not to ignore those terms, we are forced to rewrite the series to group terms according to their order. We find

$$\begin{aligned}
\epsilon_1 = \epsilon_{1\star} &- \epsilon_{1\star}\epsilon_{2\star}\left[\left(\frac{\tau}{\tau_\star} - 1\right) - \frac{1}{2}\left(\frac{\tau}{\tau_\star} - 1\right)^2 + \frac{1}{3}\left(\frac{\tau}{\tau_\star} - 1\right)^3 + \cdots\right] \\
&- \epsilon_\star^2\epsilon_{2\star}\left[\left(\frac{\tau}{\tau_\star} - 1\right) - \frac{1}{2}\left(\frac{\tau}{\tau_\star} - 1\right)^2 + \frac{1}{3}\left(\frac{\tau}{\tau_\star} - 1\right)^3 + \cdots\right] + \cdots .
\end{aligned} \tag{6.146}$$

At this point, it is clear that we are not able to evade the divergence as the limit as $\tau \to 0$ leads to a harmonic series. More importantly, we observe that this is exactly the original expansion scheme elaborated in **Sec. 6.4**. Indeed, since $\ln z = (z-1) - (z-1)^2/2 + \cdots$, we can rewrite the expansion above as

$$\epsilon_1 = \epsilon_{1*} - \epsilon_{1\star}\epsilon_{2\star}L - \epsilon_{1\star^2}\epsilon_{2\star}L + \cdots , \tag{6.147}$$

which is (6.87). Thus, the "alternative" expansion scheme above is *not* an alternative expansion scheme at all.

The natural continuation beyond this is to find other suitable expansion scheme or completely discard the use of the Hubble and sound flow parameters

and think of a better parametrization of inflationary functions. The possibility is indeed wide and varied. At this point however, we wish not to pursue this further and try solve the problem of logarithmic divergence. It is enough that we have accomplished two things:

- characterization of the form of divergence in the power spectra, and
- determination of the order in terms of the Hubble- and sound-flow parameters in the expression for the power spectra the divergence starts to appear.

The attempt at going beyond what the Hankel-function approximation through the use of the uniform approximation has essentially failed. But a good understanding has been gained as to the nature and existence of the problem we are dealing with. With regards to the existence, readers should be cautious of the results in the literature [40, 67] using fully or partly the calculation pathway we simply borrowed and elaborated in this work (see also ref. [51]). As to the nature of the problem, we wish to investigate this further in greater detail in the future to eliminate the stumbling block due to logarithmic divergence and finally arrive at a finite power spectra.

* * * *

Author's Note. A reader who might be able to read this entire manuscript might not be able to see the whole point of this chapter aside from the first section dealing with the method of Hankel-function approximation that is used in the succeeding chapters. In fact, may be it is not really essential to have an admixture discussing the method of the uniform approximation that finds no practical utility in the latter parts of this manuscript. However, it was not the original expectation. At the outset when building the results encoded in this work, the view was it could have a practical purpose namely, to provide a precise expression for the "bare" power spectrum. Unfortunately, with the all bright assets of this method, we failed to find a bright result. This prompted a thorough investigation of this method probing the subtleties of the logarithmic divergences that prevent us from finding a physically consistent calculation result. The outcomes, as one already knows after reading this chapter, are (a) characterization of the form of divergence and (b) the point of emergence of the divergence with respect to the order based on the power of slow-roll

parameters. The idea is that not all investigations lead to positive results in the usual sense and there is nothing negative with a deep insight gained about how one method fails. The topic of the uniform approximation is a part of the trajectory of this work, and hence, with the things we learned about this method, it should rightfully be included along with the rest of the manuscript.

CHAPTER

7

Adiabatic Regularization of Power Spectra in General Single-Field Inflation[73]

Those souls that breath scattered on earth
Few stalks precipitate with engine of dirt
And yet thread through the fabric of life
Quarantine the devils whose evil is ripe.

François Nemesis
The Devil is There, 1619

7.1 Divergence of the Two-Point Function in Flat and Curved Spacetime

7.2 Adiabatic Regularization

7.3 The Regularized Power Spectrum

Infinity is a time-honored hurdle in quantum field theory in (flat) Minkowski spacetime. This problem becomes more pronounced in curved spacetime because of the implicit intervention of the curved background in the lives of fields sitting in it. In inflationary cosmology, the curved background adds a layer of complexity as early as the calculation of the coincident two-point function of an otherwise, free field. This is unsettling because the power spectrum is directly related to (in fact, it is defined in terms of) the two-point function. Adiabatic regularization deals with this problem by effectively decomposing a quantity of interest into those divergent-yielding parts and finite-yielding parts, and subtracting out the dangerous terms. As applied in the calculation of coincident two-point function, consistency imposes that it be reflected in the computation of the power spectrum. In this chapter, we investigate adiabatic regularization of the power spectrum within the framework of general single-field inflation.

7.1 Divergence of the Two-Point Function in Flat and Curved Spacetime

Consider a real Klein-Gordon field ϕ of mass m in Minkowski spacetime. The action for this field is given by

$$S = \frac{1}{2}\int \mathrm{d}^4x \left(-\eta^{\mu\nu}\partial_\mu\phi\,\partial_\nu\phi - m^2\phi^2\right). \tag{7.1}$$

From this action, it is straightforward to derive the equation of motion for ϕ using the Euler-Lagrange equation. Identifying the Lagrangian $\mathcal{L}$ from the action above, we find

$$\begin{aligned}\frac{\partial\mathcal{L}}{\partial\phi} - \frac{\partial}{\partial x^\mu}\frac{\partial\mathcal{L}}{\partial\phi_{,\mu}} &= 0,\\ \Box\phi - m^2\phi &= 0,\\ \ddot{\phi} - \partial^i\partial_i\phi + m^2\phi &= 0.\end{aligned} \tag{7.2}$$

In the second line, we have identified the d'Alembertian as $\Box = \eta^{\mu\nu}\partial_\mu\partial_\nu$ with the Minkowski metric $\eta^{\mu\nu} = \mathrm{diag}(-1,+1,+1,+1)$.

The positive-frequency solution of the equation of motion is $\phi(x) \sim e^{ik\cdot x} = e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t}$. Following a standard procedure for canonical quantization, we elevate $\phi(x)$ to a status of an operator that we also simply label as ϕ for brevity. With the positive-frequency solution in hand, we can write the mode expansion (in the Heisenberg picture) as

$$\phi(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3\sqrt{2\omega}}\left(a_\mathbf{k}e^{ik\cdot x} + a_\mathbf{k}^\dagger e^{-ik\cdot x}\right), \tag{7.3}$$

where[1] $\omega^2 = \mathbf{k}^2 + m^2 = k^2 + m^2$, and $a_\mathbf{k}$ and $a_\mathbf{k}^\dagger$ are the annihilation and creation operators, respectively. The annihilation operator annihilates the Poincaré-invariant vacuum, $a_\mathbf{k}|0\rangle = 0$, and together with the creation operator, obeys the following commutation relations:

$$[a_\mathbf{k}, a_{\mathbf{k}'}^\dagger] = (2\pi)^3\delta^3(\mathbf{k}-\mathbf{k}'),$$

[1] For brevity, we simply denote $\mathbf{k}^2$ as k^2. One should see in context, that this k is *not* the same as the k in $k\cdot x$ contained in the exponential term $e^{ik\cdot x}$; that is $k\cdot x = k^\mu x_\mu$.

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0, \quad [a^\dagger_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = 0. \tag{7.4}$$

Given the above specifications, let us calculate the equal-time two point function of $\phi(x)$.

$$\begin{aligned}
\langle 0|\phi(\mathbf{x},t)\phi(\mathbf{x}',t)|0\rangle &= \int \frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k}'}{(2\pi)^6\sqrt{(2\omega)(2\omega')}}\langle 0|\left(a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}-i\omega t} + a^\dagger_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega t}\right) \\
&\qquad \times \left(a_{\mathbf{k}'}e^{i\mathbf{k}'\cdot\mathbf{x}'-i\omega' t} + a^\dagger_{\mathbf{k}}e^{-i\mathbf{k}'\cdot\mathbf{x}'+i\omega' t}\right)|0\rangle, \\
&= \int \frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k}'}{(2\pi)^6\sqrt{(2\omega)(2\omega')}}\langle 0|a_{\mathbf{k}}a^\dagger_{\mathbf{k}'}e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{x}')-i(\omega-\omega')t}|0\rangle, \\
&= \int \frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k}'}{(2\pi)^6\sqrt{(2\omega)(2\omega')}}e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{x}')-i(\omega-\omega')t}(2\pi)^3\delta^3(\mathbf{k}-\mathbf{k}'), \\
&= \int \frac{\mathrm{d}^3\mathbf{k}\,e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{(2\pi)^3(2\omega)}, \\
\langle 0|\phi(\mathbf{x},t)\phi(\mathbf{x}',t)|0\rangle &= \frac{1}{(2\pi)^2}\int_0^\infty \frac{\mathrm{d}k\,k^2}{\sqrt{k^2+m^2}}\frac{\sin k|\mathbf{x}-\mathbf{x}'|}{k|\mathbf{x}-\mathbf{x}'|}.
\end{aligned} \tag{7.5}$$

In the coincidence limit $\mathbf{x} \to \mathbf{x}'$, the cardinal sine function approaches unity and the whole integrand tends to $\sim k$ for large k; the integral is thus, quadratically divergent.

$$\langle 0|\phi(\mathbf{x},t)^2|0\rangle \sim \int_0^\infty \mathrm{d}k\,k \sim k^2. \tag{7.6}$$

The solution to this problem in quantum field theory (QFT) in Minkowski spacetime is simple. One may recall that one of the first infinities in basic QFT emerges from the calculation of the vacuum expectation of the Hamiltonian H, where the term ϕ^2 is also present. Identifying $\mathcal{H}$ as the Hamiltonian density, we find

$$\begin{aligned}
\langle 0|H|0\rangle &= \int \mathrm{d}^3\mathbf{x}\langle 0|\mathcal{H}|0\rangle = \int \mathrm{d}^3\mathbf{x}\langle 0|(\dot\phi^2 - \mathcal{L})|0\rangle, \\
&= \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\langle 0|(\dot\phi^2 + \phi^{,i}\phi_{,i} + m^2\phi^2)|0\rangle, \\
&= \frac{1}{2}\int \mathrm{d}^3\mathbf{x}\frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k}'e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}-i(\omega-\omega')t}}{(2\pi)^6\sqrt{(2\omega)(2\omega')}}(\omega\omega' + \mathbf{k}\cdot\mathbf{k}' + m^2)\langle 0|a_{\mathbf{k}}a^\dagger_{\mathbf{k}'}|0\rangle,
\end{aligned}$$

$$= \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k}'(2\pi)^3\delta^3(\mathbf{k}-\mathbf{k}')}{(2\pi)^6\sqrt{(2\omega)(2\omega')}}(\omega\omega' + \mathbf{k}\cdot\mathbf{k}' + m^2)\langle 0|a_{\mathbf{k}}a^\dagger_{\mathbf{k}'}|0\rangle,$$

$$\langle 0|H|0\rangle = \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\omega\langle 0|[a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + (2\pi)^3\delta^3(0)]|0\rangle. \tag{7.7}$$

To avoid the divergence, one prescribes **normal ordering** so that instead of $\langle 0|H|0\rangle$ one has $\langle 0|\ :H:\ |0\rangle$, where $:a_{\mathbf{k}}a^\dagger_{\mathbf{k}}:= a^\dagger_{\mathbf{k}}a_{\mathbf{k}}$. The effect of this simple rearrangement is that the vacuum expectation value (VEV) of the resulting Hamiltonian vanishes. Needless to say, applying normal ordering to the two-point function above yields zero and we avoid the problem of divergence. Qualitatively, this is physically justified by the fact that what we measure in flat spacetime is not absolute energy but difference of energies.

Now consider a Klein-Gordon field in curved spacetime[2]; specifically, we take the FLRW metric

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a^2(t)\delta_{ij}\mathrm{d}x^i\mathrm{d}x^j. \tag{7.8}$$

The corresponding action is given by

$$S = \frac{1}{2}\int \sqrt{-g}\,\mathrm{d}^4x\left(-g^{\mu\nu}\nabla_\mu\phi\,\nabla_\nu\phi - m^2\phi^2\right). \tag{7.9}$$

The Euler-Lagrange equation

$$\frac{\partial\mathcal{L}}{\partial\phi} - \nabla_\mu\frac{\partial\mathcal{L}}{\partial\phi_{;\mu}} = 0, \tag{7.10}$$

yields the same expression as the second of (7.2), $\Box\phi - m^2\phi = 0$, but this time, $\Box = g^{\mu\nu}\nabla_\mu\nabla_\nu$ where the metric is $g_{\mu\nu} = \mathrm{diag}(-1, a^2, a^2, a^2)$ instead of the flat metric $\eta_{\mu\nu} = \mathrm{diag}(-1, +1, +1, +1)$. Consequently, noting that

$$\sqrt{-g}\,\Box\phi = \partial_\mu(\sqrt{-g}\,g^{\mu\nu}\,\partial_\nu\phi), \tag{7.11}$$

we find

$$\frac{1}{a^3}\frac{\partial}{\partial t}(a^3\dot{\phi}) - \frac{\delta^{ij}}{a^2}\phi_{,ij} + m^2\phi = 0. \tag{7.12}$$

[2] Our discussion here up to the part marked by "* * * *" is based on refs. [44] and [74].

If we let $\phi = e^{i\mathbf{k}\cdot\mathbf{x}} f_k$ then

$$\frac{1}{a^3}\frac{\partial}{\partial t}(a^3 \dot{f}_k) - \omega^2 f_k = 0, \tag{7.13}$$

where we have identified $(k^2/a^2 + m^2)^{\frac{1}{2}}$ as the frequency ω.

The last equation above is not easy to solve especially that we do not have *a priori* an expression for the scale factor. To simplify our calculation, we assume that the spacetime is asymptotically flat in the far past and distant future, and expanding (non-flat spacetime) in between. Consequently, in the far past, the positive-frequency solution can simply be written as

$$f_k \sim \frac{e^{-i\omega_1 t}}{\sqrt{2a_1^3\omega_1}}, \tag{7.14}$$

where $\omega_1^2 = k^2/a_1^2 + m^2$ and $a \to a_1$ in the limit $t \to -\infty$. With this solution, the mode expansion of ϕ takes the usual form given by

$$\phi(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi^3)} \left(a_{\mathbf{k}} f_k e^{i\mathbf{k}\cdot\mathbf{x}} + a_{\mathbf{k}}^\dagger f_k^* e^{-i\mathbf{k}\cdot\mathbf{x}} \right). \tag{7.15}$$

The vacuum state in the infinite past is the usual Minkowski vacuum containing zero particles; i.e., the action of the number operator $N_{\mathbf{k}} = a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ on the vacuum state $|0\rangle$ yields a vanishing result.

In the distant future, since the spacetime is effectively also a Minkowski spacetime, we have the same mode expansion but with ω_1 replaced by $\omega_2^2 = k^2/a_2^2 + m^2$, where a_2 is the limit of a as $t \to \infty$ and $a_2 > a_1$. However, f_k is in general, a linear superposition of two linearly-independent solutions namely, the positive- and negative-frequency solutions.[3]

$$f_k = \frac{c_1 e^{-i\omega_2 t}}{\sqrt{2a_2^3\omega_2}} + \frac{c_2 e^{i\omega_2 t}}{\sqrt{2a_2^3\omega_2}}. \tag{7.16}$$

With this expression for f_k, the mode expansion of the field ϕ can be written

[3] The specific form of the constants c_1 and c_2 below depends on the specific form $a(t)$ and the hyperbolic constraint equation that we mention below. For the spacetime we are considering here, $c_2 \to 0$ in the limit that $a_2 \to a_1$.

as

$$\phi(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3\sqrt{2a_2^3\omega_2}}\Big[a_{\mathbf{k}}\left(c_1 e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_2 t} + c_2 e^{i\mathbf{k}\cdot\mathbf{x}+i\omega_2 t}\right) + a_{\mathbf{k}}^\dagger\left(c_1^* e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega_2 t} + c_2^* e^{-i\mathbf{k}\cdot\mathbf{x}-i\omega_2 t}\right)\Big],$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3\sqrt{2a_2^3\omega_2}}\Big[\left(c_1 a_{\mathbf{k}} + c_2^* a_{-\mathbf{k}}^\dagger\right) e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_2 t} + \left(c_2 a_{-\mathbf{k}} + c_1^* a_{\mathbf{k}}^\dagger\right) e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega_2 t}\Big],$$

$$\phi(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3\sqrt{2a_2^3\omega_2}}\Big[A_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}-i\omega_2 t} + A_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{x}+i\omega_2 t}\Big], \tag{7.17}$$

where we have identified

$$\begin{aligned} A_{\mathbf{k}} &= c_1 a_{\mathbf{k}} + c_2^* a_{-\mathbf{k}}^\dagger, \\ A_{\mathbf{k}}^\dagger &= c_2 a_{-\mathbf{k}} + c_1^* a_{\mathbf{k}}^\dagger, \end{aligned} \tag{7.18}$$

following the form of $\phi(x)$ in the far past.

The mapping above from $(a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger)$ to $(A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger)$ is called **Bogoliubov transformation**. The form of the mode expansion for $\phi(x)$ is suggestive that we can identify $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$ as the new creation and annihilation operators respectively, in the Minkowski spacetime of the distant future. Indeed, if the constants c_1 and c_2 satisfy the hyperbolic equation $|c_1|^2 - |c_2|^2 = 1$, then $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$ satisfy the same commutation relation as that of $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$.

$$\begin{aligned} [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger] &= [c_1 a_{\mathbf{k}} + c_2^* a_{\mathbf{k}}^\dagger, c_2 a_{\mathbf{k}} + c_1^* a_{\mathbf{k}}^\dagger], \\ &= (|c_1|^2 - |c_2|^2)(2\pi)^3\delta^3(\mathbf{k}_1 - \mathbf{k}_2), \\ [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger] &= (2\pi)^3\delta^3(\mathbf{k}_1 - \mathbf{k}_2). \end{aligned} \tag{7.19}$$

In fact, the constraint for c_1 and c_2 holds as a consequence of the constant Wronskian of f_k corresponding to (7.13) written with respect to a new time variable $\sigma = \int^t \mathrm{d}t' a(t')$. Consequently, there exists a new vacuum state $|\tilde{0}\rangle$ that is annihilated by $A_{\mathbf{k}}$; symbolically, $A_{\mathbf{k}}|\tilde{0}\rangle = 0$.

This new vacuum state is different from the vacuum state of the far past. The action of $A_{\mathbf{k}}$ on $|0\rangle$ does not in general, yield a trivial result. Furthermore,

the action of the number operator $\tilde{N}_{\mathbf{k}} \equiv A^\dagger_{\mathbf{k}} A_{\mathbf{k}}$ on $|0\rangle$ gives a nonzero result in general. In particular, in the discretized (non-continuum) case where $[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}$ we find

$$\langle 0|N_{\mathbf{k}}|0\rangle = \langle 0|(c_2 a_{-\mathbf{k}} + c_1^* a^\dagger_{\mathbf{k}})(c_1 a_{\mathbf{k}} + c_2^* a^\dagger_{-\mathbf{k}})|0\rangle = |c_2|^2 \langle 0|0\rangle. \tag{7.20}$$

Inertial observers in the distant future therefore observe particles created after the expansion of the Universe.[4] This is not to say that the vacuum changes with time from $|0\rangle$ to $|\tilde{0}\rangle$ through the expansion of the Universe, as we are using the Heisenberg picture. But to point out that the physical vacuum (with respect to inertial observers) differs for the far past and the distant future.

* * * *

The foregoing gives us a hint about the complexity associated with curved spacetime in comparison to flat spacetime. We have seen that even for a rather simple curved spacetime that is asymptotically flat at two time extremes $t \to \pm\infty$, inertial observers at these two time extremes may not agree on the physical vacuum. In between these times, where we have a fast expanding space, the situation is worse. We do not have a well-defined particle number due to the time-energy uncertainty relation associated with measurement. Furthermore, here and in general curved spacetime, the separation between positive- and negative-components of the mode expansion of ϕ is ambiguous; consequently, the identification of the creation and annihilation operators is ambiguous. Different freely-falling observers can have different physical vacua.

In Minkowski spacetime, the vacuum enjoys the full **Poincaré symmetry**; it is spacetime-translation-, rotation-, and Lorentz-invariant. The separation of the positive- and negative-frequency components allows us to consistently identify the Lorentz-covariant creation and annihilation operators. For this reason, we can consistently perform normal ordering to remove infinities in the two-point-function and Hamiltonian vacuum expectation value in general. When we consider curved spacetime however, we lose the usual symmetries of

[4] Intuitively, this is not hard to see. For a (static) Minkowski spacetime, the particle-antiparticle pairs that form by virtue of the uncertainty relation have a fleeting existence. For an expanding de Sitter spacetime, the stretching of space can separate the particle-antiparticle pairs; thus, pulling them out of the "virtual reality" to the "corporeal reality." After the expansion is finished, inertial observers can detect these created particles.

the Minkowski spacetime; the vacuum is not in general, Poincaré invariant. For this reason, we cannot consistently apply normal ordering with respect to all inertial observers; whereas we might normal order and remove infinities in one frame, this regularization is not necessarily reflected in another frame.

We are mainly interested in this work in the calculation of the power spectrum be it for the scalar perturbations or tensor perturbations. The power spectrum by definition, is directly related to the two-point function of the corresponding fields. As such, divergence in the two-point function may pose some problems in the power spectrum. This compels us to look for a way to consistently remove divergent parts in curved spacetime at least for the two-point function. In fact, such an obvious problem of divergence has already been investigated in the past considering the vacuum expectation value of energy-momentum tensor, two-point functions, etc., and we are here not going to pretend to reinvent the wheel. Various methods have been proposed and investigated including **dimensional regularization** [75, 76], **point-splitting** [77, 78, 79, 80], and **adiabatic regularization** [44, 74, 81, 82, 83, 84, 85, 86]. Among these methods, we focus on the adiabatic regularization.

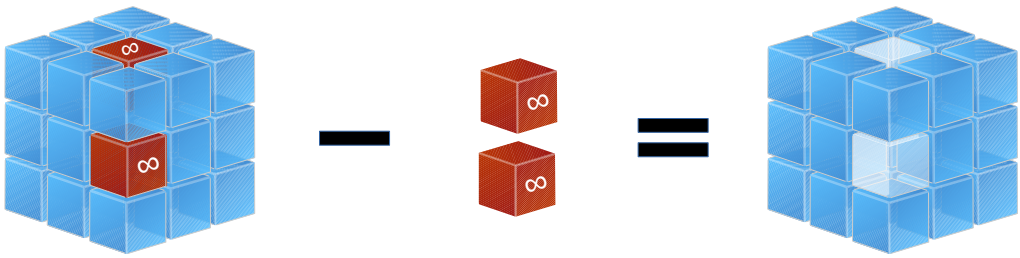


Figure 7.1: Schematic Diagram of Adiabatic Regularization. In adiabatic regularization, the divergent-yielding parts are identified and subtracted from the original quantity being considered.

Rather informally, adiabatic regularization is a method employing the adiabatic expansion of the fields involved in the calculation of the two-point (or n-point) function. In this expansion, the field is effectively decomposed into those yielding divergent expectation value and those yielding convergent expectation value. The divergent-yielding parts are identified and subtracted from the original two-point function resulting in a finite expression. In the next section,

we give the minimal necessary details to fill in this rather vague description of the method. We explain the method and its use within the context of the problem we wish to solve in this chapter namely, the adiabatic regularization of the power spectrum.

7.2 Adiabatic Regularization

The method of adiabatic regularization was proposed by Parker and Fulling [82] in 1974 to solve the divergence problem associated with the energy-momentum tensor in FLRW spacetime. Interested readers may want to refer to this work to witness the original context in which it was put forward. A rigorous and more comprehensive treatment of this method so written with relevant elementary details in place making it more accessible than the original research paper, can be found in the book [44] of the one the authors himself namely, Parker (together with D. J. Toms). Here, we are not going to repeat the full discussion in this book and in other materials but only provide the necessary background to solve the problem associated with the power spectrum that we are about to also discuss in greater detail. In so discussing the necessary background material for adiabatic regularization, we borrow the basics from refs. [44, 74].

In the previous section we have discussed the divergence associated with the two-point function of Klein-Gordon fields in Minkowski spacetime. The parallel in curved spacetime within the framework of inflation is the two-point function of scalar perturbations. (We cover the tensor perturbation later). In **Sec. 5.3**, we expressed this two-point function as (omitting the hat over ζ for brevity,)

$$\langle \zeta(\tau, \mathbf{x}_1)\zeta(\tau, \mathbf{x}_2)\rangle = \int \frac{\mathrm{d}k}{k} \frac{\sin k|\mathbf{x}_1 - \mathbf{x}_2|}{k|\mathbf{x}_1 - \mathbf{x}_2|} \Delta_s^2(k, \tau), \tag{7.21}$$

where the power spectrum is given by

$$\Delta_s^2(k, \tau) = \frac{k^3}{2\pi^2} \left| \frac{v_k(\tau)}{z} \right|^2, \tag{7.22}$$

with v_k obeying the Mukhanov-Sasaki equation,

$$v_k'' + (k^2 c_s^2 - U_s) v_k = 0. \tag{7.23}$$

In the short-wavelength limit, the coefficient of v_k tends to k^2 and by virtue of (5.37), $|v_k| \to 1/\sqrt{k}$. It follows that in this limit, $\Delta_s^2(k,\tau) \to \sim k^2$. In the coincidence limit, $\mathbf{x}_1 \to \mathbf{x}_2$, this poses a problem; the cardinal sine function in the integral above approaches unity and the integrand tends to k. The resulting two-point function is thus, *quadratically divergent*.

Adiabatic regularization solves this problem by performing a mode-by-mode subtraction effectively removing those parts of the integrand that yield divergent integrals. To implement this subtraction scheme, we label the original v_k in (7.21) as $v_k^{(b)}$, where (b) stands for "bare," and introduce $v_k^{(s)}$ corresponding to the quantity to be subtracted, the form of which is to be determined below. The resulting regularized two-point function is then calculated as

$$\langle\zeta(x)^2\rangle^{(r)} = \int \frac{\mathrm{d}k\, k^2}{2\pi^2}\left(\left|\frac{v_k^{(b)}}{z}\right|^2 - \left|\frac{v_k^{(s)}}{z}\right|^2\right). \tag{7.24}$$

Once we are able to determine $v_k^{(s)}$ and evaluate the integral above, the divergence associated with the two-point function is solved.[5] However, the form of $\langle\zeta(x)^2\rangle^{(r)}$ tells us that the power spectrum might be modified. Instead of $v_k^{(b)}$ used in standard treatments, we have to also consider the effect of $v_k^{(s)}$. We have therefore a new physical power spectrum $\Delta_s^{2(r)}$ which is the difference of $\Delta_s^{2(b)}$ and $\Delta_s^{2(s)}$,

Regularized Power Spectrum

$$\Delta_s^{2(r)} = \Delta_s^{2(b)} - \Delta_s^{2(s)}, \tag{7.25}$$

where

$$\Delta_s^{2(b)} = \frac{k^3}{2\pi^2}\left|\frac{v_k^{(b)}}{z}\right|^2 \quad \text{and} \quad \Delta_s^{2(s)} = \frac{k^3}{2\pi^2}\left|\frac{v_k^{(s)}}{z}\right|^2. \tag{7.26}$$

Should $\Delta_s^{2(r)}$ significantly differ from $\Delta_s^{2(b)}$, we will have to rethink of calculations based on $\Delta_s^{2(b)}$. In this light, our objective in this chapter is to determine the form of $\Delta_s^{2(r)}$ thereby examine the effect of adiabatic regularization on the power spectrum. At first sight, it appears $\Delta_s^{2(r)}$ could significantly deviate from $\Delta_s^{2(b)}$. However, the power spectrum we are dealing with in inflationary cosmology involves superhorizon modes; that is, frozen modes for which $aH \sim 1/|\tau|$

[5] We are only considering here the free part of the action.

is much larger than k. As such, it is possible that the adiabatic regularization being a UV regularization, might not have any effect at all. The only way to know this is of course, to perform the adiabatic regularization of the power spectrum.

We proceed to derive the subtraction term $\Delta_s^{2(s)}$ by determining $v_k^{(s)}$. In adiabatic regularization, $v_k^{(s)}$ is assumed to take the form

$$v_k^{(s)}(\tau) = \frac{1}{\sqrt{2W(\tau)}} e^{-i\int^\tau \mathrm{d}\tilde{\tau} W(\tilde{\tau})}, \tag{7.27}$$

resembling the plane-wave solution of the Klein-Gordon field in flat spacetime with W corresponding to the usual frequency ω. In fact, as part of the underlying condition of adiabatic regularization called the **adiabatic condition**, we take $W(\tau)$ to be $\omega(\tau)$ in some limit; for the case in hand, we take $\omega = kc_s$ from the Mukhanov-Sasaki equation. Such a limit corresponds to a very slow expansion of the Universe or very small wavelength of the perturbation such that the curvature of the spacetime can be ignored. From a physical perspective, the word adiabatic connotes the absence of particle creation because from the point of view of a mode being considered, the spacetime is effectively flat.

In general, W is a series of terms starting with $\omega_0 = \omega$ and continues with ω_1, ω_2, and so on; that is,

$$W = \omega_0 + \omega_1 + \omega_2 + \cdots . \tag{7.28}$$

The subscript of ω_n pertains to the so-called **adiabatic order** with ω_0 as zeroth-adiabatic order, ω_1 as first-adiabatic order, etc. Based on our description above of the adiabatic condition, the zeroth adiabatic order corresponds to ignorable expansion. The succeeding adiabatic orders must then take into account the expansion. In particular, for the FLRW spacetime, the adiabatic order is the number of the time-derivatives of the scale factor; e.g., $\ddot{a}$ is of second adiabatic order while $\dot{a}^3$ is of third adiabatic order.[6] In succession, one may see rather informally, that $\omega^{(1)}$ corresponds to velocity of expansion, $\omega^{(2)}$ corresponds to acceleration, and so on.

To determine the expansion of W up to a desired adiabatic order, we make use of the Mukhanov-Sasaki equation. Note that $v_k^{(s)}(\tau)$ satisfies the following

[6] See ref. [44] for a more rigorous description of adiabatic order. Here, our qualitative description suffices.

differential equation:

$$v_k^{(s)\prime\prime} + \left(\frac{W''}{2W} - \frac{3}{4}\frac{W'^2}{W^2} + W^2\right) v_k^{(s)} = 0, \tag{7.29}$$

while the Mukhanov-Sasaki equation can be written as

$$v_k'' + \left(\frac{W''}{2W} - \frac{3}{4}\frac{W'^2}{W^2} + W^2\right) v_k = \left(\frac{W''}{2W} - \frac{3}{4}\frac{W'^2}{W^2} + W^2 - k^2c_s^2 + U_s\right) v_k. \tag{7.30}$$

Now, based on ref. [44], if we choose W such that $v_k^{(s)}$ is a solution of the Mukhanov-Sasaki equation above up to a certain adiabatic order, the right hand side of the last equation above is of higher adiabatic order. To see this, note that if $v_k^{(s)}$ is determined up to a certain adiabatic order, plugging this truncated $v_k^{(s)}$ in (7.29) would allow us to move higher-adiabatic-order terms to the right hand side. Consequently, the difference of the last two equations above with v_k taken as the untruncated $v_k^{(s)}$ will be of higher adiabatic order. If $v_k^{(s)}$ is chosen to be up to third adiabatic order, the resulting difference will be at least fourth adiabatic order and if $v_k^{(s)}$ is chosen to be up to second adiabatic order, the resulting difference will be at least third adiabatic order. This sequence continues until we hit zero. Equating the right hand side to zero allows us to determine W to all adiabatic orders. Symbolically, we have

Working Equation for the Adiabatic Expansion of W

$$\frac{W''}{2W} - \frac{3}{4}\frac{W'^2}{W^2} + W^2 - k^2c_s^2 + U_s = 0, \tag{7.31}$$

as our working equation for the determination of W to all adiabatic orders.

It is now straightforward to determine W to any desired adiabatic order. We solve it up to fourth adiabatic order and see if the result suffices.

$$\frac{W''}{2W} = \frac{\omega_0''}{2\omega_0} + \left(\frac{\omega_1''}{2\omega_0} - \frac{\omega_0''\omega_1}{2\omega_0^2}\right) + \left(\frac{\omega_2''}{2\omega_0} - \frac{\omega_1''\omega_2}{2\omega_0^2} - \frac{\omega_0''\omega_2}{2\omega_0^2} - \frac{\omega_1\omega_1''}{2\omega_0^2} + \frac{\omega_0''\omega_1^2}{2\omega_0^3}\right),$$

$$-\frac{3}{4}\frac{W'^2}{W^2} = -\frac{3\omega_0'^2}{4\omega_0^2} + \left(\frac{3\omega_0'^2\omega_1}{2\omega_0^3} - \frac{3\omega_0'\omega_1'}{2\omega_0^2}\right) + \left(\frac{3\omega_0'^2\omega_2}{2\omega_0^3} - \frac{3\omega_0'\omega_2'}{2\omega_0^2} - \frac{3\omega_1'^2}{4\omega_0^2} + \frac{3\omega_0'\omega_1\omega_1'}{\omega_0^3} - \frac{9\omega_0'^2\omega_1^2}{4\omega_0^4}\right),$$

$$W^2 = 2\omega_0\omega_4 + 2\omega_1\omega_3 + 2\omega_0\omega_3 + \omega_2^2 + 2\omega_1\omega_2 + 2\omega_0\omega_2 + \omega_1^2 + 2\omega_0\omega_1 + \omega_0^2$$

We substitute these results in the working equation above for W and set the terms in the left hand side to zero order-by-order. Note that $k^2c_s^2$ is zeroth adiabatic order while $U_s \sim H^2$ is second adiabatic order.

$$\begin{aligned}
\omega_0 &= kc_s, \\
\omega_1 &= \omega_3 = 0, \\
\omega_2 &= \frac{1}{2\omega_0}\left(\frac{3\omega_0'^2}{4\omega_0^2} - \frac{\omega_0''}{2\omega_0} - U_s\right), \\
\omega_4 &= \frac{1}{2\omega_0}\left(\frac{3\omega_0'\omega_2'}{2\omega_0^2} - \frac{\omega_2''}{2\omega_0} + \frac{\omega_0''\omega_2}{2\omega_0^2} - \frac{3\omega_0'^2\omega_2}{2\omega_0^3} - \omega_2^2\right).
\end{aligned} \tag{7.32}$$

The form of ω_0 tells us that $\omega_2 \sim 1/k$ while $\omega_4 \sim 1/k^3$. As such, since

$$|v_k^{(s)}|^2 = \tfrac{1}{2}\,W^{-1}, \quad \text{and} \quad W^{-1} = \frac{1}{\omega_0} - \frac{\omega_2}{\omega_0^2} + \left(\frac{\omega_2^2}{\omega_0^3} - \frac{\omega_4}{\omega_0^2}\right), \tag{7.33}$$

in order to just sufficiently remove the divergence in the two-point function given by (7.21), we only need to find $|v_k^{(s)}|^2$ up to second adiabatic order; the term ω_4 is unnecessary. Such a scheme of using only those terms needed to remove the divergence is called the **minimal subtraction scheme**. It is crucial to consistently implement adiabatic regularization because "in general, the adiabatic expansion yields asymptotic, not convergent, series" [44]. Going beyond this would lead to arbitrariness as to the limit of the adiabatic order of the subtraction term. For the case in hand, it is also possible that the power spectrum can become negative, which is unphysical.

The truncation of $v_k^{(s)}$ leaves us with only few simple terms to calculate the subtraction term $\Delta_k^{2(s)}$. We find using the expressions for ω_0 and U_s given by the first of (7.32) and (5.23) respectively, and the definitions of the Hubble and sound flow functions given by (4.16) and (4.17),

$$\begin{aligned}
\frac{3}{4}\frac{\omega_0'^2}{\omega_0^2} &= \frac{3}{4}(aH)^2\delta_1^2, \\
-\frac{\omega_0''}{2\omega_0} &= \frac{(aH)^2}{2}(\delta_1 - \delta_1^2 + \delta_1\delta_2 - \epsilon_1\delta_1),
\end{aligned}$$

$$-U_s = -(aH)^2\Big[2-\epsilon_1+\tfrac{3}{2}\,\epsilon_2-\tfrac{1}{2}\,\epsilon_1\epsilon_2+\tfrac{1}{4}\,\epsilon_2^2+\tfrac{1}{2}\,\epsilon_2\epsilon_3+\delta_1(3-\epsilon_1+\epsilon_2+\delta_1+\delta_2)\Big],$$

$$\omega_2 = -\frac{(aH)^2}{kc_s}\Big(1-\tfrac{1}{2}\,\epsilon_1+\tfrac{3}{4}\,\epsilon_2+\tfrac{5}{4}\,\delta_1+\cdots\Big),$$

where the dots represent higher-order terms in (ϵ_1, δ_1). Using this result in the expression for $\Delta_s^{2(s)}$, up to first order in the slow-roll parameters, we get

$$\Delta_s^{2(s)} = \frac{k^3}{2\pi^2}\left|\frac{v_k^{(s)}}{z}\right|^2 = \frac{k^2}{4\pi^2 z^2 c_s}\left[1+\left(\frac{aH}{kc_s}\right)^2\Big(1-\tfrac{1}{2}\,\epsilon_1+\tfrac{3}{4}\,\epsilon_2+\tfrac{5}{4}\,\delta_1\Big)\right],$$

$$= \frac{k^2 c_s}{8\pi^2 a^2\epsilon_1}\left[1+\left(\frac{aH}{kc_s}\right)^2\Big(1-\tfrac{1}{2}\,\epsilon_1+\tfrac{3}{4}\,\epsilon_2+\tfrac{5}{4}\,\delta_1\Big)\right],$$

$$\boxed{\Delta_s^{2(s)} = \frac{H^2}{8\pi^2\epsilon_1 c_s}(1+\alpha_s),} \qquad \text{Subtraction Term (Scalar)} \tag{7.34}$$

where in the last line we have taken the limit $|kc_s/aH| \ll 1$ and $\alpha_s = -\frac{1}{2}\,\epsilon_1 + \frac{3}{4}\,\epsilon_2 + \frac{5}{4}\,\delta_1$. This is our sought-for expression for the subtraction term. In the next section, we investigate the behavior of the $\Delta_s^{2(s)}$ and its effect on the regularized power spectrum.

7.3 The Regularized Power Spectrum

Before dealing with the more general case, we consider the canonical inflation model where the speed of sound is constant; $c_s^2 = 1$. In this limit, all the Hubble flow functions vanish and the subtraction term tends to

$$\Delta_s^{2(s)}\Big|_{c_s=1} = \frac{H^2}{8\pi^2\epsilon_1}\Big(1-\tfrac{1}{2}\,\epsilon_1+\tfrac{3}{4}\,\epsilon_2\Big). \tag{7.35}$$

The "bare" power spectrum is given by (6.26),

$$\Delta_s^{2(b)}\Big|_{c_s=1} = \frac{H_*^2}{8\pi^2\epsilon_{1*}}(1+\mu_{s*}), \tag{7.36}$$

where $\mu_{s*} \equiv (2\epsilon_{1*}+\epsilon_{2*})(2-\gamma-\ln 2)-2\epsilon_{1*}$. Observe that it has the same form as that of the subtraction term; the main difference is that it is a constant.

We subtract from this constant expression the quantity $\Delta_s^{2(s)}$ and gain the regularized power spectrum,

$$\Delta_s^{2(r)}\Big|_{c_s=1} = \frac{H_*^2}{8\pi^2\epsilon_{1*}}\left[1+\mu_{s*}-\left(1-\tfrac{1}{2}\,\epsilon_1+\tfrac{3}{4}\,\epsilon_2\right)\frac{H^2}{H_*^2}\frac{\epsilon_{1*}}{\epsilon_1}\right]. \tag{7.37}$$

This is the same result derived by Urakawa and Starobinsky [87]. In essence, our work is a generalization of their calculation to the case of general single-field inflation wherein $c_s^2 = 1$. Their analysis of the adiabatic regularization in the canonical case indicates that the subtraction term decays with the expansion of the Universe mainly during inflation. To see this, note that for the factor involving the Hubble parameter inside the pair of square brackets in the equation for $\Delta_s^{2(r)}$ above,

$$\epsilon_1 = -\frac{\dot{H}}{H^2} = -\frac{1}{H}\frac{\mathrm{d}H}{\mathrm{d}N}, \tag{7.38}$$

where we have used the definition $\mathrm{d}N \equiv \mathrm{d}\ln a$ in the second equality. In effect,

$$\left(\frac{H}{H_*}\right)^2 = \exp\left(-2\int_{N_*}^{N}\mathrm{d}\tilde{N}\,\epsilon_1(\tilde{N})\right). \tag{7.39}$$

Furthermore, for the factor involving the first slow-roll parameter, because $\dot{\epsilon}_1 = H\epsilon_1\epsilon_2$, then

$$\frac{\epsilon_1}{\epsilon_{1*}} = \exp\left(\int_{N_*}^{N}\mathrm{d}\tilde{N}\,\epsilon_2(N)\right). \tag{7.40}$$

The product of the last two expressions above is then simply

$$\left(\frac{H}{H_*}\right)^2\left(\frac{\epsilon_1}{\epsilon_{1*}}\right) = \exp\left(-\int_{N*}^{N}\mathrm{d}\tilde{N}\,(2\epsilon_1+\epsilon_2)\right). \tag{7.41}$$

Now, during inflation, ϵ_1 goes from near 0 to unity marking the end of inflation. On the other hand, consistent with this behavior of ϵ_1, the second slow-roll parameter must be positive on average. As such, the product above exponentially decays with the number of e-folds.[7] Consequently, the subtraction term also exponentially decays and the regularized power spectrum tends to the "bare" power spectrum. Hence, if we follow the subtraction term long enough with

[7] Post inflation, the product can continue to decrease even with vanishing ϵ_2 because ϵ_1 can stay near unity and the Universe can continue to expand for some time.

the evolution of the Universe, we eventually ends up with the "bare" power spectrum.

Now suppose the speed of sound is not constant. Then the "bare" power spectrum can be written as

$$\Delta_s^{2(b)} = \frac{H_*^2}{8\pi^2\epsilon_{1*}c_{s*}}(1+\mu_{cs*}), \tag{7.42}$$

where μ_{cs*} is a correction involving the Hubble- and sound-flow parameters. On the other hand, the subtraction term is generalized to that given by the third of (7.34). We can then write the regularized power spectrum as

Regularized Power Spectrum (Scalar Perturbation)

$$\Delta_s^{2(r)} = \frac{H_*^2}{8\pi^2\epsilon_{1*}c_{s*}}\left[1+\mu_{cs*}-(1+\alpha_s)\frac{H^2}{H_*^2}\frac{\epsilon_{1*}}{\epsilon_1}\frac{c_{s*}}{c_s}\right]. \tag{7.43}$$

Scale Invariance and the Speed of Sound

The effect of the generalization of the Lagrangian from $X-V$ to the functional $P(X,\phi)$ is reflected in the presence of the speed of sound. In view of the adiabatic regularization, all the complications are shouldered by the behavior of c_s present in the subtraction term. We thus need to find the dependence of c_s on the number of e-folds in a similar way we did for H and ϵ_1. Unlike that of H and ϵ_1 however, due to the wide array of possibilities for the general function $P(X,\phi)$, we have a seemingly limitless number of choices for c_s. To evade this "paradox of choice," we invoke symmetry in the form of **scale invariance**. Following the idea of Khoury and Piazza [88] we determine the simplest condition on c_s so that the power spectrum is *exactly* scale-invariant. Then after this, we relax the condition to accommodate the more realistic condition of *near* scale-invariance.

To proceed, we go back to the second-order action for the scalar perturbation given by (5.4) and rewrite it as follows:

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}\tau\,\mathrm{d}^3\mathbf{x}\,z^2(\zeta'^2 - c_s^2\zeta_{,i}\zeta^{,i}); \quad \left(z^2 = 2a^2\epsilon/c_s^2\right)$$

$$= \frac{1}{2}\int \mathrm{d}\tau\, \mathrm{d}^3\mathbf{x}\left(\frac{2a^2\epsilon}{c_s^2}\right)\left[\left(\frac{\mathrm{d}\zeta}{\mathrm{d}\tau}\right)^2 - c_s^2\zeta_{,i}\zeta^{,i}\right]; \quad (\mathrm{d}y \equiv c_s\mathrm{d}\tau),$$

$$= \frac{1}{2}\int \mathrm{d}y\, \mathrm{d}^3\mathbf{x}\left(c_s\frac{2a^2\epsilon}{c_s^2}\right)\left[\left(\frac{\mathrm{d}\zeta}{\mathrm{d}y}\right)^2 - \zeta_{,i}\zeta^{,i}\right]; \qquad (q \equiv z\sqrt{c_s}),$$

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}y\, \mathrm{d}^3\mathbf{x}\, q^2\left[\left(\frac{\mathrm{d}\zeta}{\mathrm{d}y}\right)^2 - \zeta_{,i}\zeta^{,i}\right]. \tag{7.44}$$

In the derivation of the original Mukhanov-Sasaki equation, we took $v = z\zeta$; here, we take $\tilde{v} = q\zeta$. In effect,

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}y\, \mathrm{d}^3\mathbf{x}\left[\left(\frac{\mathrm{d}\tilde{v}}{\mathrm{d}y}\right)^2 - \frac{2\tilde{v}}{q}\frac{\mathrm{d}q}{\mathrm{d}y}\frac{\mathrm{d}v}{\mathrm{d}y} + \frac{\tilde{v}^2}{q^2}\left(\frac{\mathrm{d}q}{\mathrm{d}y}\right)^2 - \tilde{v}_{,i}\tilde{v}^{,i}\right],$$

$$= \frac{1}{2}\int \mathrm{d}y\, \mathrm{d}^3\mathbf{x}\left[\left(\frac{\mathrm{d}\tilde{v}}{\mathrm{d}y}\right)^2 - \frac{2\tilde{v}}{q}\frac{\mathrm{d}q}{\mathrm{d}y}\frac{\mathrm{d}v}{\mathrm{d}y} - \tilde{v}^2\frac{\mathrm{d}q}{\mathrm{d}y}\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{1}{q}\right) - \tilde{v}_{,i}\tilde{v}^{,i}\right],$$

$$S^{(2)} = \frac{1}{2}\int \mathrm{d}y\, \mathrm{d}^3\mathbf{x}\left[\left(\frac{\mathrm{d}\tilde{v}}{\mathrm{d}y}\right)^2 + \frac{\tilde{v}^2}{q}\frac{\mathrm{d}^2q}{\mathrm{d}y^2} - \tilde{v}_{,i}\tilde{v}^{,i}\right]. \tag{7.45}$$

It is then straightforward to determine the equation of motion for $\tilde{v}$ from the last equation above. In Fourier space we have

$$\frac{\mathrm{d}^2\tilde{v}_k}{\mathrm{d}y^2} + \left[k^2 - \frac{1}{q}\frac{\mathrm{d}^2q}{\mathrm{d}y^2}\right]\tilde{v}_k = 0. \tag{7.46}$$

A scale-invariant power spectrum results when

$$\frac{1}{q}\frac{\mathrm{d}^2q}{\mathrm{d}y^2} = \frac{2}{y^2}. \tag{7.47}$$

Indeed, when the above condition holds, we have the analytic solution given by (see **Sec. 5.1** for a similar calculation)

$$\tilde{v}_k(y) = \frac{1}{\sqrt{2k}}\left(1 - \frac{i}{ky}\right)e^{-iky}, \tag{7.48}$$

which gives

$$\frac{\mathrm{d}}{\mathrm{d}\ln k}\ln(k^3|v_k|^2) = 0, \tag{7.49}$$

in the limit $k \to 0$.

There are two solutions to the differential equation above for q namely,[8]

$$q \sim -\frac{1}{y} \quad \text{and} \quad q \sim y^2. \tag{7.50}$$

If we assume that the relative rate of change of the speed of sound is constant, that is,

$$\delta \equiv \frac{\dot{c}_s}{H c_s} = \text{constant}, \tag{7.51}$$

and ϵ is also constant, then the scale factor and the speed of sound are constrained to take the form [88]

$$a(y) \sim (-y)^{\frac{1}{\delta+\epsilon-1}} \quad \text{and} \quad c_s(y) \sim (-y)^{\frac{\delta}{\delta+\epsilon-1}}, \tag{7.52}$$

respectively. For the first relation involving a, note that when $\delta \to 0$ and $\epsilon \to 0$, then $a \sim -\tau^{-1} \sim aH$, implying that $H =$ constant, consistent with the inflationary setting $\epsilon \approx 0$. For the second relation involving c_s, the limit $\delta \to 0$ corresponds to $c_s \sim$ constant, as it should be.

The relationship for the scale factor follows from the definition of ϵ and δ, and their constancy. It can be derived in a two-step process involving the calculation of H starting with ϵ and then using the relationship between a and c_s through the definition of δ in the resulting expression for H to finally find a.

$$\begin{aligned}
\epsilon \equiv -\frac{\dot{H}}{H^2} &= -\frac{1}{H^2}\frac{\mathrm{d}H}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t}, \\
&= -\frac{1}{H^2}\frac{\mathrm{d}H}{\mathrm{d}y}\frac{c_s}{a}; \quad \left(\delta \equiv \frac{\dot{c}_s}{H c_s} = \frac{1}{H c_s}\frac{\mathrm{d}c_s}{\mathrm{d}y}\frac{c_s}{a}\right), \\
-\frac{1}{H}\frac{\mathrm{d}H}{\mathrm{d}y} &= \left(\frac{1}{c_s}\frac{\mathrm{d}c_s}{\mathrm{d}y}\right)\frac{\epsilon}{\delta}, \\
\frac{H}{H_0} &= \left(\frac{c_{s,0}}{c_s}\right)^{\frac{\epsilon}{\delta}}.
\end{aligned} \tag{7.53}$$

Here, the subscript 0 denotes the time $y = 0$. Next, we find an expression

[8] Since y runs from $-\infty$ to zero, $q \geq 0$ for both solutions above.

relating c_s and a through the definition of δ.

$$\begin{aligned}
\delta &= \frac{1}{Hc_s}\frac{\mathrm{d}c_s}{\mathrm{d}y}\frac{c_s}{a} = \frac{1}{\dot{a}}\frac{\mathrm{d}c_s}{\mathrm{d}y}, \\
\frac{1}{c_s}\frac{\mathrm{d}c_s}{\mathrm{d}y} &= \frac{\delta}{a}\frac{\mathrm{d}a}{\mathrm{d}y}, \\
c_s &= c_{s,0}\left(\frac{a}{a_0}\right)^{\delta}
\end{aligned} \tag{7.54}$$

We then use this result in the equation for H above.

$$\begin{aligned}
\frac{H}{H_0} &= \left(\frac{c_{s,0}}{c_s}\right)^{\frac{\epsilon}{\delta}}, \\
\frac{1}{a}\frac{\mathrm{d}a}{\mathrm{d}y}\frac{c_s}{a} &= H_0\left(\frac{c_{s,0}}{c_s}\right)^{\frac{\epsilon}{\delta}}, \\
\frac{1}{a^2}\frac{\mathrm{d}a}{\mathrm{d}y} &= H_0(c_{s,0})^{\frac{\epsilon}{\delta}}(c_s)^{-1-\frac{\epsilon}{\delta}}, \\
\frac{1}{a^2}\frac{\mathrm{d}a}{\mathrm{d}y} &= \frac{H_0}{c_{s,0}}\left(\frac{a}{a_0}\right)^{-\delta-\epsilon}, \\
(a_0)^{-\delta-\epsilon}\int_{a_0}^{a}\mathrm{d}a\, a^{\epsilon+\delta-2} &= \int_0^y \mathrm{d}y\,\frac{H_0}{c_{s,0}}, \\
\frac{1}{a_0}\frac{1}{\delta+\epsilon-1}\left[\left(\frac{a}{a_0}\right)^{\delta+\epsilon-1}-1\right] &= y\frac{H_0}{c_{s,0}}, \\
\left(\frac{a}{a_0}\right)^{\delta+\epsilon-1} - 1 &= (-y)\frac{a_0H_0}{c_{s,0}}(1-\delta-\epsilon)
\end{aligned} \tag{7.55}$$

This gives us the desired result $a(y) \sim (-y)^{\frac{1}{\delta+\epsilon-1}}$ for large $(-y)$ corresponding to the inflationary period. Note that although we have used $y = 0$ (for simplicity) as a reference time in the calculation above for a, far beyond the inflationary period, the relation $a(y) \sim (-y)^{\frac{1}{\delta+\epsilon-1}}$ no longer holds; the behavior of a depends on the presence of radiation and/or matter after inflation.

For the speed of sound, we use the intermediate result above for the derivation for a given by the third of (7.54). We have

$$c_s \sim a^{\delta} \sim (-y)^{\frac{\delta}{\delta+\epsilon-1}}, \tag{7.56}$$

which was to be shown.

With the analytic expressions for the scale factor and the speed of sound in terms of y, ϵ, and δ in hand, let us find the consequence of the condition of exact scale invariance given by the differential equation for q; c.f.(7.47). From the first of (7.50) we have

$$\begin{aligned} q &\sim (-y)^{-1}, \\ \frac{a\sqrt{2\epsilon}}{\sqrt{c_s}} &\sim (-y)^{-1}, \\ \frac{a}{\sqrt{c_s}} \sim y^{-\frac{\delta-2}{2(\delta+\epsilon-1)}} &\sim (-y)^{-1}, \\ -1 &= \frac{2-\delta}{2(\delta+\epsilon-1)}, \\ \boxed{\delta &= -2\epsilon.} \end{aligned} \tag{7.57}$$

This relationship ties the rate of change of the speed of sound and the slow-roll parameter together. By virtue of the first of (7.52) expressing the dependence of a on y and the definition of δ, we see that it corresponds to an *expanding* universe $[a \sim (-y)^{\frac{-1}{1+\epsilon}}]$ with a *decreasing* speed of sound. In the limit $\delta \to 0$, the quantity ϵ also approaches zero giving us a perfect de Sitter space.

The other solution to the differential equation for q namely, $q \sim y^2$, leads to the relation between δ and ϵ given by [88]

$$\delta = \frac{2}{5}(3 - 2\epsilon). \tag{7.58}$$

For $0 < \epsilon < \frac{3}{2}$, the speed of sound is *increasing*. Furthermore, by virtue of the first of (7.52), the scale factor *decreases* with time $[a \sim (-y)^{\frac{5}{\epsilon}}]$—the universe is contracting. We will be setting aside this second possibility and focus on the more realistic solution above where $\delta = -2\epsilon$, in our analysis of the subtraction term for the power spectrum.

Behavior of the Regularized Scalar Power Spectrum

The condition of exact scale invariance, $\delta = -2\epsilon_1 = \text{const}$, gives us a good framework to relate the speed of sound with the number of e-folds in the way

we did for ϵ_1 and H. However, we cannot use this expression the way it is because it completely "entangles" δ and ϵ. When we consider the limit $\delta \to 0$ for instance, it also forces ϵ_1 to vanish. Physically, this is problematic because a constant speed of sound—something not necessarily unphysical—implies a never ending inflation. For this reason, we relax the mentioned condition with an addition of a correction β describing the deviation from exact scale invariance. Furthermore, we generalize the relationship such that both δ and ϵ depend on time. Symbolically,

$$\delta(\tau) = -2\epsilon_1(\tau) + \beta(\tau). \tag{7.59}$$

We take β to be at least $\mathcal{O}(\epsilon^2)$ when δ is away from zero so that $\delta \approx -2\epsilon_1$. When $\delta \to 0$, β grows to $2\epsilon_1$. In the usual calculation of the power spectrum (involving only the "bare" part), the above relationship implies that the spectral tilt,

$$n_s - 1 \equiv \frac{\mathrm{d}\ln \Delta_s^2(k)}{\mathrm{d}\ln k}, \tag{7.60}$$

using the usual slow-roll approximation, is $n_s = -2\epsilon_1 - \delta - \epsilon_2$ [88] in accord with existing results in the literature [2, 89].

With the above near-scale-invariant condition for δ, the evolution of the speed of sound with respect to the number of e-folds can be calculated as

$$\begin{aligned} \frac{\dot{c}_s}{c_s H} &= -2\epsilon_1 + \beta, \\ \int_{N_*}^{N} \frac{\mathrm{d}c_s}{c_s} &= \int_{N_*}^{N} \mathrm{d}\tilde{N}\,(-2\epsilon_1 + \beta), \\ \frac{c_{s*}}{c_s} &= \exp\left(\int_{N_*}^{N} \mathrm{d}\tilde{N}\,(2\epsilon_1 - \beta)\right). \end{aligned} \tag{7.61}$$

Referring back to the expression for the regularized power spectrum given by (7.43) and the expressions for H and ϵ_1 given by (7.39) and (7.40) respectively, we find that the integral involving ϵ_1 in the last equation above is exactly canceled by that coming from the equation for H. The regularized power spectrum then becomes

$$\Delta_s^{2(r)} = \frac{H_*^2}{8\pi^2 \epsilon_{1*} c_{s*}} \left[1 + \mu_{cs*} - (1 + \alpha_s) \exp\left(-\int_{N*}^{N} \mathrm{d}\tilde{N}\,(\epsilon_2 + \beta)\right)\right]. \tag{7.62}$$

On average if not monotonically, the first slow-roll parameter grows with N during inflation. It follows that the second slow-roll parameter is positive because $\mathrm{d}\epsilon_1/\mathrm{d}N = \epsilon_1\epsilon_2$, by definition. In general, $\beta \sim \mathcal{O}(\epsilon^2)$ unless $\delta \to 0$ in which case the regularized power spectrum given by (7.43) or (7.62) above tends to that of the canonical case. Consequently, the second term inside the pair of square brackets in the last equation above is exponentially decaying with N. Similar to that of the canonical case, if we follow the subtraction term long enough after horizon crossing, it becomes negligible and the regularized power spectrum tends to the "bare" power spectrum.

In retrospect, the adiabatic regularization of the power spectrum was proposed by Parker[9] [90] following a successful application of the technique he and Fulling [81] pioneered several decades ago in taming the divergence of the energy-momentum tensor in curved spacetime. He reported a "very significant correction (of several orders of magnitude) to the predicted amplitude of the power spectrum." This unorthodox prediction has called the attention of several researchers in the field. Durrer, Marozzi, and Rinaldi [94] casting doubt on the application of adiabatic regularization on the power spectrum, argued that "adiabatic expansion does not seem physically meaningful" in the far-infrared regime because at this regime, the expansion of the Universe is not adiabatic. In a review paper by Bastero-Gil et al [95], they pointed out that since $\mathbf{x} \neq \mathbf{y}$ in practical applications involving the CMB, then there is no need to perform adiabatic regularization. In a separate paper, Finelli et al [96] performed a calculation demonstrating that adiabatic regularization utilizing up to fourth adiabatic order can lead to negative power spectrum; thus, giving another blow against the use of adiabatic regularization.

The three main points above starting with the group of Durrer, are all against the use of adiabatic regularization thus, aiming to restore the power spectrum that way it is. Although the end seems consistent with the agreement between theory and experiment as the "bare" power spectrum is the one used in standard calculations, the arguments in support to fulfill this aim seem to have some deficiencies.[10] First, consistency calls that adiabatic regularization be applied following the minimal subtraction scheme. This is so because

[9] For follow-up and related investigations by the group of Parker, see refs. [91, 92, 93].

[10] Here, we are not going to present a full argumentative defense of the use of adiabatic regularization but leave some words for our chosen reconciliatory position that adiabatic regularization may be necessary albeit it may not have any effect at all.

the adiabatic expansion is in general, not convergent but only asymptotic. Going beyond the minimal subtraction scheme begs the question concerning the appropriate adiabatic order to use beyond those that only cause divergence problem. Naturally, a negative power spectrum may be expected when one truncates the subtraction beyond that prescribed by the minimal subtraction scheme. Second, the limitation imposed by the condition $\mathbf{x} \neq \mathbf{y}$ is only as good as the number of practical applications that it can correspond to. The divergence in the coincidence limit is indeed, unphysical but it is a mathematical defect in our calculations that cannot simply be evaded by the existence of few cases where such a limit may not hold. Moreover, the inclusion of self-interactions in the two-point function definitely calls for regularization. Third and last, deciding whether to apply adiabatic regularization or not depending on the value of k seems to put an unnecessary complication whenever we deal with quantities in Fourier space. This calls for a difficult auxiliary condition on top of an otherwise simple and sound method, that should determine a definite cut on the range of k beyond which one can decidedly apply or not to apply the adiabatic regularization.

Here, following the lead by Urakawa and Starobinsky, we take a different stand that adiabatic regularization may be necessary. As what we have seen however, in the canonical case and in its extension to the case of general single-field inflation, the subtraction term exponentially decays with the expansion of the Universe leaving us with only the "bare" power spectrum. The key as pointed out by Urakawa and Starobinsky is to go beyond the horizon crossing and follow the subtraction term long enough as the Universe expands. On physical ground, the result $\Delta^{2(r)} \to \Delta_s^{2(b)}$ with increasing N might be expected from the beginning if adiabatic regularization is to be considered a consistent method of removing infinities. We recall that it is a form of UV regularization. As such, it seems justified to think that it can only affect the UV modes.[11] Hence, the power spectrum "constituted" by frozen superhorizon modes should in the long run be unaffected by a subtraction process aiming to remove UV divergence; inflation washes out the subtraction term. This way of seeing things reconcile two seemingly conflicting points namely, (a) the adiabatic regularization of two-point functions in the coincidence limit extends to the power spectrum as

[11] Although this seems a reasonable claim, we have so far only shown this to be valid for the cases we have investigated so far in this chapter. In the next chapter, we deal with a non-minimally coupled inflation model where the Lagrangian includes a term involving the inflaton explicitly coupled to gravity; ie., ϕR where R is the Ricci scalar.

argued by Parker and his collaborators, but (b) the regularized power spectrum is simply the "bare" power spectrum for large enough N in agreement with the idea that the physical power spectrum is simply the "bare" power spectrum as implicitly/explicitly assumed or taken by the group of Durrer, Bastero-Gil, and Finelli.

Adiabatic Regularization of the Tensor Power Spectrum

The calculation in **Sec. 5.3** for the tensor two-point function given by (5.105) tells us that

$$\langle \hat{\gamma}_{ij}(\tau, \mathbf{x}_1)\hat{\gamma}^{ij}(\tau, \mathbf{x}_2)\rangle = \int \frac{\mathrm{d}k}{k}\frac{\sin k|\mathbf{x}_1 - \mathbf{x}_2|}{k|\mathbf{x}_1 - \mathbf{x}_2|}\Delta_t^2(k, \tau), \tag{7.63}$$

where the tensor power spectrum is given by (5.106) namely,[12]

$$\Delta_t^2(k, \tau) = \frac{2k^3}{\pi^2}\left|\frac{u_k(\tau)}{a}\right|^2, \tag{7.64}$$

and u_k satisfies the Mukhanov-Sasaki equation for tensor perturbations given by (5.101), namely,

$$u_k'' + \left(k^2 - U_t\right)u_k = 0. \qquad \left(U_t = \frac{a''}{a}\right) \tag{7.65}$$

Similar to that of the scalar perturbation, in the coincidence limit $\mathbf{x} \to \mathbf{y}$, the two-point function diverges owing to the contribution of the short-wavelength modes. To see this, note that for very-large wavenumber, the solution of the Mukhanov-Sasaki equation above indicates $\Delta_t^2(k, \tau) \sim k$. As such, the integral above is quadratically divergent in k. This calls for some form of regularization for a physically meaningful two-point function. Such a regularization is then reflected in the tensor power spectrum.

The adiabatic regularization of the tensor power spectrum has already been carried out by Urakawa and Starobinsky for the case of canonical inflation. The generalization to general single-field inflation where $X - V \to P(X, \phi)$, adds nothing new to the result of their investigation because the second-order action is the same; the Mukhanov-Sasaki equation for tensor perturbations does not

[12] Here, we assume to have already taken the summation over the polarization modes thus, we simply write u_k instead of u_k^s; see **Sec. 5.4**.

involve c_s^2 (or more formally, the speed of sound c_t^2 for tensor perturbations is unity). Nevertheless, we find this chapter somewhat incomplete without at least including the basic calculation and results. We have the framework in place and it should be straightforward to do the derivation following an approach similar to that of the scalar perturbation.

To find the subtraction term we exploit the fact that the Mukhanov-Sasaki equations for scalar and tensor perturbations have exactly the same form; the only important differences are the absence of c_s and the potential is the less complicated $U_t = a''/a$ instead of $U_s = z''/z$. As such, to find W following the ansatz

$$u_k^{(s)}(\tau) = \frac{1}{\sqrt{W(\tau)}} e^{-i\int^\tau \mathrm{d}\tilde{\tau} W(\tilde{\tau})}, \tag{7.66}$$

we borrow the working equation for scalar perturbation given by (7.31) and replace c_s by unity and U_s by U_t.

Working Equation for the Adiabatic Expansion of W (Tensor Perturbations)

$$\frac{W''}{2W} - \frac{3}{4}\frac{W'^2}{W^2} + W^2 - k^2 + U_t = 0, \tag{7.67}$$

The expansion $W = \omega_0 + \omega_1 + \omega_2 + \cdots$ together with the working equation above then leads to the identifications

$$\omega_0 = k, \quad \omega_1 = \omega_3 = 0, \quad \omega_2 = -\frac{U_t}{2\omega_0}, \tag{7.68}$$

which in turn, give us up to second adiabatic order,

$$\begin{aligned} |u_k^{(s)}|^2 &= W^{-1} = \frac{1}{\omega_0} - \frac{\omega_2}{\omega_0^2}, \\ |u_k^{(s)}|^2 &= \frac{1}{k} + (2-\epsilon_1)\frac{(aH)^2}{2k^3}. \end{aligned} \tag{7.69}$$

Following the form of the "bare" power spectrum with $u_k^{(b)}$ to be replaced by $u_k^{(s)}$ we find

$$\Delta_t^{2(s)} = \frac{2k^3}{\pi^2}\left|\frac{u_k^{(s)}}{a}\right|^2,$$

$$= \frac{2k^2}{a^2\pi^2}\left[1 + (1 - \tfrac{1}{2}\,\epsilon_1)\frac{(aH)^2}{k^2}\right],$$

$$\Delta_t^{2(s)} = \frac{2H^2}{\pi^2}\Big(1 - \tfrac{1}{2}\,\epsilon_1\Big), \qquad \text{Subtraction Term (Tensor)} \tag{7.70}$$

where in the last line we have taken the superhorizon limit, $k/aH \ll 1$.

On the other hand, the "bare" power spectrum has already been solved in **Sec. 6.1**.

$$\Delta_t^{2(b)} = \frac{2H_*^2}{\pi^2}(1 + \mu_{t*}) \tag{7.71}$$

Taking the difference of $\Delta_t^{2(b)}$ and $\Delta_t^{2(s)}$ gives us the regularized power spectrum.

Regularized Power Spectrum (Tensor Perturbation)

$$\Delta_t^{2(r)} = \frac{2H_*^2}{\pi^2}\left[1 + \mu_{t*} - \Big(1 - \tfrac{1}{2}\,\epsilon_1\Big)\frac{H^2}{H_*^2}\right]. \tag{7.72}$$

In comparison to that of the scalar perturbation, the factors ϵ_{1*}/ϵ_1 and c_{s*}/c_s accompanying H^2/H_*^2 are absent making this much easier to analyze. In fact, since the behavior of H has already been spelled out above, c.f. (7.39), we do not need to perform any additional calculation at all. The last term inside the pair of square brackets in the expression for $\Delta_t^{2(r)}$ above exponentially decays with the number of e-folds. As the expansion of the Universe (during and right after inflation) washes out the subtraction term, the regularized power spectrum tends to the bare power spectrum.

CHAPTER

8

Adiabatic Regularization of Power Spectra in Nonminimally Coupled Chaotic Inflation[97]

His soul is infected with a disease called vanity;
Enlarged head and fixated eyes looking always down.
Play by the rules, nonminimally coupled with the academe,
Eternal damnation, regularize him away...

Holloine Nickaulaus
The Mechanism of the Devil, 1868

8.1 Minimally Coupled Chaotic Inflation

8.2 Nonminimally Coupled Chaotic Inflation

8.3 The "Bare" Power Spectrum

8.4 Adiabatic Regularization of Power Spectra

8.5 Implications of Differing Regularized and "Bare" Power Spectra

From a field-theoretic perspective, it is obvious that gravity couples with matter; otherwise, the gravitational attraction between two objects would be improbable. Starting from the second chapter up until the previous chapter, we have been mainly dealing with single-field inflation where the coupling between matter and gravity is "implicit." In this last chapter, we explore the case when such a coupling is "explicit," termed more formally as nonminimal coupling. Within the framework of adiabatic regularization, the question we tackle involves the regularization of the power spectra. As we shall see, the divergence in the two-point function of primordial cosmological perturbations is left unaffected by the addition of nonminimal coupling term. For this reason, we investigate how the adiabatic subtraction could affect one of most important quantities in inflationary cosmology—the power spectrum.

8.1 Minimally Coupled Chaotic Inflation

In **Sec. 2.3** we introduced the canonical inflation model through the action[1]

$$S = \frac{1}{2}\int \mathrm{d}^4x\sqrt{-g}\left[M_{\mathrm{Pl}}^2 R - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V(\phi)\right], \tag{8.1}$$

and the two slow-roll conditions $\epsilon \ll 1$ and $|\eta| \ll 1$ where

$$\epsilon \equiv -\frac{\dot{H}}{H^2}, \qquad \eta \equiv \epsilon - \frac{1}{2H}\frac{\dot{\epsilon}}{\epsilon}, \tag{8.2}$$

The first inequality constrains H to be nearly constant telling us that inflation is a quasi-de Sitter (accelerated) expansion while the second inequality ensures that the Hubble friction term in the equation of motion for the inflaton is large enough to prolong inflation.

In the following calculation, we explicitly relate the two slow-roll parameters ϵ and η to the derivatives of the potential (first-order and second-order) through two new slow-roll parameters defined in terms of these derivatives. Following this calculation is an introduction to the notion of chaotic inflation utilizing the important ideas in the example below.



Example 1. ***Slow-Roll Parameters in Terms of the Potential.*** Let us define two new slow-roll parameters ϵ_V and η_V in terms of the derivative(s) of the potential $V(\phi)$.

$$\epsilon_V \equiv \frac{M_{\mathrm{Pl}}^2}{2}\left(\frac{V_{,\phi}}{V}\right)^2, \qquad \eta_V \equiv M_{\mathrm{Pl}}^2\frac{V_{,\phi\phi}}{V}. \tag{8.3}$$

Show that $\epsilon_V \approx \epsilon$ and $\eta_V \approx \eta + \epsilon$ in the slow-roll approximation.

Solution. The slow-roll parameter ϵ can be related to ϵ_V through the equation of motion for ϕ containing $V_{,\phi}$.

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = 0. \tag{8.4}$$

[1] In this chapter, we make the Planck mass $M_{\mathrm{Pl}}^2 = (8\pi G)^{-1} \approx 2.4 \times 10^{18}\,\mathrm{GeV}$ explicit to easily compare energy values.

During inflation, the friction term dominates over the first term in the left hand side; that is, $\dot{\phi} \approx -V_{,\phi}/3H$. On the other hand, $\dot{H}$ in the definition of ϵ can be related to $\dot{\phi}$ through the relationship between pressure and energy density, and $\dot{H}$.

$$\begin{aligned}
\dot{H} &= -\tfrac{1}{2}\, M_{\rm Pl}^{-2}(\rho + p), \\
&= -\tfrac{1}{2}\, M_{\rm Pl}^{-2}\Big(\tfrac{1}{2}\,\dot{\phi}^2 + V + \tfrac{1}{2}\,\dot{\phi}^2 - V\Big), \\
\dot{H} &= -\tfrac{1}{2}\, M_{\rm Pl}^{-2}\dot{\phi}^2, \\
\epsilon &= \frac{\dot{\phi}^2}{2M_{\rm Pl}^2 H^2}.
\end{aligned} \tag{8.5}$$

The last two results above for ϵ and $\dot{\phi}$ together with the first Friedmann equation,

$$H^2 = \frac{\rho}{3M_{\rm Pl}^2} \approx \frac{V}{3M_{\rm Pl}^2}, \tag{8.6}$$

then yield

$$\epsilon \approx \frac{M_{\rm Pl}^2}{2}\left(\frac{V_{,\phi}}{V}\right)^2 = \epsilon_V, \tag{8.7}$$

which was to be shown.

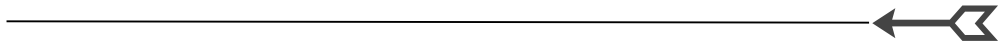
To establish the approximation $\eta_V \approx \eta + \epsilon$, we start again with the equation of motion for ϕ where we can get $V_{,\phi\phi}$ in the definition of η_V.

$$\begin{aligned}
3H\dot{\phi} &\approx -V_{,\phi}, \\
3\dot{H}\dot{\phi} + 3H\ddot{\phi} &\approx -V_{,\phi\phi}\dot{\phi}, \\
-3\epsilon + \frac{3\ddot{\phi}}{H\dot{\phi}} &= -\frac{V_{,\phi\phi}}{H^2}.
\end{aligned} \tag{8.8}$$

Based on the last of (2.32), we know that $\eta = -\ddot{\phi}/H\dot{\phi}$. As such, upon invoking the first Friedmann equation again, we find

$$-3\epsilon - 3\eta \approx -3M_{\rm Pl}^2\frac{V_{,\phi\phi}}{V} \quad \Rightarrow \quad \eta_V \approx \eta + \epsilon, \tag{8.9}$$

which was to be shown.



Based on the above calculation, the slow-roll conditions $\epsilon, |\eta| \ll 1$, constrain the form of the potential through the corresponding conditions $\epsilon_V, |\eta_V| \ll 1$. If the magnitudes of the first and second derivatives of the potential are very small, (or more formally, ϵ_V, $|\eta_V| \ll 1$,) then this is suggestive of an almost flat potential. Or, even if it might not be almost flat, our pair of constraints seems to call for a special condition on the potential that is correspondingly reflected in its argument ϕ, to initiate and sustain inflation making it quite unnatural.

One way to solve this possible **naturalness** problem is to declare that the special condition (or set of conditions) on the potential is not unnatural; thus, denying that the problem exists. Based on the **anthropic principle** [98], the Universe is the way it is and the way it was because otherwise, we would not be here. In other words, the existence of man may be seen as a testament of the fine-tuned conditions necessary for his emergence and life. Following this reasoning, one may then think that if there had been no such special potential in the past satisfying the pair of constraints ϵ_V, $|\eta_V| \ll 1$, then we would not be here today.

This resolution although quite interesting due to its simplicity, looks too simple that it is *simpler* (in reference to the quote "Everything should be made as simple as possible but not simpler.") The anthropic principle as applied at least to the current problem, seems to cut our pursuit of inquiry that could otherwise give us a better understanding of the machinery of the Universe, by essentially denying the existence of a problem. If at all possible, we do not want to default to this resolution.

Another way to solve the problem of unnaturalness mentioned above is through **chaotic inflation** put forward by Linde [18]. In the literature, this is also often called **large-field inflation** for a reason that will become apparent in a short while. Suppose for the sake of argument, we assume that

$$V(\phi) = M_{\rm Pl}^4 \frac{\lambda}{2n} \left(\frac{\phi}{M_{\rm Pl}} \right)^n , \tag{8.10}$$

where λ is a coupling constant. Then the condition $\epsilon_V \ll 1$ implies

$$\epsilon_V \equiv \frac{M_{\rm Pl}^2}{2}\left(\frac{V_{,\phi}}{V}\right)^2 = \frac{n^2}{2}\frac{M_{\rm Pl}^2}{\phi^2} \ll 1,$$
$$\phi \gg \frac{n}{\sqrt{2}} M_{\rm Pl}, \tag{8.11}$$

This means that the condition $\epsilon_V \ll 1$ can be realized even if the potential is not apparently flat. For potentials polynomial in the scalar field, inflation can happen as a large-field inflation. In particular, by large, the above inequality indicates that ϕ should be super-Planckian for a quasi-de Sitter expansion characteristic of inflation to occur.

At first sight, a super-Planckian field seems conceptually dangerous as we do not have a suitable quantum theory of gravity yet. However, this is permissible within the domain of applicability of general relativity as long as we require the potential to be sub-Planckian; i.e., $V(\phi) \ll M_{\rm Pl}^4$. Under this condition, the field ϕ is further restricted by the inequality $\phi \ll M_{\rm Pl}(2n/\lambda)^{1/n}$. As such,

$$\frac{n}{\sqrt{2}} M_{\rm Pl} \ll \phi \ll M_{\rm Pl}\left(\frac{2n}{\lambda}\right)^{\frac{1}{n}}. \tag{8.12}$$

Inflation starts with a large value of ϕ and then it decreases halting the accelerated expansion at some small field value (see **Fig. 8.1**).

Linde imagines that the Universe was initially in a chaotic quantum state. In such a state, due to quantum fluctuations, ϕ can take on more or less "random" values. Now, there could exist a small region of space where "accidentally" ϕ could be much larger than the Planck mass; thus, satisfying the condition $\epsilon_V \ll 1$. That region of space would then inflate and give birth to a new universe. Our Universe could have started this way and possibly a part of a multi-verse system. In this setting, there is a no need for a specifically fine-tuned complicated potential necessary to initiate inflation; the uncertainty principle permits inflation to occur out of chaos.

* * * *

One curious thing about the restriction on ϕ given by the last inequality above is the existence of the coupling constant in the right hand side. If λ is

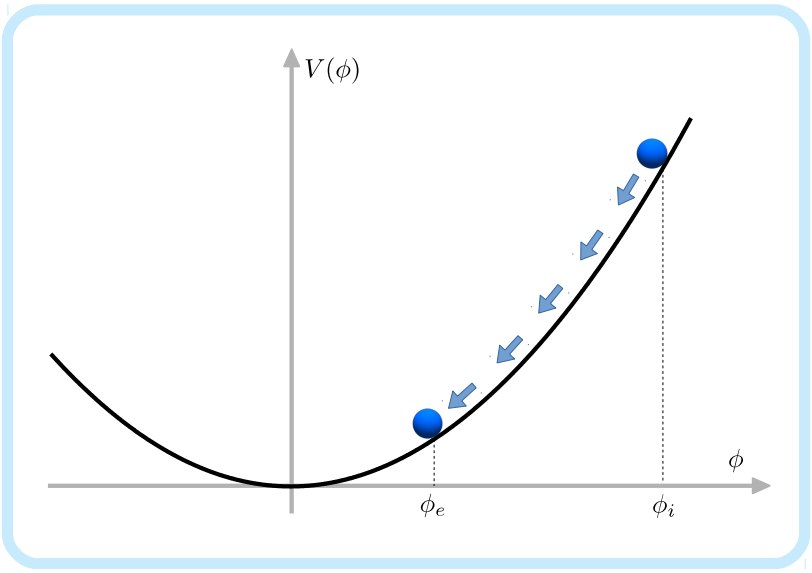


Figure 8.1: Large-field inflation. In large-field inflation (or chaotic inflation), the field starts at super-Planckian value ϕ_i corresponding to $\epsilon \ll 1$ and then it goes down to ϕ_e marking the end of inflation, $\epsilon \sim 1$.

very large, the inequality might not be satisfied. If follows that it must have a non-vanishing small value. How small this value is remains to be seen. To determine the approximate value of λ, we relate it to the scalar power spectrum given by (6.26) namely,[2]

$$\Delta_s^2(k) = \frac{H_*^2}{8\pi^2\epsilon_* M_{\rm Pl}^2}(1+\mu_{s*}) \approx \frac{H_*^2}{8\pi^2\epsilon_* M_{\rm Pl}^2} \tag{8.13}$$

This power spectrum on the other hand, is linked with the CMB temperature fluctuations the value of which can be determined experimentally.

In relation to CMB measurement, the power spectrum is usually assumed

[2] The Planck mass comes from the numerical coefficient $1/8\pi G = M_{\rm Pl}^2$ in the geometric part of the action (originally, the Einstein-Hilbert action). This is then absorbed in the definition $z^2 = 2a^2\epsilon/M_{\rm Pl}^2$.

to take the power-law form given by

$$\Delta_s^2(k) = A_s(k_\diamond)\left(\frac{k}{k_\diamond}\right)^{n_s(k_\diamond)-1+\frac{1}{2}\alpha_s(k_\diamond)\ln(k/k_\diamond)}, \tag{8.14}$$

where $k_\diamond$ is some pivot scale, n_s is the spectral index (or spectral tilt), and α_s is the running of the spectral index. The latter two are defined as

$$n_s - 1 \equiv \frac{\mathrm{d}\ln\Delta_s^2(k)}{\mathrm{d}\ln k}, \qquad \alpha_s \equiv \frac{\mathrm{d}n_s}{\mathrm{d}\ln k}. \tag{8.15}$$

The power spectrum is nearly scale-invariant with a tilt[3] $n_s = 0.97$ based on Planck 2015 results [99]. We may then take the power spectrum to be simply $A_s(k_\diamond)$ where $k_\diamond = 0.002\,\mathrm{Mpc}^{-1}$. Based on the same reference, $\ln(10^{10}A_s) = 3.06$. As such,

$$\Delta_s^2(k) \approx 2.13 \times 10^{-9}. \tag{8.16}$$

To relate λ to the power spectrum, knowing that $V = M_{\mathrm{Pl}}^4(\lambda/2n)(\phi/M_{\mathrm{Pl}})^n$, we use the first Friedmann equation as given by the approximation (8.6).

$$\begin{aligned}\Delta_s^2 &\approx \frac{H_*^2}{8\pi^2\epsilon_* M_{\mathrm{Pl}}^2} \approx \frac{V_*}{8(3)\pi^2\epsilon_* M_{\mathrm{Pl}}^4},\\ \Delta_s^2 &\approx \frac{\lambda\phi_*^n}{8(3)(2n)\pi^2\epsilon_* M_{\mathrm{Pl}}^n}\end{aligned} \tag{8.17}$$

Then, since $\epsilon \approx \epsilon_V$ we have

$$\epsilon_* \approx \frac{M_{\mathrm{Pl}}^2}{2}\left(\frac{V_{,\phi}}{V}\right)^2 = \frac{n^2}{2}\frac{M_{\mathrm{Pl}}^2}{\phi_*^2}. \tag{8.18}$$

Substitution in the last expression for Δ_s^2 yields

$$\Delta_s^2 \approx \frac{\lambda\phi_*^{n+2}}{8(3)n^3\pi^2 M_{\mathrm{Pl}}^{n+2}}. \tag{8.19}$$

The value of ϕ can be related to the number of e-folds through the definition

[3] For all the values we quote in this paragraph, the small uncertainty is in the last digit.

of N.

$$\mathrm{d}N \equiv \mathrm{d}\ln a = H\mathrm{d}t = H\frac{\mathrm{d}\phi}{\dot{\phi}} \tag{8.20}$$

For the derivative $\dot{\phi}$, we use the equation of motion for ϕ namely,

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = 0. \tag{8.21}$$

Assuming that the friction term is dominant over $\ddot{\phi}$, we can have the approximation

$$\dot{\phi} \approx -\frac{V_{,\phi}}{3H}. \tag{8.22}$$

Then

$$\begin{aligned}
\mathrm{d}N &= -\mathrm{d}\phi\frac{3H^2}{V_{,\phi}} = -\frac{\mathrm{d}\phi}{M_{\mathrm{Pl}}^2}\frac{V}{V_{,\phi}}, \\
\mathrm{d}N &= -\frac{\phi}{nM_{\mathrm{Pl}}^2}\mathrm{d}\phi
\end{aligned} \tag{8.23}$$

We integrate from the time corresponding to (N, ϕ) up to the end of inflation corresponding to (N_e, ϕ_e).

$$\begin{aligned}
\int_N^{N_e} \mathrm{d}\tilde{N} &= -\int_\phi^{\phi_e} \frac{\mathrm{d}\tilde{\phi}\,\tilde{\phi}}{nM_{\mathrm{Pl}}^2}, \\
N_e - N &= -\frac{\phi_e^2}{2nM_{\mathrm{Pl}}^2} + \frac{\phi^2}{2nM_{\mathrm{Pl}}^2}, \\
N_e &\approx \frac{\phi^2}{2nM_{\mathrm{Pl}}^2}.
\end{aligned} \tag{8.24}$$

The third line follows from taking (N, ϕ) at the start of inflation. For chaotic (large-field) inflation (we are considering here), this time corresponds to a super-Planckian field in accord with the condition (8.12), that is, $\phi \gg \phi_e$, and to the number of e-folds $N = 0$.

Using the result above for N_e in the approximation for Δ_s^2 given by (8.19)

we find

$$\Delta_s^2 \approx \lambda \frac{(2nN_e)^{\frac{n+2}{2}}}{3(8)\pi^2 n^3} \quad \Rightarrow \quad \lambda \approx \frac{3(8)\pi^2 n^3}{(2nN_e)^{\frac{n+2}{2}}} \Delta_s^2 \tag{8.25}$$

It is customary to set $N_e \approx 60$ for a successful inflation (see **Sec. 2.2** for a sample calculation of N_e). With this value of N_e, for the phi-fourth model for instance, we get $\lambda \approx 3 \times 10^{-13}$. While we have mentioned that λ is small, this value is surprisingly very small in comparison to that of typical field theories; for example, the Standard Model Higgs boson has a self coupling $\lambda \simeq 0.1$ [100]. The large-field inflation successfully evades the problem of unnaturalness associated with the initial condition, yet given the form of the potential we are considering, we are facing another problem of unnaturalness.

Fakir and Unruh [101] proposed a simple solution to this problem by removing "one of the assumptions common to almost all previous models: that of minimal coupling between the inflaton field and the scalar curvature." Specifically, they added the nonminimal coupling term

$$\frac{\xi \phi^2}{2M_{\rm Pl}^2} R, \tag{8.26}$$

where ξ is the curvature coupling parameter, in the Lagrangian. With this addition, they found out that chaotic inflation can push through for arbitrarily large values of ξ and emphasized that the "larger ξ is, the better the model behaves." Moreover, λ is not necessarily small; that is, for $n = 4$ considered by the authors,

$$\lambda^{(\xi>1)} \approx 48 N_e \xi^2 \lambda^{(\xi=0)} \tag{8.27}$$

For $\xi \sim 10^3$, $N_e \approx 60$, and $\lambda^{(\xi=0)} \approx 3 \times 10^{-13}$, the self-coupling constant $\lambda^{(\xi=1000)} \sim 10^{-2}$; thus, leveling λ with that of typical field theories.

In the next couple of sections, we lay down the set up for and details of nonminimal ($\xi \neq 0$) chaotic inflation. In so doing, we start shifting our attention to the main concern of this chapter namely, adiabatic regularization of the power spectrum. The calculations that follow shall then be geared towards the computation of the regularized power spectrum and not simply the "bare" quantity used in standard calculations. However, after we have provided an ample space for the discussion of minimal ($\xi = 0$) chaotic inflation with respect

to the unnaturalness of the initial condition for inflation and the detailed calculation for $\lambda^{(\xi=0)}$, we wish not to leave (8.27) devoid of detailed calculation. What we do then so as not to leave (8.27) hanging but at the same time keep our main track on adiabatic regularization, is to proceed with the adiabatic regularization as usual—deriving the "bare" power spectrum and the subtraction term following the discussion of nonminimally coupled chaotic inflation—and then along the way, when the "bare" power spectrum has been established, insert the calculation for $\lambda^{(\xi>1)}$ as given by (8.27); see **Example 3** in **Sec. 8.3**.

8.2 Nonminimally Coupled Chaotic Inflation

The full action for nonminimally coupled chaotic inflation[4] can be written as

$$S = \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{-g}\Big[M_{\rm Pl}^2 f(\phi)R - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V(\phi)\Big], \tag{8.28}$$

where $f(\phi) = 1 + \psi(\phi)$. Needless to say, for $\psi(\phi) = 0$, the action reduces to that of the canonical case. For the most part, we assume that[5]

$$V(\phi) = \frac{\lambda}{8}\phi^4 \quad \text{and} \quad \psi(\phi) = \frac{\xi\phi^2}{M_{\rm Pl}^2}, \tag{8.29}$$

(although we try to keep the intermediate calculations as general as possible for possible future use.) From a field-theoretic point of view, given a Klein-Gordon matter Lagrangian with a self-interaction term $\sim \phi^4$, the nonminimal coupling term above emerges as a necessary component for renormalization.[44] This justifies the inclusion of the nonminimal coupling term in addition to the justification based on the resolution of the problem concerning the unnaturalness of λ in the minimal coupling case, covered in the previous section.

[4] We cannot certainly do justice to the full treatment of this well-studied subject matter here. In addition to the pioneering work by Fakir and Unruh [101], and Futamase and Maeda [102], interested readers may consult (a) refs. [103, 104] for the rigorous calculation of and constraints on several physical observables associated with nonminimally coupled chaotic inflation, (b) refs. [105, 106] for loop corrections and Higgs inflation, (c) refs. [107] for observational consequences when a potential quadratic in the scalar field is added, (d) ref. [108] for non-Gaussianity, among others.

[5] Based on the 2013 and 2015 Planck results, the *minimally* coupled case involving quartic potential is strongly disfavored. This does not hold however, for the *nonminimally* coupled case. [34, 99]

The curvature coupling constant indicates the strength of nonminimal coupling. It has a value of $\xi = -\frac{1}{6}$ for a conformally invariant action; that is, for $m = V = 0$, the action is invariant under the conformal transformation $g_{\mu\nu}(x) \to \tilde{g}_{\mu\nu} = \Omega^2(x) g_{\mu\nu}(x)$. [44, 74, 109] Here, we consider ξ to take non-negative values in general. For $\xi < 0$ the effective gravitational constant,

$$G_{\text{eff}} = G\left(1 + \frac{\xi\phi^2}{M_{\text{Pl}}^2}\right)^{-1}, \tag{8.30}$$

can become negative (see ref. [102] for further details); we do not consider this scenario here. For positive values of ξ, a large value can mean small effective gravitational constant. This possible pitfall can be evaded if after starting with large value of ϕ to trigger inflation, it could end up with small ϕ corresponding to small ψ.

Set up: Background Equations

Given the action (8.28) we now proceed to derive the usual equations for the set up of our model namely, equation of motion, Friedmann equation, energy density, and pressure. We begin the derivation of the equation of motion with the identification

$$\mathcal{L} = \tfrac{1}{2}\sqrt{-g}[M_{\text{Pl}}^2 f(\phi)R - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V], \tag{8.31}$$

where g is the determinant of the background (FLRW) metric namely,

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a^2(t)\delta_{ij}\mathrm{d}x^i\mathrm{d}x^j. \tag{8.32}$$

It follows from the Euler-Lagrange equation that

$$\begin{aligned} \frac{\partial\mathcal{L}}{\partial\phi} - \nabla_\mu\frac{\partial\mathcal{L}}{\partial\phi_{;\mu}} &= 0, \\ M_{\text{Pl}}^2 f_{,\phi}R - 2V_{,\phi} + 2\nabla_\mu(g^{\mu\nu}\nabla_\nu\phi) &= 0, \\ \Box\phi - V_{,\phi} + \frac{M_{\text{Pl}}^2}{2}f_{,\phi}R &= 0. \end{aligned} \tag{8.33}$$

Since $\sqrt{-g}\,\Box\phi = \partial_\mu(\sqrt{-g}\,g^{\mu\nu}\,\partial_\nu\phi)$ then

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} - \frac{M_{\text{Pl}}^2}{2}f_{,\phi}R = 0. \tag{8.34}$$

The derivative of $f(\phi)$ vanishes in the minimal coupling case and the equation of motion reduces to the familiar form $\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = 0$.

The energy-momentum tensor containing the energy density and pressure can be derived by varying the action with respect to $\delta g^{\mu\nu}$. We have from the action above,

$$S = \frac{1}{2}\int \mathrm{d}t\,\mathrm{d}x\sqrt{-g}[M_{\mathrm{Pl}}^2 f(\phi)R - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V],$$

$$\delta S = \frac{1}{2}\int \mathrm{d}t\,\mathrm{d}x\Big\{\delta\sqrt{-g}[M_{\mathrm{Pl}}^2 fR - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V] + \sqrt{-g}[M_{\mathrm{Pl}}^2 f\delta R - \delta g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi]\Big\},$$

$$\delta\sqrt{-g} = -\frac{1}{2}\sqrt{-g}(g_{\mu\nu}\delta g^{\mu\nu})$$

$$\delta S = \frac{1}{2}\int \mathrm{d}t\,\mathrm{d}x\Big\{ -\frac{1}{2}\sqrt{-g}(g_{\mu\nu}\delta g^{\mu\nu})[M_{\mathrm{Pl}}^2 fR - g^{\alpha\beta}\nabla_\alpha\phi\nabla_\beta\phi - 2V],$$

$$+\ \sqrt{-g}[M_{\mathrm{Pl}}^2 f\delta R - \delta g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi]\Big\}. \tag{8.35}$$

Ordinarily, we can simply take $\delta R = R_{\mu\nu}\delta g^{\mu\nu}$, but with the extra factor $f(\phi)$, we have a more complicated situation; the integration by parts which normally ignores $\sqrt{-g}$ because its covariant derivative vanishes, has to take into account $f\sqrt{-g}$.

To continue, we take $\delta R = R_{\mu\nu}\delta g^{\mu\nu} + g^{\mu\nu}\,\delta R_{\mu\nu}$. From the calculation in the example below, we find

$$\delta R = R_{\mu\nu}\delta g^{\mu\nu} + g_{\mu\nu}\nabla_\alpha\nabla^\alpha(\delta g^{\mu\nu}) - \nabla_\mu\nabla_\nu(\delta g^{\mu\nu}). \tag{8.36}$$

Performing integration by parts then gives us the contribution due to δR in the variation of the action.

$$\int \mathrm{d}^4x\sqrt{-g}f\delta R = \int \mathrm{d}^4x\sqrt{-g}f[R_{\mu\nu}\delta g^{\mu\nu} + g_{\mu\nu}\nabla_\alpha\nabla^\alpha(\delta g^{\mu\nu}) - \nabla_\mu\nabla_\nu(\delta g^{\mu\nu})],$$

$$\int \mathrm{d}^4x\sqrt{-g}f\delta R = \int \mathrm{d}^4x\sqrt{-g}[fR_{\mu\nu} + g_{\mu\nu}\nabla_\alpha\nabla^\alpha f - \nabla_\mu\nabla_\nu f]\delta g^{\mu\nu} \tag{8.37}$$

Using this in the last expression for δS above then gives

$$\delta S = \frac{1}{2}\int \mathrm{d}t\,\mathrm{d}x\Big\{ -\frac{1}{2}\sqrt{-g}(g_{\mu\nu}\delta g^{\mu\nu})[M_{\mathrm{Pl}}^2 fR - g^{\alpha\beta}\nabla_\alpha\phi\nabla_\beta\phi - 2V] \tag{8.38}$$

$$+\sqrt{-g}\left[M_{\rm Pl}^2 f R_{\mu\nu}+M_{\rm Pl}^2 g_{\mu\nu}\Box f-M_{\rm Pl}^2\nabla_\mu\nabla_\nu f-\nabla_\mu\phi\nabla_\nu\phi\right]\delta g^{\mu\nu}\Big\},$$

from which follows the field equation

$$R_{\mu\nu}-\tfrac{1}{2}g_{\mu\nu}R=M_{\rm Pl}^{-2}\Big[\nabla_\mu\phi\nabla_\nu\phi-g_{\mu\nu}\left(\tfrac{1}{2}\nabla^\alpha\phi\nabla_\alpha\phi+V\right)\Big]$$
$$+\nabla_\mu\nabla_\nu\psi-g_{\mu\nu}\Box\psi-\psi G_{\mu\nu}, \tag{8.39}$$

where $G_{\mu\nu}\equiv R_{\mu\nu}-\frac{1}{2}g_{\mu\nu}R$ is the Einstein tensor. This field equation gives us the expression for the conserved energy-momentum tensor; cf. $R_{\mu\nu}-\frac{1}{2}g_{\mu\nu}R=M_{\rm Pl}^{-2}T_{\mu\nu}$.

$$T_{\mu\nu}=\phi_{;\mu}\phi_{;\nu}-g_{\mu\nu}\left(\tfrac{1}{2}\phi^{;\alpha}\phi_{;\alpha}+V\right)+M_{\rm Pl}^2\left(\psi_{;\mu\nu}-g_{\mu\nu}\Box\psi-\psi G_{\mu\nu}\right), \tag{8.40}$$

Needless to say, it is the same expression that will result from the definition given by

$$T_{\mu\nu}\equiv-\frac{2}{\sqrt{-g}}\frac{\delta S_{\rm matter}}{\delta g^{\mu\nu}}, \tag{8.41}$$

where $S_{\rm matter}$ includes all those terms in the action containing ϕ, namely,

$$S_{\rm matter}=\frac{1}{2}\int {\rm d}t\,{\rm d}x\sqrt{-g}\left[M_{\rm Pl}^2\psi(\phi)R-g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi-2V\right]. \tag{8.42}$$



Example 2. ***Variation of the Ricci Scalar.*** Show that the variation of the Ricci scalar is as given by (8.36) namely,

$$\delta R=R_{\mu\nu}\delta g^{\mu\nu}+g_{\mu\nu}\nabla_\alpha\nabla^\alpha(\delta g^{\mu\nu})-\nabla_\mu\nabla_\nu(\delta g^{\mu\nu}). \tag{8.43}$$

Solution. The contraction of the Ricci tensor is the Ricci scalar; that is, $R=g^{\mu\nu}R_{\mu\nu}$. Consequently, $\delta R=R_{\mu\nu}\delta g^{\mu\nu}+g^{\mu\nu}\delta R_{\mu\nu}$. For the last term, we start with the expression for the Riemann tensor in terms of the Christoffel symbols.

$$R^\alpha{}_{\mu\beta\nu}=-\Gamma^\alpha_{\mu\beta,\nu}+\Gamma^\alpha_{\mu\nu,\beta}-\Gamma^\rho_{\mu\beta}\Gamma^\alpha_{\rho\nu}+\Gamma^\rho_{\mu\nu}\Gamma^\alpha_{\rho\beta},$$

$$\delta R^\alpha{}_{\mu\beta\nu}=-\delta\Gamma^\alpha_{\mu\beta,\nu}+\delta\Gamma^\alpha_{\mu\nu,\beta}-\delta\Gamma^\rho_{\mu\beta}\Gamma^\alpha_{\rho\nu}-\Gamma^\rho_{\mu\beta}\delta\Gamma^\alpha_{\rho\nu}+\delta\Gamma^\rho_{\mu\nu}\Gamma^\alpha_{\rho\beta}+\Gamma^\rho_{\mu\nu}\delta\Gamma^\alpha_{\rho\beta},$$

$$
\begin{aligned}
&= -\delta\Gamma^{\alpha}_{\mu\beta,\nu} - \Gamma^{\alpha}_{\rho\nu}\delta\Gamma^{\rho}_{\mu\beta} + \Gamma^{\rho}_{\mu\nu}\delta\Gamma^{\alpha}_{\rho\beta} + \Gamma^{\rho}_{\beta\nu}\delta\Gamma^{\alpha}_{\mu\rho} \\
&\quad + \delta\Gamma^{\alpha}_{\mu\nu,\beta} + \Gamma^{\alpha}_{\rho\beta}\delta\Gamma^{\rho}_{\mu\nu} - \Gamma^{\rho}_{\mu\beta}\delta\Gamma^{\alpha}_{\rho\nu} - \Gamma^{\rho}_{\beta\nu}\delta\Gamma^{\alpha}_{\mu\rho}, \\
\delta R^{\alpha}{}_{\mu\beta\nu} &= -(\delta\Gamma^{\alpha}_{\mu\beta})_{;\nu} + (\delta\Gamma^{\alpha}_{\mu\nu})_{;\beta}. \qquad (8.44)
\end{aligned}
$$

In the third equality, we have added and subtracted the term $\Gamma^{\rho}_{\beta\nu}\delta\Gamma^{\alpha}_{\mu\rho}$. Note that although the Christoffel symbol itself is *not* a tensor, its *variation* is a tensor. It follows that we are free to take its covariant derivative.

From the expression for the Christoffel symbol in terms of the metric, we calculate its variation (with respect to the metric)

$$
\begin{aligned}
\Gamma^{\alpha}_{\mu\beta} &= \tfrac{1}{2}\, g^{\alpha\rho}(g_{\rho\mu,\beta} + g_{\beta\rho,\mu} - g_{\mu\beta,\rho}), \\
\delta\Gamma^{\alpha}_{\mu\beta} &= \tfrac{1}{2}\, g^{\alpha\rho}\big[(\delta g_{\rho\mu})_{,\beta} + (\delta g_{\beta\rho})_{,\mu} - (\delta g_{\mu\beta})_{,\rho}\big] + \tfrac{1}{2}\,\delta g^{\alpha\rho}(g_{\rho\mu,\beta} + g_{\beta\rho,\mu} - g_{\mu\beta,\rho}).
\end{aligned}
$$

To simplify the last equation above, we imagine $\Gamma^{\alpha}_{\mu\beta}$ being evaluated in a small enough space such that the metric takes the canonical form. Then $\delta g^{\alpha\rho}$ vanishes. This leaves us with[6]

$$
\delta\Gamma^{\alpha}_{\mu\beta} = \tfrac{1}{2}\, g^{\alpha\rho}\big[(\delta g_{\rho\mu})_{,\beta} + (\delta g_{\beta\rho})_{,\mu} - (\delta g_{\mu\beta})_{,\rho}\big]. \qquad (8.45)
$$

Invoking the "comma-to-semicolon" rule (or more formally, from the principle of covariance), the above equation generalizes to curved spacetime as

$$
\delta\Gamma^{\alpha}_{\mu\beta} = \tfrac{1}{2}\, g^{\alpha\rho}\big[(\delta g_{\rho\mu})_{;\beta} + (\delta g_{\beta\rho})_{;\mu} - (\delta g_{\mu\beta})_{;\rho}\big]. \qquad (8.46)
$$

In the equation above for δR we have $\delta g^{\mu\nu}$ instead of $\delta g_{\mu\nu}$ so we "shift" δ to the inverse metric components. After this, we take the covariant derivative according to the expression for $\delta R^{\alpha}{}_{\mu\beta\nu}$ above.

$$
\begin{aligned}
\delta\Gamma^{\alpha}_{\mu\beta} &= -\tfrac{1}{2}\,\big[g_{\rho\mu}(\delta g^{\alpha\rho})_{;\beta} + g_{\beta\rho}(\delta g^{\alpha\rho})_{;\mu} + (\delta g_{\mu\beta})^{;\alpha}\big], \\
&\qquad \big[\text{Note:}\quad -g_{\mu\rho}g_{\beta\sigma}\delta g^{\rho\sigma} = g_{\mu\rho}(\delta g_{\beta\sigma})g^{\rho\sigma} = \delta g_{\beta\mu}\big],
\end{aligned}
$$

[6] Needless to say, even though we can take $\delta g^{\alpha\rho} = 0$, we cannot take the derivative of $\delta g_{\alpha\rho}$ as vanishing because the curvature tensor is proportional to the second-order derivative of the metric; unless otherwise, the spacetime under consideration is flat, which we assume it is not in general.

$$\begin{aligned}
\delta\Gamma^{\alpha}_{\mu\beta} &= -\tfrac{1}{2}\left[g_{\rho\mu}(\delta g^{\alpha\rho})_{;\beta} + g_{\beta\rho}(\delta g^{\alpha\rho})_{;\mu} - g_{\mu\rho}g_{\beta\sigma}(\delta g^{\rho\sigma})^{;\alpha}\right],\\
\Rightarrow (\delta\Gamma^{\alpha}_{\mu\beta})_{;\nu} &= -\tfrac{1}{2}\left[g_{\rho\mu}(\delta g^{\alpha\rho})_{;\beta\nu} + g_{\beta\rho}(\delta g^{\alpha\rho})_{;\mu\nu} - g_{\mu\rho}g_{\beta\sigma}(\delta g^{\rho\sigma})^{;\alpha}{}_{\nu}\right],\\
\Rightarrow (\delta\Gamma^{\alpha}_{\mu\nu})_{;\beta} &= -\tfrac{1}{2}\left[g_{\rho\mu}(\delta g^{\alpha\rho})_{;\nu\beta} + g_{\nu\rho}(\delta g^{\alpha\rho})_{;\mu\beta} - g_{\mu\rho}g_{\nu\sigma}(\delta g^{\rho\sigma})^{;\alpha}{}_{\beta}\right]
\end{aligned} \tag{8.47}$$

Contracting the indices α and β, and then raising the index μ we find

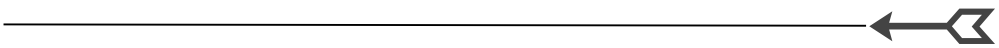
$$\begin{aligned}
(\delta\Gamma^{\alpha}_{\mu\alpha})_{;\nu} &= -\tfrac{1}{2}\left[g_{\rho\mu}(\delta g^{\alpha\rho})_{;\alpha\nu} + g_{\alpha\rho}(\delta g^{\alpha\rho})_{;\mu\nu} - g_{\mu\rho}(\delta g^{\rho\sigma})_{;\sigma\nu}\right],\\
-g^{\mu\nu}(\delta\Gamma^{\alpha}_{\mu\alpha})_{;\nu} &= +\tfrac{1}{2}\left[(\delta g^{\alpha\rho})_{;\alpha\rho} + g_{\alpha\rho}(\delta g^{\alpha\rho})_{;}{}^{\mu} - (\delta g^{\rho\sigma})_{;\sigma\rho}\right],
\end{aligned}$$

$$\begin{aligned}
(\delta\Gamma^{\alpha}_{\mu\nu})_{;\alpha} &= -\tfrac{1}{2}\left[g_{\rho\mu}(\delta g^{\alpha\rho})_{;\nu\alpha} + g_{\nu\rho}(\delta g^{\alpha\rho})_{;\mu\alpha} - g_{\mu\rho}g_{\nu\sigma}(\delta g^{\rho\sigma})^{;\alpha}{}_{\alpha}\right],\\
g^{\mu\nu}(\delta\Gamma^{\alpha}_{\mu\nu})_{;\alpha} &= -\tfrac{1}{2}\left[(\delta g^{\alpha\rho})_{;\rho\alpha} + (\delta g^{\alpha\rho})_{;\rho\alpha} - g_{\rho\sigma}(\delta g^{\rho\sigma})^{;\alpha}{}_{\alpha}\right].
\end{aligned} \tag{8.48}$$

Then

$$\begin{aligned}
g^{\mu\nu}\delta R_{\mu\nu} &= -g^{\mu\nu}(\delta\Gamma^{\alpha}_{\mu\alpha})_{;\nu} + (\delta\Gamma^{\alpha}_{\mu\nu})_{;\alpha},\\
\delta R &= R_{\mu\nu}\delta g^{\mu\nu} + g_{\mu\nu}\nabla_{\alpha}\nabla^{\alpha}(\delta g^{\mu\nu}) - \nabla_{\mu}\nabla_{\nu}(\delta g^{\mu\nu}),
\end{aligned} \tag{8.49}$$

which was to be shown.



The energy density and pressure form the diagonal components of the energy-momentum tensor; i.e., $T^{\mu}{}_{\nu} = \mathrm{diag}(-\rho, p, p, p)$. For the energy density, we have

$$\begin{aligned}
T^{\mu}{}_{\nu} &= \phi^{;\mu}\phi_{;\nu} - \delta^{\mu}_{\nu}\left(\tfrac{1}{2}\,\phi^{;\alpha}\phi_{;\alpha} + V\right) + M_{\mathrm{Pl}}^2\left(\psi^{;\mu}{}_{\nu} - \delta^{\mu}_{\nu}\Box\psi - \psi G^{\mu}{}_{\nu}\right),\\
T^{0}{}_{0} &= -\tfrac{1}{2}\,\dot{\phi}^2 - V + M_{\mathrm{Pl}}^2\left(\psi^{;0}{}_{0} - \Box\psi - \psi G^{0}{}_{0}\right),\\
-\rho &= \frac{1}{f}\left[-\tfrac{1}{2}\,\dot{\phi}^2 - V + M_{\mathrm{Pl}}^2\left(\psi^{;0}{}_{0} - \Box\psi\right)\right]
\end{aligned} \tag{8.50}$$

For the first term inside the pair of parentheses, we expand the covariant derivative.

$$\psi^{;0}{}_{0} = \psi^{;0}{}_{,0} + \Gamma^{\alpha}_{0\alpha}\psi^{;\alpha}; \quad (\Gamma^{0}_{00} = 0),$$

$$\psi^{;0}{}_{0} = -\ddot{\psi}. \tag{8.51}$$

On the other hand, the d'Alembertian of ψ can be expressed in terms of time derivative by using the formula $\sqrt{-g}\,\Box\psi = \partial_\mu(\sqrt{-g}g^{\mu\nu}\partial_\nu\psi)$. Noting that $\sqrt{-g} = a^3$, we find $\Box\psi = -3H\dot{\psi} - \ddot{\psi}$. Consequently,

$$\psi^{;0}{}_{0} - \Box\psi = 3H\dot{\psi}, \tag{8.52}$$

and we can write our sought-for equation for the energy density as

$$\boxed{\rho = \frac{1}{f}\left(\tfrac{1}{2}\,\dot{\phi}^2 + V - 3M_{\rm Pl}^2 H\dot{\psi}\right).} \tag{8.53}$$

The pressure is one-third of the spatial trace of the energy-momentum tensor. From the equation for $T^{\mu}{}_{\nu}$ above we have

$$\begin{aligned}
T^{i}{}_{i} &= \tfrac{3}{2}\,\dot{\phi}^2 - 3V + M_{\rm Pl}^2\left(\psi^{;i}{}_{i} - 3\Box\psi - \psi G^{i}{}_{i}\right),\\
p &= \frac{1}{3f}\left[\tfrac{3}{2}\,\dot{\phi}^2 - 3V + M_{\rm Pl}^2\left(\psi^{;i}{}_{i} - 3\Box\psi\right)\right],\\
&= \frac{1}{3f}\left[\tfrac{3}{2}\,\dot{\phi}^2 - 3V + M_{\rm Pl}^2\left(-\psi^{;0}{}_{0} - 2\Box\psi\right)\right],\\
&= \frac{1}{3f}\left[\tfrac{3}{2}\,\dot{\phi}^2 - 3V + M_{\rm Pl}^2\left(3\ddot{\psi} + 6H\dot{\psi}\right)\right],
\end{aligned}$$

$$\boxed{p = \frac{1}{f}\left[\tfrac{1}{2}\,\dot{\phi}^2 - V + M_{\rm Pl}^2\left(2H\dot{\psi} + \ddot{\psi}\right)\right],} \tag{8.54}$$

which is our sought-for expression for the pressure.

The sum of pressure and energy density is related to the time derivative of the Hubble parameter by (1.13). Using the expressions for ρ and p above, we can then calculate ϵ as

$$\begin{aligned}
\dot{H} &= -\frac{1}{2M_{\rm Pl}^2}(\rho + p),\\
&= -\frac{1}{2M_{\rm Pl}^2 f}\left[\dot{\phi}^2 + M_{\rm Pl}^2\left(\ddot{\psi} - H\dot{\psi}\right)\right],
\end{aligned}$$

$$\epsilon = \frac{1}{f}\left(\frac{\dot{\phi}^2}{2M_{\rm Pl}^2H^2} - \frac{\dot{\psi}}{2H} + \frac{\ddot{\psi}}{2H^2}\right),$$

$$\boxed{\epsilon = \frac{1}{f}\left(\bar{\epsilon} - \frac{\dot{\psi}}{2H} + \frac{\ddot{\psi}}{2H^2}\right),} \tag{8.55}$$

where $\bar{\epsilon}$ is the first slow-roll parameter corresponding to the minimally coupled case[7], namely,

$$\bar{\epsilon} \equiv \frac{\dot{\phi}^2}{2M_{\rm Pl}^2H^2} \tag{8.56}$$

With the expressions for energy density and pressure, we can also write the equation of motion for ϕ so that the Ricci scalar is not explicitly included. The idea is to rewrite R in terms of ρ and p and then perform a substitution from the expressions for ρ and p so that R is expressed in terms of ϕ and H.

$$\begin{aligned} R^{\mu}{}_{\mu} - \tfrac{1}{2}\,\delta^{\mu}_{\mu}R &= M_{\rm Pl}^{-2}T^{\mu}{}_{\mu}, \\ -R &= T^{0}{}_{0} + T^{i}{}_{i}, \\ R &= M_{\rm Pl}^{-2}(\rho - 3p), \\ R &= \frac{1}{f}\left(-M_{\rm Pl}^{-2}\dot{\phi}^2 + 4M_{\rm Pl}^{-2}V - 9H\dot{\psi} - 3\ddot{\psi}\right). \end{aligned} \tag{8.57}$$

This last equation for R allows us to update the equation of motion for ϕ given by (8.34) as

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} + \frac{f_{,\phi}}{2f}\left(\dot{\phi}^2 - 4V + 9M_{\rm Pl}^2H\dot{\psi} + 3M_{\rm Pl}^2\ddot{\psi}\right) = 0. \tag{8.58}$$

Noting that $\dot{\psi} = \psi_{,\phi}\dot{\phi}$ and $\ddot{\psi} = \psi_{,\phi\phi}\dot{\phi}^2 + \psi_{,\phi}\ddot{\phi}$, we regroup terms involving $\ddot{\phi}$, $\dot{\phi}$ and $\dot{\phi}^2$.

$$\ddot{\phi} + 3H\dot{\phi} + \frac{f_{,\phi}}{2f}\left(9M_{\rm Pl}^2H\dot{\psi} + 3M_{\rm Pl}^2\ddot{\psi}\right)$$

[7] Word of caution here: Although $\epsilon \equiv -\dot{H}/H^2 = \dot{\phi}^2/(2M_{\rm Pl}^2H^2)$ in the minimally coupled case, one should note that the field ϕ in $\bar{\epsilon} = \dot{\phi}^2/2M_{\rm Pl}^2H^2$ may behave differently compared to ϕ in the former. The two epsilons here $(\epsilon, \bar{\epsilon})$ are not exactly the same.

$$
\begin{aligned}
&= \ddot{\phi} + 3H\dot{\phi} + \frac{\psi_{,\phi}}{2f}\left(9M_{\rm Pl}^2 H\psi_{,\phi}\dot{\phi} + 3M_{\rm Pl}^2\psi_{,\phi}\ddot{\phi} + 3M_{\rm Pl}^2\psi_{,\phi\phi}\dot{\phi}^2\right), \\
&= \ddot{\phi}\left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{f}\right) + 3H\dot{\phi}\left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{f}\right) + \frac{3}{2}M_{\rm Pl}^2\frac{\psi_{,\phi}\psi_{,\phi\phi}}{f}\dot{\phi}^2, \\
&= \left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{f}\right)\left(\ddot{\phi} + 3H\dot{\phi}\right) + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}\psi_{,\phi\phi}}{f}\dot{\phi}^2. \qquad (8.59)
\end{aligned}
$$

It follows that

$$
\begin{aligned}
&\ddot{\phi} + 3H\dot{\phi} + \left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{f}\right)^{-1} V_{,\phi} \\
&\quad + \frac{\psi_{,\phi}}{2f}\left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{f}\right)^{-1}\left(1 + 3M_{\rm Pl}^2\psi_{,\phi\phi}\right)\dot{\phi}^2 \\
&\quad - \frac{2\psi_{,\phi}}{f}\left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{f}\right)^{-1} V = 0. \qquad (8.60)
\end{aligned}
$$

For $\psi = \xi\phi^2/M_{\rm Pl}^2$, this equation reduces to [101, 104]

$$
\begin{aligned}
&\ddot{\phi} + 3H\dot{\phi} + \frac{1 + \xi M_{\rm Pl}^{-2}\phi^2}{1 + \xi M_{\rm Pl}^{-2}\phi^2(1 + 6\xi)} V_{,\phi} \\
&+ \frac{\xi M_{\rm Pl}^{-2}\phi^2(1 + 6\xi)}{1 + \xi M_{\rm Pl}^{-2}\phi^2(1 + 6\xi)}\frac{\dot{\phi}^2}{\phi} - \frac{4\xi M_{\rm Pl}^{-2}\phi}{1 + \xi M_{\rm Pl}^{-2}\phi^2(1 + 6\xi)} V = 0.
\end{aligned}
$$

Nonminimally Coupled Slow-roll Inflation[8]

Large-field corresponds to $\psi = \xi\phi^2 M_{\rm Pl}^{-2} \gg 1$ (see also the discussion in the preceding section for ϵ_V). For slow-roll inflation, the term involving $\dot{\phi}^2$ is much smaller than the rest of the terms in the equation of motion for ϕ. Furthermore, to prolong inflation, the drag term $3H\dot{\phi}$ should be also much larger than $\ddot{\phi}$. For

[8] Our discussion here is based mainly on the works of Fakir and Unruh [101], and Komatsu and Futamase [104].

the potential $V = \lambda\phi^4/8$, these conditions imply

$$\begin{aligned} 3H\dot{\phi} &\approx -\frac{1+\xi M_{\rm Pl}^{-2}\phi^2}{1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)}V_{,\phi} + \frac{4\xi M_{\rm Pl}^{-2}\phi}{1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)}V, \\ &= -\frac{1+\xi M_{\rm Pl}^{-2}\phi^2}{1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)}\frac{\lambda}{2}\phi^3 + \frac{\xi M_{\rm Pl}^{-2}}{1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)}\frac{\lambda}{2}\phi^5, \\ 3H\dot{\phi} &\approx -\frac{\lambda\phi^3}{2[1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)]}. \end{aligned} \tag{8.61}$$

The time derivative of the Hubble parameter should be nearly vanishing for a quasi-de Sitter expansion; more formally, $\epsilon \ll 1$. From the Friedmann equation with ρ given by (8.53) and using the result above for $3H\dot{\phi}$ we have

$$\begin{aligned} H^2 &= \frac{\rho}{3M_{\rm Pl}^2}, \\ &= \frac{1}{3M_{\rm Pl}^2 f}\left(\frac{1}{2}\dot{\phi}^2 + V - 3M_{\rm Pl}^2 H\dot{\psi}\right), \\ &\approx \frac{1}{3M_{\rm Pl}^2 f}\left[V - 2\xi\phi(3H\dot{\phi})\right], \\ &\approx \frac{1}{3M_{\rm Pl}^2 f}\left[V + \frac{\xi\lambda\phi^4}{1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)}\right], \\ H^2 &\approx \frac{\lambda\phi^4}{24M_{\rm Pl}^2(1+\xi M_{\rm Pl}^{-2}\phi^2)}\left[1 + \frac{8\xi}{1+\xi M_{\rm Pl}^{-2}\phi^2(1+6\xi)}\right] \end{aligned} \tag{8.62}$$

Further assuming that $\xi \gg 1$, we see that the second term inside the pair of square brackets can be neglected. The Friedmann equation then simplifies to

$$H^2 \approx \frac{\lambda\phi^2}{24\xi}. \tag{8.63}$$

The time derivative of H is

$$\begin{aligned} \dot{H} &\approx \frac{\lambda\phi}{24(3)\xi}\frac{3H\dot{\phi}}{H^2}, \\ &\approx -\frac{\lambda\phi}{24(3)\xi}\frac{\lambda\phi^3}{12\xi^2 M_{\rm Pl}^{-2}\phi^2}\frac{24\xi}{\lambda\phi^2}, \end{aligned}$$

$$-\dot{H} \approx \frac{\lambda M_{\rm Pl}^2}{36\xi^2}. \tag{8.64}$$

Dividing this by H^2 brings us back to[9]

$$\epsilon = -\frac{\dot{H}}{H^2} \approx \frac{2}{3}\left(\frac{\xi\phi^2}{M_{\rm Pl}^2}\right)^{-1} \ll 1, \tag{8.65}$$

indicating a self-consistent inflationary solution for $\psi \gg 1$.

From a large value of ϕ corresponding to $\psi \gg 1$ inflation continues until $\psi \sim 1$. The total number of e-folds can be calculated following an approach similar to that in the previous section (see (8.20)). Here, instead of directly using ϕ, we use ψ.

$$\mathrm{d}N = \mathrm{d}\ln a = H\frac{\mathrm{d}\psi}{\dot{\psi}}. \tag{8.66}$$

From the approximation for $3H\dot{\phi}$ given by the last of (8.61) we have

$$\begin{aligned}
3H\dot{\phi} &\approx -\frac{\lambda}{2}\phi^3\left[1+\psi(1+6\xi)\right]^{-1}, \\
3HM_{\rm Pl}^2\dot{\psi} &\approx -\xi\lambda\phi^4\left[1+\psi(1+6\xi)\right]^{-1}, \\
\frac{\dot{\psi}}{H} &\approx -\frac{\xi\lambda\phi^4}{3M_{\rm Pl}^2H^2}\left[1+\psi(1+6\xi)\right]^{-1}, \\
\frac{\dot{\psi}}{H} &\approx -\frac{\xi\lambda\phi^4}{M_{\rm Pl}^2\psi(1+6\xi)}\left(\frac{1}{3H^2}\right).
\end{aligned} \tag{8.67}$$

But from (8.63), $3H^2 \approx \lambda\phi^2/8\xi$. It follows that

$$\frac{\dot{\psi}}{H} \approx -\frac{8\xi}{1+6\xi}. \tag{8.68}$$

Substituting this in the expression for the number of e-folds above and performing integration yields

$$N_e \approx \frac{1+6\xi}{8\xi}(\psi_i - \psi_e) \approx \frac{1+6\xi}{8\xi}\psi_i, \tag{8.69}$$

[9] Equivalently, we can also obtain the same result following the equation for ϵ given by the last of (8.55) and ignoring terms involving $\bar{\epsilon}$ and $\ddot{\psi}$.

since $N_i = 0$ and $\psi_i \gg \psi_e$. For $N_e \geq 60$ and large ξ, this implies $\psi_i \geq 80$.

8.3 The "Bare" Power Spectrum

"Bare" Scalar Power Spectrum

We recall that the calculation of the "bare" power spectrum in the canonical inflation wherein the inflaton is minimally coupled with gravity, proceeds with the decomposition of the action into $S = S^{(0)} + S^{(2)} + S^{(3)} + \cdots$, where n in $S^{(n)}$ denotes the order with respect to ζ. (As usual, we discuss the tensor perturbations later.) Then we focus on $S^{(2)}$ and solve for the equation of motion the solution of which, upon quantization, gives us the power spectrum. In nonminimally coupled chaotic inflation, this whole procedure is complicated, starting at the decomposition of the action, by the presence of the nonminimal coupling term. This does not mean however, that such decomposition is impossible; it can be challenging but still doable. In the paper of Qiu and Yang [108], the authors decomposed the action for general nonminimally coupled single-field inflation up to third order to calculate the power spectrum from $S^{(2)}$ and the so-called **non-Gaussianity**[10] from $S^{(3)}$.

Our interest in this section is the "bare" power spectrum and it might be good to simply borrow the result in ref. [108]. However, the authors used slightly different set of parameters in their calculations. The power spectrum also involves $f(\phi)$ that is evaluated at an unusual value of the conformal time $\tau = -1$. This is in addition to the suspicious neglect of some terms involving the slow-roll parameters.[11] For these reasons we opt to perform our own calculation of the "bare" power spectrum. With such a choice, although it might be a good

[10] Rather informally, the non-Gaussianity is a measure of deviation of the probability distribution of ζ from the normal (or Gaussian) distribution. In canonical inflation, the slow-roll parameter successively suppresses the n-th order action with n; thus, the non-Gaussianity is predicted to be very small. For more information on this concept, interested readers are referred to refs. [43, 108, 111, 112, 113] and the references therein. We do not cover non-Gaussianity in this work.

[11] By so making these comments, we aim not to significantly water down the work of Qiu and Yang [108]. In fact, their calculation results, at least for the decomposed actions, can serve as a good basis for checking the results following simpler methods. Part of the progression of theoretical physics and science in general, is finding more and more simple ways of doing things; often, the first one is not readily the optimal approach.

option, we wish not to repeat the seemingly tedious pathway in ref. [108], only trying to follow a slightly different pathway to yield an expression that would fit our need here. Instead, we follow a much simpler method employing the trick of frame transformation.

The action S given by (8.28) in the previous section, where the inflaton is *nonminimally* coupled with the Ricci scalar, is written in the **Jordan frame**. This action can be rewritten such that matter is *minimally* coupled with gravity by performing **conformal transformation** namely, $\mathrm{d}\widehat{s}^2 = \Omega^2 \mathrm{d}s^2$. (Note that in this context, the term conformal transformation usually used in GR treatments, is simply the Weyl transformation.) In other words, under such transformation, the resulting action takes the form of the canonical action but (following the notation for the metric $\mathrm{d}\widehat{s}^2$,) with all other variables rewritten with a hat signifying transformed variables as a consequence of metric rescaling. The resulting action resembling the original Einstein-Hilbert action plus matter term, is said to be written in the **Einstein frame**.

To rewrite the action from the Jordan frame to the Einstein frame, we rewrite all segments of the action in the Jordan frame one-by-one, to the Einstein frame. First, as a consequence of the metric rescaling we can define a hatted time coordinate and a hatted scale factor as

$$\mathrm{d}\widehat{t} \equiv \Omega \, \mathrm{d}t \quad \text{and} \quad \widehat{a} \equiv \Omega a, \tag{8.70}$$

respectively, such that

$$\widehat{g}_{00} = g_{00}, \quad \widehat{g}_{0i} = \Omega g_{0i}, \quad \text{and} \quad \widehat{g}_{ij} = \Omega^2 g_{ij}, \tag{8.71}$$

(implying that in this treatment, $\mathrm{d}\widehat{s}^2 = \Omega^2 \mathrm{d}s^2$ does not necessarily mean $\widehat{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$ as is usually the case in many textbooks on general relativity). For the background FLRW metric, the above choice of hatted metric components implies $\mathrm{d}\widehat{s}^2 = -\mathrm{d}\widehat{t}^{\,2} + \widehat{a}^2 \delta_{ij} \mathrm{d}x^i \mathrm{d}x^j$, taking exactly the same form as the original metric.

Second, noting the above convention for the metric components, the integral measures in the two frames can be related by

$$\mathrm{d}\widehat{t}\, \mathrm{d}^3\mathbf{x} \sqrt{-\widehat{g}} = \mathrm{d}^4\widehat{x} \sqrt{-\widehat{g}} = \Omega^4 \mathrm{d}t\, \mathrm{d}^3\mathbf{x} \sqrt{-g}, \tag{8.72}$$

where we have defined $\mathrm{d}^4\widehat{x} \equiv \mathrm{d}\widehat{t}\, \mathrm{d}^3\mathbf{x}$ and used the relation $\widehat{g} = \Omega^6 g$ for the

background FLRW metric. Third, using $\widehat{g}_{\mu\nu}$ we can calculate $\widehat{R}$ and relate it to R computed using $g_{\mu\nu}$. This has already been done before—see ref. [114] or ref. [8] (or **Appendix C**)—with the following result

$$R = \Omega^2 \left[\widehat{R} + 6\widehat{\Box}\ln\Omega - 6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu \ln\Omega)(\widehat{\nabla}_\nu \ln\Omega)\right], \tag{8.73}$$

where $\widehat{\Box} \equiv \widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\widehat{\nabla}_\nu$ and $\widehat{\nabla}_\mu$ acts on an operand with respect to the metric $\widehat{g}_{\mu\nu}$. Moreover, due to our convention given by (8.70) and (8.71), the covariant derivative above is evaluated with respect to the coordinates $\{\widehat{x}^\mu\}$ and *not* with respect to $\{x^\mu\}$.[12] Furthermore, in performing integration involving $\widehat{\nabla}_\mu$, the metric compatibility in the Jordan frame, $\nabla_\mu g_{\alpha\beta} = 0$, is correspondingly reflected in the Einstein frame, $\widehat{\nabla}_\mu \widehat{g}_{\alpha\beta} = 0$.

The rest of the procedure for writing S in the Einstein frame from the Jordan frame can be implemented following the idea that the final form of the action should be that of the canonical case; that is, minimally coupled. From the action given by (8.28) we have

$$\begin{aligned}
S &= \frac{1}{2}\int \mathrm{d}^4x\,\sqrt{-g}\Big[M_{\rm Pl}^2 f R - g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi - 2V(\phi)\Big],\\
&= \frac{1}{2}\int \mathrm{d}\widehat{t}\,\mathrm{d}^3\mathbf{x}\,\sqrt{-\widehat{g}}\,\Omega^{-4}\Big[M_{\rm Pl}^2 f\Omega^2(\widehat{R} + 6\widehat{\Box}\ln\Omega - 6\widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\ln\Omega\,\widehat{\nabla}_\nu\ln\Omega)\\
&\qquad\qquad - \Omega^2\widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\phi\,\widehat{\nabla}_\nu\phi - 2V\Big]; \quad (\Omega^2 = f),\\
&= \frac{1}{2}\int \mathrm{d}^4\widehat{x}\sqrt{-\widehat{g}}\Big(M_{\rm Pl}^2\widehat{R} - 6M_{\rm Pl}^2\widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\ln\Omega\,\widehat{\nabla}_\nu\ln\Omega - \Omega^{-2}\widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\phi\,\widehat{\nabla}_\nu\phi - 2\Omega^{-4}V\Big),\\
&= \frac{1}{2}\int \mathrm{d}^4\widehat{x}\sqrt{-\widehat{g}}\Big[M_{\rm Pl}^2\widehat{R} - \tfrac{6}{4}M_{\rm Pl}^2\Omega^{-4}\widehat{g}^{\mu\nu}(\psi_{,\phi})^2\widehat{\nabla}_\mu\phi\,\widehat{\nabla}_\nu\phi - \Omega^{-2}\widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\phi\,\widehat{\nabla}_\nu\phi - 2\Omega^{-4}V\Big],\\
&= \frac{1}{2}\int \mathrm{d}^4\widehat{x}\sqrt{-\widehat{g}}\Big\{M_{\rm Pl}^2\widehat{R} - \widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\phi\,\widehat{\nabla}_\nu\phi\,\Omega^{-2}\Big[1 + \tfrac{6}{4}\,M_{\rm Pl}^2\Omega^{-2}(\psi_{,\phi})^2\Big] - 2\Omega^{-4}V\Big\},\\
S &= \frac{1}{2}\int \mathrm{d}^4\widehat{x}\sqrt{-\widehat{g}}\Big[M_{\rm Pl}^2\widehat{R} - \widehat{g}^{\mu\nu}\widehat{\nabla}_\mu\widehat{\phi}\,\widehat{\nabla}_\nu\widehat{\phi} - 2\widehat{V}(\phi)\Big],
\end{aligned} \tag{8.74}$$

[12] As noted in **Appendix C**, the equation above relating R and $\widehat{R}$ is also valid if we take $\widehat{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$ with all the derivatives evaluated with respect to $\{x^\mu\}$ (which is equal to $\{\widehat{x}^\mu\}$).

where we have chosen $\Omega^2 = f(\phi)$ and

$$\frac{\mathrm{d}\hat{\phi}}{\mathrm{d}\phi} = \Omega^{-1}\Big[1 + \tfrac{6}{4}\, M_{\rm Pl}^2 \Omega^{-2} (\psi_{,\phi})^2\Big]^{\frac{1}{2}} \quad \text{and} \quad V(\phi) = \Omega^{-4} V. \tag{8.75}$$

For $f(\phi) = 1 + \psi = 1 + M_{\rm Pl}^{-2}\xi\phi^2$, these imply

$$\frac{\mathrm{d}\hat{\phi}}{\mathrm{d}\phi} = \frac{\sqrt{1 + \psi(1 + 6\xi)}}{(1 + \psi)} \quad \text{and} \quad \widehat{V}(\phi) = \frac{V(\phi)}{(1 + \psi)^2}. \tag{8.76}$$

The good thing about the transformation to the Einstein frame is that all the background equations in the canonical case including the Friedmann equation, equation of motion, etc., are carried to the Einstein frame corresponding to the nonminimally coupled case in the Jordan frame, but with all the variables wearing a hat. Surprisingly, this correspondence also applies to all equations involving perturbations. This means that we can find the decomposition of the action into $S = S^{(0)} + S^{(2)} + S^{(3)} + \cdots$ with respect to ζ by following the decomposition $\widehat{S} = \widehat{S}^{(0)} + \widehat{S}^{(2)} + \widehat{S}^{(3)} + \cdots$ with respect to[13] $\widehat{\zeta}$ with the latter simply borrowing the results from the canonical case and putting a hat over all variables involved. Consequently, the Mukhanov-Sasaki equation, derivable from $\widehat{S}^{(2)}$,

$$\widehat{S}^{(2)} = \int \mathrm{d}\widehat{t}\, \mathrm{d}^3x \left[\widehat{a}^3 \widehat{\epsilon} \left(\frac{\mathrm{d}\widehat{\zeta}}{\mathrm{d}\widehat{t}}\right)^2 - \widehat{a}\, \widehat{\epsilon} (\partial\widehat{\zeta})^2\right], \tag{8.77}$$

from which we can compute the "bare" power spectrum, can simply be written following that of the canonical case. We have

$$\widehat{v}_k'' + \left(k^2 - \frac{\widehat{z}''}{\widehat{z}}\right)\widehat{v}_k = 0, \tag{8.78}$$

where

$$\widehat{\zeta} \equiv \frac{\widehat{v}}{\widehat{z}} \quad \text{and} \quad \widehat{z}^2 = 2\widehat{a}^2\widehat{\epsilon}, \tag{8.79}$$

[13] The quantity $\widehat{\zeta}$ should not be confused with the hatted ζ in **Sec. 5.1** denoting the operator $\hat{\zeta}$. In this section, we do not put hats on operators as operators are already clear from the context of discussion.

with

$$\widehat{\epsilon} \equiv -\frac{1}{\widehat{H}}\frac{\mathrm{d}\widehat{H}}{\mathrm{d}\widehat{t}} \quad \text{and} \quad \widehat{H} \equiv \frac{1}{\widehat{a}}\frac{\mathrm{d}\widehat{a}}{\mathrm{d}\widehat{t}}. \tag{8.80}$$

Observe that the derivative with respect to the conformal time has been written in the same way as that in the Jordan frame even though $\mathrm{d}\widehat{t} \neq \mathrm{d}t$, in general. This is because no distinction is necessary; that is, $\mathrm{d}\widehat{\tau} = \mathrm{d}\tau$, as can be easily verified.

Now, to solve for the "bare" power spectrum in nonminimally coupled chaotic inflation from the Mukhanov-Sasaki equation written in the Einstein frame above, we need to find $\widehat{\zeta}$ first and then relate it to ζ. The form of the scalar perturbation as defined by (4.37),

$$\zeta \equiv -\Psi - H\frac{\delta\rho}{\dot{\bar{\rho}}}, \tag{8.81}$$

seems to suggest a complex relationship between $\widehat{\zeta}$ and ζ. But as it turns out, surprisingly, $\widehat{\zeta} = \zeta$ (see refs. [33, 103, 115, 117])[14]. To see this, we follow the simple argument presented in ref. [117] applied to the case in hand. Under conformal transformation, the metric transforms to $\mathrm{d}\widehat{s}^2 = \Omega^2\mathrm{d}s^2$. It follows that

$$\widehat{g}_{ij} = \Omega^2 a^2 e^{2\zeta}\left(e^{\gamma}\right)_{ij}\mathrm{d}x^i\mathrm{d}x^j, \tag{8.82}$$

where we have also included the tensor perturbations so as not to repeat this simple calculation later. From the definition given by (8.70), namely, $\widehat{a} \equiv \Omega a$, we can rewrite this equation as

$$\widehat{g}_{ij} = \widehat{a}^2 e^{2\zeta}\left(e^{\gamma}\right)_{ij}\mathrm{d}x^i\mathrm{d}x^j. \tag{8.83}$$

However, we know that

$$\widehat{g}_{ij} = \widehat{a}^2 e^{2\widehat{\zeta}}\left(e^{\widehat{\gamma}}\right)_{ij}\mathrm{d}x^i\mathrm{d}x^j. \tag{8.84}$$

Consequently, $\widehat{\zeta} = \zeta$ and $\widehat{\gamma}_{ij} = \gamma_{ij}$.

This tells us that solving for $\widehat{\zeta}$ in the Mukhanov-Sasaki equation in the

[14] The last reference covers the proof considering the more general disformal transformation namely, $\widehat{g}_{\mu\nu} = \Omega^2(\phi)g_{\mu\nu} + \Gamma(\phi, X)\nabla_\mu\phi\,\nabla_\nu\phi$.

Einstein frame directly translates to solving for ζ. Should we then proceed with (8.78), all we need is to spell out $\widehat{z}''/\widehat{z}$ up to the desired order in the slow-roll parameters (that is, first order, as we previously mentioned,) and then use the method involving the Hankel-function approximation. And this is what we follow here except that at the outset, we express $\widehat{z}''/\widehat{z}$ in terms of the slow-roll parameters in the Jordan frame so as to avoid the difficulty expressing the result in the Jordan frame later.

Since $\widehat{z}^2 = 2\widehat{a}^2\,\widehat{\epsilon}$, and we have to find $\widehat{z}''$, then $\widehat{H}$ should be related to H and then $\widehat{\epsilon}$ to ϵ. For the Hubble parameter, we have from the second of (8.80),

$$\widehat{H} = \frac{1}{\Omega}\left(H + \frac{\dot{\Omega}}{\Omega}\right). \tag{8.85}$$

The relationship for the first slow-roll parameter in the two frames then follows by using the first of (8.80) and performing differentiation.

$$\widehat{\epsilon} = \left(1 + \frac{1}{H}\frac{\dot{\Omega}}{\Omega}\right)^{-2}\left[\epsilon + \frac{1}{H}\frac{\dot{\Omega}}{\Omega} + \frac{1}{H^2}\left(2\frac{\dot{\Omega}^2}{\Omega^2} - \frac{\ddot{\Omega}}{\Omega}\right)\right]. \tag{8.86}$$

This expression can be written in a more compact form by using the last of (8.55), leading to

$$\widehat{\epsilon} = \frac{\bar{\epsilon}}{\Omega^2}\left(1 + \frac{\dot{\psi}}{2H\Omega^2}\right)^{-2}\left(1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{\Omega^2}\right), \tag{8.87}$$

and then defining

$$p_1 \equiv 1 + \beta \quad \text{and} \quad p_2 \equiv 1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{\Omega^2}, \tag{8.88}$$

where $\beta = \dot{\psi}/2H\Omega^2$ is another slow-roll parameter introduced in ref. [104], resulting in

$$\widehat{\epsilon} = \frac{\bar{\epsilon}}{\Omega^2}\frac{p_2}{p_1^2}. \tag{8.89}$$

It follows that in terms of quantities in the Jordan frame, $\widehat{z}$ can be written as

$$\widehat{z} = \frac{a\sqrt{2\bar{\epsilon}p_2}}{p_1}. \tag{8.90}$$

Double differentiation and division by $\widehat{z}$ then yields

$$\frac{\widehat{z}''}{\widehat{z}} = (aH)^2\bigg[2-\epsilon+\frac{3}{2}\frac{\dot{\bar{\epsilon}}}{H\bar{\epsilon}}+\frac{\ddot{\bar{\epsilon}}}{2H^2\bar{\epsilon}}-\frac{\dot{\bar{\epsilon}}^2}{4H^2\bar{\epsilon}^2}-\left(\frac{3}{H}+\frac{\dot{\bar{\epsilon}}}{H^2\bar{\epsilon}}\right)\left(\frac{\dot{p}_1}{p_1}-\frac{\dot{p}_2}{2p_2}\right)$$
$$-\frac{1}{H^2}\left(\frac{\ddot{p}_1}{p_1}-\frac{\ddot{p}_2}{2p_2}\right)+\frac{1}{H^2}\left(\frac{2\dot{p}_1^2}{p_1^2}-\frac{\dot{p}_1\dot{p}_2}{p_1p_2}-\frac{\dot{p}_2^2}{4p_2^2}\right)\bigg],$$
$$\frac{\widehat{z}''}{\widehat{z}} = (aH)^2\Big[2-\epsilon+\tfrac{3}{2}\bar{\epsilon}_2+\epsilon_s+\mathcal{O}(\epsilon^2)\Big], \tag{8.91}$$

where $\epsilon_s = \epsilon_s(p_1, p_2, \dot{p}_1, \dot{p}_2)$ includes the first-order terms due to the nonminimal-coupling term, and $\bar{\epsilon}_2$ is defined as $\dot{\bar{\epsilon}} \equiv H\bar{\epsilon}\bar{\epsilon}_2$ following the definition of the Hubble-flow parameters given in **Sec. 4.1**; that is, $\dot{\bar{\epsilon}}_n \equiv H\bar{\epsilon}_n\bar{\epsilon}_{n+1}$ with $n = 1, 2, 3, \cdots$.

The Mukhanov-Sasaki equation for $\widehat{v}_k$ can be written in terms of the conformal time as the independent variable (and slow-roll parameters) by relating the coefficient $(aH)^2$ above in the expression for $\widehat{z}''/\widehat{z}$, to τ. From (6.4) or more practically, (6.7), we have

$$(aH)^2 = \frac{1}{\tau^2}(1+\epsilon+\cdots)^2. \tag{8.92}$$

Then

$$\widehat{v}_k'' + \left[k^2 - \frac{1}{\tau^2}\Big(2+3\tilde{\epsilon}_s+\tfrac{3}{2}\,\bar{\epsilon}_2\Big)\right]\widehat{v}_k = 0,$$
$$\widehat{v}_k'' + \left[k^2 - \frac{1}{\tau^2}\left(\tilde{\nu}_s^2-\frac{1}{4}\right)\right]\widehat{v}_k = 0, \tag{8.93}$$

where $\tilde{\epsilon}_s \equiv \epsilon + \epsilon_s/3$ and $\tilde{\nu}_s \equiv \frac{3}{2} + \tilde{\epsilon}_s + \frac{1}{2}\bar{\epsilon}_2$.

Observe that the last numbered equation above takes the same form as that of the minimal case. Noting that

$$\widehat{\zeta}_k = \frac{\widehat{v}_k}{\widehat{z}} \quad \text{and} \quad \zeta_k = \frac{v_k}{z}, \tag{8.94}$$

with $\widehat{\zeta}_k = \zeta_k$, we find that in the short-wavelength limit, $\widehat{v}_k \sim 1/\sqrt{k}$ and $v_k \sim 1/\sqrt{k}$. It follows that $k^3v_k^2 \sim k^2$ in the mentioned limit, and the two-point

function (see (7.21) and (7.22))

$$\langle\zeta(\tau,\mathbf{x}_1)\zeta(\tau,\mathbf{x}_2)\rangle = \int \frac{\mathrm{d}k}{k}\frac{\sin k|\mathbf{x}_1-\mathbf{x}_2|}{k|\mathbf{x}_1-\mathbf{x}_2|}\Delta_s^2(k,\tau), \tag{8.95}$$

is quadratically divergent in the coincidence limit $\mathbf{x}_1 \to \mathbf{x}_2$. We thus, see that the divergence of the two-point function in the minimally coupled case is carried to the nonminimally coupled case in exactly the same form. As such, based on the argument in the previous chapter, this calls for a regularization procedure that when applied to the two-point function is correspondingly reflected in the regularization of the power spectrum.

In the next section we concentrate on the subtraction term and adiabatic regularization, while in this section, as we have already mentioned in the beginning, we deal with the "bare" power spectrum. With the form of the Mukhanov-Sasaki equation given by the last of (8.93), it is now straightforward to use the method based on Hankel-function approximation to find the "bare" power spectrum. In fact, because it shares exactly the same form as that of the minimal case, we can simply borrow the result in **Sec. 6.1** given by (6.19).

$$\begin{aligned}
\widehat{v}_k &= -\frac{i}{\sqrt{\pi k}}\frac{2^{\tilde{\nu}_s}}{2}e^{i\frac{\pi}{4}(2\tilde{\nu}_s+1)}x^{\frac{1}{2}-\tilde{\nu}_s}\Gamma(\tilde{\nu}_s); \quad (x=-k\tau),\\
|\widehat{v}_{k*}| &= \frac{1}{\sqrt{\pi k}}\frac{2^{\tilde{\nu}_{s*}}}{2}(1+\epsilon_*)^{\frac{1}{2}-\tilde{\nu}_{s*}}\Gamma(\tilde{\nu}_{s*}),\\
&= \frac{\sqrt{2}}{\sqrt{\pi k}}\Big[1+(\tilde{\epsilon}_{s*}+\tfrac{1}{2}\,\bar{\epsilon}_{2*})\ln 2\Big](1-\epsilon_*)\Big[\Gamma(\tfrac{3}{2})+(\tilde{\epsilon}_{s*}+\tfrac{1}{2}\,\bar{\epsilon}_{2*})\Gamma'(\tfrac{3}{2})\Big],\\
|\widehat{v}_{k*}| &= \frac{\sqrt{2}}{2\sqrt{k}}\Big[1-\epsilon_*+\Big(\tilde{\epsilon}_{s*}+\tfrac{1}{2}\,\bar{\epsilon}_{2*}\Big)(2-\gamma-\ln 2)\Big].
\end{aligned} \tag{8.96}$$

Note that starting from the second equality, each expression is evaluated at the horizon crossing in the Jordan frame ($k=aH$) and *not* in the Einstein frame ($k=\widehat{a}\widehat{H}$) since we are after $\Delta_s^{2(b)}$ in the former frame where the original model is in place. It is worth noting that $aH \neq \widehat{a}\widehat{H}$ so the times of horizon crossing in the two frames differ; however, since $\widehat{\tau}=\tau$ then

$$(\widehat{a}\widehat{H}) = -\frac{1}{\widehat{\tau}}(1+\widehat{\epsilon}+\cdots) \approx (aH)(1+\text{small correction}), \tag{8.97}$$

provided that the slow-roll parameters in the Einstein frame like those in the Jordan frame, are small in comparison to unity. (This means $|\dot{\Omega}/\Omega H| \ll$

1, $|\ddot{\Omega}/\Omega H^2| \ll 1$, etc.)

Continuing, we perform a substitution from the last expression above for $\widehat{v}_k$ in the equation for the "bare" power spectrum.

$$\begin{aligned}
\Delta_s^{2(b)} &= \frac{k^3}{2\pi^2}\left|\frac{\widehat{v}_{k*}}{\widehat{z}_*}\right|^2, \\
&= \frac{k^2}{4\pi^2}\Big[1-2\epsilon_* + (2\tilde{\epsilon}_{s*}+\bar{\epsilon}_{2*})(2-\gamma-\ln 2)\Big]\left(\frac{p_{1*}^2}{2a_*^2\bar{\epsilon}_* p_{2*}}\right), \\
&= \frac{H_*^2}{8\pi^2\bar{\epsilon}_* p_{2*}}\big[1-2\epsilon_*+2\beta_*+(2\tilde{\epsilon}_{s*}+\bar{\epsilon}_{2*})(2-\gamma-\ln 2)\big], \\
\Delta_s^{2(b)} &= \frac{H_*^2}{8\pi^2 p_{2*}\bar{\epsilon}_*}(1+\tilde{\mu}_{s*}),
\end{aligned} \tag{8.98}$$

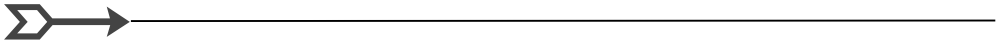
Analogous to μ_{s*} in the minimally coupled case, we have defined $\tilde{\mu}_{s*} \equiv -2\epsilon_* + 2\beta_* + (2\tilde{\epsilon}_{s*}+\bar{\epsilon}_{2*})(2-\gamma-\ln 2)$ for the nonminimally coupled case.

For $\psi = \xi\phi^2/M_{\rm Pl}^2$, the quantity $p_2 \approx 1+6\xi$ and we can rewrite the "bare" power spectrum as

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$$\Delta_s^{2(b)} = \frac{H_*^2}{8\pi^2\bar{\epsilon}_*(1+6\xi)}(1+\tilde{\mu}_{s*}), \tag{8.99}$$

which is our desired expression. Apart from the small correction $\tilde{\mu}_{s*}$ due to the contribution from slow-roll parameters, this result is in agreement[15] with refs. [104, 103] obtained using a slightly different method. Ignoring the difference in the magnitudes of μ_{s*} and $\tilde{\mu}_{s*}$, this is the same as that of canonical case—see the last of (6.26)—except for the extra divisor $(1+6\xi)$ (that seems to have been missed or intentionally omitted in the more recent calculation in ref. [116]) marking the effect of nonminimal coupling.



[15] The authors did not include the slow-roll correction $\tilde{\mu}_{s*}$ in their result. In fact, as far as adiabatic regularization is concerned, the small correction is unnecessary and we could have just simply borrowed the results in refs. [104, 103]. However, as we have already witnessed in the previous chapter, there are indications that in general, the regularized power spectrum is simply the "bare" power spectrum. As such, there is no harm and in fact, we view it as practically useful for comparison with experiments, that we have a relatively more precise expression for the "bare" power spectrum.

Example 3. ***Comparison of*** $\lambda^{(\xi>1)}$ ***and*** $\lambda^{(\xi=0)}$**.** The addition of nonminimal-coupling term in the form $\xi\phi^2 R/M_{\rm Pl}^2$ changes the constraint on the self-coupling constant λ in the potential $V = \lambda\phi^4/8$, depending on the value of ξ. In **Sec. 8.1**, we quoted one of the main results of the work of Fakir and Unruh [101] namely,

$$\lambda^{(\xi>1)} \approx 48 N_e \xi^2 \lambda^{(\xi=0)}, \tag{8.100}$$

establishing the relationship between λ in minimally and nonminimally coupled cases. Show this relationship.

Solution. To establish the relationship above between $\lambda^{(\xi>1)}$ and $\lambda^{(\xi=0)}$ we equate the two expressions for the power spectra corresponding to the minimally and nonminimally coupled cases. For the former we have from (8.25),

$$\Delta_s^{2(\xi=0)} \approx \frac{\lambda^{(\xi=0)} N_e^3}{3\pi^2}. \tag{8.101}$$

For the latter we have from (8.99),

$$\Delta_s^{2(\xi>1)} = \frac{H_*^2}{8\pi^2 \bar{\epsilon}_* (1+6\xi)}, \tag{8.102}$$

where $\bar{\epsilon}_* = \dot{\phi}^2/2H^2$. We can write $\dot{\phi}$ in terms of ϕ using the expression for $3H\dot{\phi}$ and H^2 given by the last of (8.61) and (8.63) respectively.

$$\begin{aligned}
\bar{\epsilon} &\approx \left\{ \frac{1}{3H} \frac{\lambda\phi^3}{2[1+\psi(1+6\xi)]} \right\}^2 \frac{1}{2H^2}, \\
&\approx \frac{\lambda^2\phi^6}{2(36)[1+\psi(1+6\xi)]^2} \frac{24(24)\xi^2}{\lambda^2\phi^4}, \\
\bar{\epsilon} &\approx \frac{8\xi^2\phi^2}{\psi^2(1+6\xi)^2}.
\end{aligned} \tag{8.103}$$

Substituting this in the expression for $\Delta_s^{2(\xi>1)}$ above we find

$$\begin{aligned}
\Delta_k^{2(\xi>1)} &\approx \frac{H_*^2}{8\pi^2(1+6\xi)} \frac{\psi_*^2(1+6\xi)^2}{8\xi^2\phi_*^2}, \\
\Delta_k^{2(\xi>1)} &\approx \frac{\lambda\psi_*^2(1+6\xi)}{24(8)(8)\pi^2\xi^3}.
\end{aligned} \tag{8.104}$$

In the previous section, we calculated the number of e-folds as (see (8.69))

$$N_e \approx \frac{1+6\xi}{8\xi}\psi_i, \tag{8.105}$$

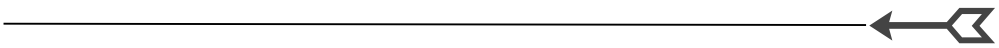
where we may take $\psi_i \approx \psi_*$. Then

$$\Delta_s^{2(\xi>1)} \approx \frac{\lambda N_e^2}{24\pi^2\xi(1+6\xi)} \approx \frac{\lambda N_e^2}{24(6)\pi^2\xi^2}. \tag{8.106}$$

Equating the right hand side to that of the approximation for $\Delta_s^{2(\xi=0)}$ above yields

$$\lambda^{(\xi>1)} \approx 48 N_e \xi^2 \lambda^{(\xi=0)}, \tag{8.107}$$

which was to be shown. As already discussed in the last part of **Sec. 8.1**, for large enough ξ, say 10^3, the inflaton self-coupling constant avoids getting too close to zero (e.g., less than 10^{-10}), leveling it to typical field theory values (e.g., $\sim 10^{-2}$).



"Bare" Tensor Power Spectrum

Let us now turn our attention to tensor perturbations. To write the equation of motion, we simply borrow the expression from the canonical case and put a hat over the variables involved. From (7.65) or (5.101) we have

$$\begin{aligned}
\widehat{u}_k'' + \left(k^2 - \frac{\widehat{a}''}{a}\right)\widehat{u}_k &= 0,\\
\widehat{u}_k'' + \left[k^2 - (aH)^2\left(2 - \epsilon + \frac{3}{H}\frac{\dot{\Omega}}{\Omega} + \frac{1}{H^2}\frac{\ddot{\Omega}}{\Omega}\right)\right]\widehat{u}_k &= 0,\\
\widehat{u}_k'' + \left[k^2 - \frac{1}{\tau^2}\left(2 + 3\epsilon + \frac{3\dot{\psi}}{2H\Omega^2} + \frac{\ddot{\psi}}{2H^2\Omega^2} - \frac{\dot{\psi}^2}{4H^2\Omega^4}\right)\right]\widehat{u}_k &= 0,\\
\widehat{u}_k'' + \left[k^2 - \frac{1}{\tau^2}(2 + 3\tilde{\epsilon}_t)\right]\widehat{u}_k &= 0,
\end{aligned} \tag{8.108}$$

where $\tilde{\epsilon}_t \equiv \epsilon + \epsilon_t/3$ and

$$\epsilon_t \equiv \frac{3\dot{\psi}}{2H\Omega^2} + \frac{\ddot{\psi}}{2H^2\Omega^2} - \frac{\dot{\psi}^2}{4H^2\Omega^4}. \tag{8.109}$$

Similar to that of the scalar perturbations, the exact matching of the form of the Mukhanov-Sasaki equations for the minimally and nonminimally coupled cases, cf. first of (6.32), and the relation we established above that $\widehat{\gamma}_{ij} = \gamma_{ij}$, tell us that in the short-wavelength limit, $k^3|u_k/a|^2 \sim k^2$. This renders the two-point function of tensor perturbations,

$$\langle \gamma_{ij}(\tau, \mathbf{x}_1)\gamma^{ij}(\tau, \mathbf{x}_2)\rangle = \int \frac{\mathrm{d}k}{k} \frac{\sin k|\mathbf{x}_1 - \mathbf{x}_2|}{k|\mathbf{x}_1 - \mathbf{x}_2|} \left(\frac{2k^3}{\pi^2}\left|\frac{u_k^s}{a}\right|^2\right) \tag{8.110}$$

(see (5.105)) quadratically divergent in the coincident limit $\mathbf{x}_1 \to \mathbf{x}_2$, indicating that the divergence in the two-point function is carried from the minimal case to the nonminimal case. Similar to that of the minimal case, adiabatic regularization removes this divergence by consistently subtracting out the problematic terms. The consistent application of such a subtraction procedure is correspondingly reflected as a regularization of the power spectrum which is the main subject of this work. We perform such regularization after we finish computing the "bare" power spectrum, in the next section.

Continuing from the last equation above for $\widehat{u}_k$, we let $\tilde{\nu}_t^2 \equiv \frac{3}{2} + \tilde{\epsilon}_t$. Then

$$\widehat{u}_k'' + \left[k^2 - \frac{1}{\tau^2}\left(\tilde{\nu}_t^2 - \frac{1}{4}\right)\right]\widehat{u}_k = 0. \tag{8.111}$$

Following the logic leading to the first of (8.96) for scalar perturbations[16] we find upon taking into account that $\tilde{\nu}_t$ does not involved the term $\bar{\epsilon}_2$ in $\tilde{\nu}_s$ to first-order approximation,

$$\widehat{u}_k = -\frac{i}{\sqrt{\pi k}}\frac{2^{\tilde{\nu}_t}}{\sqrt{2}} e^{i\frac{\pi}{4}(2\tilde{\nu}_t+1)} x^{\frac{1}{2}-\tilde{\nu}_t}\Gamma(\tilde{\nu}_t); \quad (x = -k\tau),$$

$$|\widehat{u}_{k*}| = \frac{2^{\tilde{\nu}_{t*}}}{\sqrt{2\pi k}}(1+\epsilon_*)^{\frac{1}{2}-\tilde{\nu}_{t*}}\Gamma(\tilde{\nu}_{t*}),$$

[16] Note that one might be tempted to simply copy the result from (6.34) in the minimal case and change ϵ to $\tilde{\epsilon}_t$. One should however, be careful since the *same* two epsilons in (6.34) are not the same in the nonminimal case. They become ϵ and $\tilde{\epsilon}_t$ as is shown in the detailed calculation below.

$$= \frac{2}{\sqrt{\pi k}}(1+\tilde{\epsilon}_{t*}\ln 2)(1-\epsilon_*)\Big[\Gamma(\tfrac{3}{2}) + (\tilde{\epsilon}_{t*} + \tfrac{1}{2}\,\bar{\epsilon}_{2*})\Gamma'(\tfrac{3}{2})\Big],$$

$$|\widehat{u}_{k*}| = \frac{1}{\sqrt{k}}\Big[1-\epsilon_* + \tilde{\epsilon}_{t*}(2-\gamma-\ln 2)\Big]. \tag{8.112}$$

Substituting this in the working equation for the "bare" power spectrum gives us

$$\Delta_t^{2(b)} = \frac{2k^3}{\pi^2}\left|\frac{\widehat{u}_k}{\widehat{a}}\right|^2_{k=aH},$$

$$= \frac{2k^2}{\pi^2}\frac{1-2\epsilon_* + 2\tilde{\epsilon}_{t*}(2-\gamma-\ln 2)}{\widehat{a}_*^2},$$

$$\boxed{\Delta_t^{2(b)} = \frac{2H_*^2}{\pi^2\Omega_*^2}(1+\tilde{\mu}_{t*}),} \tag{8.113}$$

"Bare" Tensor Power Spectrum
Nonminimally Coupled
Chaotic Inflation

which is our sought-for expression. Here, $\tilde{\mu}_t \equiv 2\tilde{\epsilon}_{t*}(2-\gamma-\ln 2) - 2\epsilon_*$. In comparison to that of the minimal case, there is an extra divisor Ω_*^2 marking the effect of nonminimal coupling. This extra divisor apart from $\bar{\epsilon}_*$, is also what makes it different from that of the scalar perturbation in the nonminimally coupled case; see (8.99).

8.4 Adiabatic Regularization of Power Spectra

In the previous section we have calculated the "bare" power spectra of scalar and tensor perturbations. In so doing, we took advantage of the invariance of these perturbations under frame transformation from the Jordan frame to the Einstein. The flow of the calculation went from the Jordan frame where the original model was in place, then in the Einstein frame to easily solve the Mukhanov-Sasaki equation, and then back to the Jordan frame where we expressed the "bare" power spectra. We are now facing the task of performing adiabatic regularization and one may ask if we can easily follow the same route in the computation of $\Delta^{2(s)}$. Crucial in answering this question, in the same way as that for $\Delta^{2(b)}$, is the frame invariance of $\zeta^{(s)}$ and $\gamma_{ij}^{(s)}$.

A moment's thought on this matter may lead us to the idea that if adiabatic regularization is a consistent regularization procedure then, if $\zeta_k^{(b)}$ and$\gamma_{ij,k}^{(b)}$

are frame-invariant then $\zeta_k^{(s)}$ and $\gamma_{ij,k}^{(s)}$ should also be frame-invariant. Rather informally, what adiabatic regularization does is simply isolate the divergent-yielding parts of $(\zeta_k^{(b)}, \gamma_{ij,k}^{(b)})$ through the adiabatic decomposition and then subtract them away. Since $(\zeta_k^{(b)}, \gamma_{ij,k}^{(b)})$ are frame-invariant, the divergent-yield parts are also frame-invariant. To argue in support of this position, we need to only look at the "sources" of $(\zeta_k^{(b)}, \gamma_{ij,k}^{(b)})$ and $(\zeta_k^{(s)}, \gamma_{ij,k}^{(s)})$. The former quantities are solutions of their corresponding Mukhanov-Sasaki equations. The latter quantities on the other hand, satisfy the *same* pair of Mukhanov-Sasaki equations (for scalar and tensor perturbations) up to a certain desired adiabatic order (that we choose consistent with the minimal subtraction scheme). As such, consistency-wise, the frame invariance of $\zeta_k^{(b)}$ implies the same for $\zeta_k^{(s)}$, and the same goes for tensor perturbations.[17]

Behavior of the Regularized Scalar Power Spectrum

Having established the frame invariance of $\zeta_k^{(s)}$, it is now straightforward to calculate the subtraction term for scalar perturbations, namely,

$$\Delta_s^{2(s)} = \frac{k^3}{2\pi^2}\left|\zeta_k^{(s)}\right|^2. \tag{8.114}$$

(As usual, we tackle the tensor perturbations later.) Since

$$\zeta_k^{(s)} = \widehat{\zeta}_k^{(s)} = \frac{\widehat{v}_k^{(s)}}{\widehat{z}}, \quad \text{and} \quad \left|\widehat{v}_k^{(s)}\right|^2 = \frac{1}{2\widehat{W}}, \tag{8.115}$$

we need to find $\widehat{W}$. From the working equation for the minimal case given by (7.31) we have

$$\frac{\widehat{W}''}{2\widehat{W}} - \frac{3}{4}\frac{\widehat{W}'^2}{\widehat{W}^2} + \widehat{W}^2 - k^2 + \frac{\widehat{z}''}{\widehat{z}} = 0. \tag{8.116}$$

It is then a matter of decomposing $\widehat{W}$ into $\widehat{\omega}_0 + \widehat{\omega}_1 + \widehat{\omega}_2 + \cdots$, and solving the above equation order-by-order, to calculate $v_k^{(s)}$, and then $\zeta_k^{(s)}$ which in turn, leads to $\Delta_s^{2(s)}$.

The potential term in the working equation for $\widehat{W}$ is given by the second of

[17] For an explicit calculation demonstrating this up to second adiabatic order, interested readers are referred to ref. [73].

(8.91), namely,

$$\widehat{U}_s = \frac{\widehat{z}''}{\widehat{z}} = (aH)^2\Big[2 - \epsilon + \tfrac{3}{2}\bar{\epsilon}_2 + \epsilon_s + \mathcal{O}(\epsilon^2)\Big]. \tag{8.117}$$

Observe that it is second adiabatic order (due to the double prime on $\widehat{z}$ or, the factor H^2). Taking this into consideration in the order-by-order calculation of $\widehat{W}$, following essentially the same computation given by (7.32), we find

$$\widehat{\omega}_0 = k, \qquad \widehat{\omega}_1 = \widehat{\omega}_3 = 0, \qquad \widehat{\omega}_2 = -\frac{U_s}{2\widehat{\omega}_0}. \tag{8.118}$$

Noting that the odd-ordered parts at least up to third adiabatic order are vanishing, we have essentially calculated $\widehat{W}$ up to second adiabatic order only, consistent with the prescription of the minimal subtraction scheme. To see this once again, now in the nonminimally coupled case, we substitute the results above in the expression for $|\widehat{v}_k^{(s)}|^2$ above.

$$\begin{aligned}
\Big|\widehat{v}_k^{(s)}\Big|^2 &= \frac{1}{2\widehat{W}} = \frac{1}{2\widehat{\omega}_0} - \frac{\widehat{\omega}_2}{2\widehat{\omega}_0^2},\\
\Big|\widehat{v}_k^{(s)}\Big|^2 &= \frac{1}{2k} + \frac{(aH)^2}{2k^3}\Big(1 - \tfrac{1}{2}\,\epsilon + \tfrac{3}{4}\,\bar{\epsilon}_2 + \tfrac{1}{2}\,\epsilon_s\Big).
\end{aligned} \tag{8.119}$$

The first term in the right hand side is $\sim 1/k$ while the second term is $\sim 1/k^3$. Following the logic leading to (7.33) suggesting a sequence $1/k$, $1/k^3$, $1/k^5$, $\cdots$, the third term in line would have been $\sim 1/k^5$ which would overshoot the requirement to just remove the divergence in the two-point function $\langle\zeta(\tau,\mathbf{x}_1)\zeta(\tau,\mathbf{x}_2)\rangle$ in the coincident limit (see (8.95)).

With $|v_k^{(s)}|$ in hand, we can now finally write down the expression for the subtraction term using the expression for $\Delta_s^{2(s)}$ above. We have upon further using (8.90) for $\widehat{z}$

$$\begin{aligned}
\Delta_s^{2(s)} &= \frac{k^3}{2\pi^2}|\zeta_k^{(s)}|^2 = \frac{k^3}{2\pi^2}|\widehat{\zeta}_k^{(s)}|^2,\\
&= \frac{k^3}{2\pi^2}\left|\frac{\widehat{v}_k^{(s)}}{\widehat{z}}\right|^2,\\
\Delta_s^{2(s)} &= \frac{k^2 p_1^2}{8\pi^2 a^2 \bar{\epsilon} p_2}\left[1 + \frac{(aH)^2}{k^2}\Big(1 - \tfrac{1}{2}\,\epsilon + \tfrac{3}{4}\,\bar{\epsilon}_2 + \tfrac{1}{2}\,\epsilon_s\Big)\right].
\end{aligned} \tag{8.120}$$

Since $p_1 \equiv 1+\beta$ from the first of (8.88) and we are considering the superhorizon limit $k \ll aH$, then

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$$\Delta_s^{2(s)} = \frac{H^2}{8\pi^2 \bar{\epsilon} p_2}(1+\tilde{\alpha}_s), \tag{8.121}$$

where $\tilde{\alpha} \equiv 2\beta - \frac{1}{2}\,\epsilon + \frac{3}{4}\,\bar{\epsilon}_2 + \frac{1}{2}\,\epsilon_s$. Comparing it with that of the canonical case computable by setting $c_s^2 = 1$ in the third of (7.34), we see that the only essential difference attributable to the nonminimal coupling is the presence of the term p_2 in the denominator. We will see below how it may possibly affect the behavior of the regularized power spectrum.

The regularized power spectrum is the difference between the "bare" power spectrum and the subtraction term.

$$\Delta_s^{2(r)} = \Delta_s^{2(b)} - \Delta_s^{2(s)}. \tag{8.122}$$

Performing substitution from the equation for the "bare" power spectrum given by the last of (8.98) of the previous section, and the expression for the subtraction term above we find

Regularized Scalar Power Spectrum (Nonminimally Coupled)

$$\Delta_s^{2(r)} = \frac{H_*^2}{8\pi^2 p_{2*}\bar{\epsilon}_*}\left[1+\tilde{\mu}_{s*} - (1+\tilde{\alpha}_s)\frac{H^2}{H_*^2}\frac{\bar{\epsilon}_*}{\bar{\epsilon}}\frac{p_{2*}}{p_2}\right],$$

which is our sought-for expression for the regularized power spectrum. Observe that in the limit as $\xi \to 0$, the quantity p_2 defined by the second of (8.88) behaves as

$$p_2 \equiv 1 + \frac{3M_{\rm Pl}^2}{2}\frac{\psi_{,\phi}^2}{\Omega^2} \to 1 \tag{8.123}$$

because $\psi = \xi\phi^2/M_{\rm Pl}^2$ and $\Omega^2 = 1+\psi$. In such a limit $\Delta_s^{2(r)}$ reduces to the result of Urakawa and Starobinsky [87] for scalar perturbations in the canonical case; see (7.37).

In the nonminimally coupled case we have to mind the behavior of p_2 in addition to those of H and $\bar{\epsilon}$. It has already been established in the previous chapter dealing with the minimal case, that H exponentially decays with the

number of e-folds; that is, from (7.39),

$$\left(\frac{H}{H_*}\right)^2 = \exp\left(-2\int_{N_*}^{N} \mathrm{d}\tilde{N}\,\epsilon(\tilde{N})\right). \tag{8.124}$$

This equation holds even in the nonminimal case because the nonminimal coupling term is *not* directly involved in the equation for H/H_*. Likewise, $\bar{\epsilon}$ at least on average, increases as inflation progresses. Now, for the term p_{2*} we have

$$p_{2*} = 1 + \frac{6\xi^2 M_{\mathrm{Pl}}^{-2}\phi_*^2}{1+\xi M_{\mathrm{Pl}}^{-2}\phi_*^2},$$
$$p_{2*} \approx 1 + 6\xi. \tag{8.125}$$

On the other hand,

$$p_2 = \frac{1+\xi M_{\mathrm{Pl}}^{-2}\phi^2 + 6\xi^2 M_{\mathrm{Pl}}^{-2}\phi^2}{1+\xi M_{\mathrm{Pl}}^{-2}\phi^2}. \tag{8.126}$$

Near the end of inflation $\xi M_{\mathrm{Pl}}^{-2}\phi^2 \sim 1$ (see ref. [101] or the last subsection under **Sec. 8.2**.) As such, in the long run, $p_2 \sim 1 + 3\xi$. Although the ratio p_{2*}/p_2 increases with N, it is bounded from above by a constant number of the order unity. It follows that it cannot compete with the multiplicative decaying effect due to H/H_* and $\bar{\epsilon}_*/\bar{\epsilon}$. Hence, similar to that of the minimally coupled case, the expansion of the Universe during inflation (and even after but before structure formation) effectively washes out the subtraction term, and the regularized power spectrum tends to the "bare" power spectrum.

Behavior of the Regularized Tensor Power Spectrum

Following the same logical pathway as that for scalar perturbation, noting that we already have the "bare" power spectrum, we calculate the second piece namely, the subtraction term,

$$\Delta_t^{2(s)} = \frac{2k^3}{\pi^2}\left|\frac{\widehat{u}_k^{(s)}}{\widehat{a}}\right|^2, \tag{8.127}$$

to finally accomplish adiabatic regularization. To derive the subtraction term, we need to find

$$|u_k^{(s)}|^2 = \frac{1}{\widehat{W}}, \tag{8.128}$$

using the working equation for $\widehat{W}$. Such a working equation should be straightforward from that of the scalar perturbation given by (8.116); we need to simply change the potential term $\widehat{z}''/\widehat{z}$ to $\widehat{a}''/\widehat{a}$.

$$\frac{\widehat{W}''}{2\widehat{W}} - \frac{3}{4}\frac{\widehat{W}'^2}{\widehat{W}^2} + \widehat{W}^2 - k^2 + \frac{\widehat{a}''}{\widehat{a}} = 0. \tag{8.129}$$

The potential term can be written out explicitly in terms of H, ϵ, and Ω as

$$\begin{aligned} U_t &= (aH)^2\left(2 - \epsilon + 3\beta - \beta\epsilon + \beta^2 + \frac{\dot{\beta}}{H}\right), \\ U_t &= 2(aH)^2(1 + \tilde{\alpha}_t), \end{aligned} \tag{8.130}$$

where $\tilde{\alpha}_t \equiv -\frac{1}{2}\epsilon + \frac{3}{2}\beta - \frac{1}{2}\beta\epsilon + \frac{1}{2}\beta^2 + \frac{1}{2}\frac{\dot{\beta}}{H}$ with being β given by the definition stated below (8.88); that is, $\beta \equiv \dot{\psi}/2H\Omega^2$. Noting that the potential is second adiabatic order, the decomposition $\widehat{W} = \widehat{\omega}_0 + \widehat{\omega}_1 + \widehat{\omega}_2 + \widehat{\omega}_3 + \cdots$ results in

$$\widehat{\omega}_0 = k, \qquad \widehat{\omega}_1 = \widehat{\omega}_3 = 0, \qquad \widehat{\omega}_2 = -\frac{U_t}{2\widehat{\omega}_0}. \tag{8.131}$$

It follows that

$$\begin{aligned} \left|\widehat{u}_k^{(s)}\right|^2 &= \widehat{W}^{-1} = \frac{1}{\widehat{\omega}_0} - \frac{\widehat{\omega}_2}{\widehat{\omega}_0^2}, \\ \left|\widehat{u}_k^{(s)}\right|^2 &= \frac{1}{k} + \frac{(aH)^2}{k^3}(1 + \tilde{\alpha}_t). \end{aligned} \tag{8.132}$$

Performing substitution from the last equation above for $|\widehat{u}_k^{(s)}|^2$ into the expression for the subtraction term, we get

$$\Delta_t^{2(s)} = \frac{2k^2}{\pi^2\Omega^2 a^2}\left[1 + \left(\frac{aH}{k}\right)^2(1 + \tilde{\alpha}_t)\right],$$

$$\Delta_t^{2(s)} = \frac{2H^2}{\pi^2\Omega^2}(1+\tilde{\alpha}_t), \tag{8.133}$$

Subtraction Term (Tensor)
Nonminimally Coupled
Chaotic Inflation

where we have taken the limit $k \ll |aH|$ corresponding to superhorizon modes. The last equation above is our sought-for expression for the subtraction term. Note that apart from the small correction due to the slow-roll parameters encoded in $\tilde{\alpha}$, the only main difference with the minimal case (see (7.70)) is the presence of the extra factor Ω^2 in the denominator, marking the effect of nonminimal coupling. This same term can be found in the equation for the "bare" power spectrum in the form of Ω_*. We will see below how this might affect the behavior of the regularized power spectrum.

The regularized power spectrum of tensor perturbations is the difference between $\Delta_t^{2(b)}$ given by the last of (8.113) and $\Delta_t^{2(s)}$ given by the equation we have just derived above. We have

$$\Delta_t^{2(r)} = \frac{2H_*^2}{\pi^2\Omega_*^2}(1+\tilde{\mu}_{t*}) - \frac{2H^2}{\pi^2\Omega^2}(1+\tilde{\alpha}_t),$$

$$\Delta_t^{2(r)} = \frac{2H_*^2}{\pi^2\Omega_*^2}\left[1+\tilde{\mu}_{t*} - (1+\tilde{\alpha}_t)\frac{H^2}{H_*^2}\frac{\Omega_*^2}{\Omega^2}\right], \tag{8.134}$$

Regularized Tensor
Power Spectrum
(Nonminimally Coupled)

which was to be derived. In the limit as $\xi \to 0$, the conformal scale factor Ω^2 tends to unity, and the expression above reduces to that of the (minimally coupled) canonical case.

The behavior of the regularized power spectrum depends on the behavior of Ω^2 in addition to that of H. The latter has already been elaborated in the previous chapter and reiterated above (see (8.124)) for the scalar perturbation; that is, it is exponentially decaying with the number of e-folds. For the factor Ω_*^2/Ω^2 we note that inflation starts with large field value; in particular, $\psi_* = \xi\phi_*^2/M_{\rm Pl}^2 \gg 1$. Then it continues until $\psi \sim 1$. As such, Ω_*^2/Ω^2 is increasing during the course of inflation, but it is bounded from above. Based on (8.69) (or see ref. [101] or ref. [104]), $\Omega_*^2 \sim \mathcal{O}(N_e)$. Consequently, $\Omega_*^2/\Omega^2 \sim \mathcal{O}(N_e)$ long after horizon crossing and we find that the factor involving Ω cannot compete with the exponential "damping" due to the factor involving H. Hence, similar to that of the minimally coupled case, if we follow the subtraction term long enough, it becomes insignificant compared to the "bare" power spectrum; the

regularized power spectrum approaches the "bare" power spectrum.

8.5 Implications of Differing Regularized and "Bare" Power Spectra

Our current understanding tells us that the primordial cosmological perturbations gave rise to the Universe that we have today. Since the power spectrum is a statistical measure of dispersion of the primordial cosmological perturbations, "altering" its value possibly by way of regularization must have some experimental/physical consequences; that is, some predictions might be modified or if the use of the "bare" power spectrum within the framework of one model is consistent with experiment, such consistency might be broken. In this section, we ask the question, "What would change if the (physical) regularized power spectrum would significantly deviate from the 'bare' power spectrum?" Here, we consider three quantities of observational and theoretical interest namely, the power spectrum itself, the spectral tilt, and the tensor-to-scalar ratio.[18]

Based on the latest CMB measurement made by the Planck collaboration, the scalar power spectrum is $\Delta_s^2(k) \approx 2.13 \times 10^{-9}$ [99]; see the part of **Sec. 8.1** containing (8.16). Since the power spectrum depends on H^2 which in turn is related to the potential by the Friedmann equation, the change in Δ_s^2 would be reflected in the effective coupling constant of, or the parameters involved with, the field(s) contained in V. Such change would have important implications in our understanding of the relevant field interaction strength during the inflationary era, reheating, and energy scale at which inflation started.

For the spectral tilt, we note that adiabatic regularization does not alter the near-scale-invariant property of the power spectrum at least in the canonical case [90]. For more general single-field slow-roll inflation models, we expect (although this still requires a rigorous proof) the same should hold even in cases where the regularized power spectrum could be different from the "bare" power spectrum. The reason is that during inflation, the *physical* Hubble horizon $aR_H = a(1/aH) = 1/H$ is essentially constant because ϵ is closed to zero

[18] **Appendix D** gives a short discussion relating CMB temperature fluctuations and power spectrum of primordial cosmological perturbations.

during inflation. It follows that each mode follows essentially the same evolutionary pathway. The small deviation from perfect scale-invariance (to near scale-invariance) stems from the fact that ϵ is not exactly zero during inflation.

Lastly, the tensor-to-scalar ratio r would change if the tensor and scalar power spectra are not proportionately modified by regularization. Since adiabatic regularization involves subtraction instead of multiplication, we expect r to change if $\Delta^{2(r)}$ is significantly different from $\Delta^{2(b)}$. The latest Planck result tells us that[19] $r < 0.09$ at the 95% upper limits [99]. Some models of inflation have actually been strongly disfavored because of this result; e.g., *minimally* coupled chaotic inflation model with phi-fourth potential. If $\Delta^{2(r)}$ would be far different from $\Delta^{2(b)}$, some of the disfavored models of inflation could come back to life and some of those favored could fall out of acceptance.

The result of this study together with that of Urakawa and Starobinsky dealing with the canonical case, encompasses a wide variety of single-field inflation models namely, (minimally coupled) general single-field inflation and nonminimally coupled chaotic inflation—the regularized power spectrum is simply the "bare" power spectrum both for the tensor and scalar perturbations. It serves to strengthen if not restore the use of the "bare" power spectra in standard calculations. Had it been the other way around, the three implications above would make us rethink of the way we perform calculations of several physical observables in inflationary cosmology.

[19] This is with respect to the pivot scale 0.002 Mpc^{-1}.

Summary

Research Summary and Future Prospects

The power spectrum of primordial cosmological perturbations is one of the most significant physical quantities in inflationary cosmology. Because the Universe that we have today originated from these primordial cosmological perturbations (as what our current understanding tells us), the power spectrum bears an important relationship with the distribution of cosmic microwave background radiation, of galaxy clusters, and perhaps of the yet "undetected" dark matter. From theoretical-physics point of view, it is thus natural to demand a self-consistent calculation of the power spectrum. Part of the demand for this self-consistency is the absence of questionable divergences that could be present in the power spectrum itself as a mathematical artifact of one calculation scheme, or, in the two-point function of the cosmological perturbations in terms of which the power spectrum is defined.

It is along this line of thinking that this study is geared—a consistent calculation of the power spectrum. In particular, we explored two main areas of concern namely, (a) calculation of the power spectrum using one implementation of a promising semi-analytic method called the uniform approximation, and (b) adiabatic regularization of the power spectrum. The former is done within the framework of (minimally coupled) general single-field inflation where the part of the action involving the inflaton is a general functional of inflaton and the kinetic term. The latter is performed within the frameworks of two models of inflation namely, that of (a), and nonminimally coupled chaotic inflation. In both of these models, we assume the slow-roll inflation scenario.

Uniform Approximation. Setting aside the idea of quantization, the power spectrum is basically derived from the solution of Mukhanov-Sasaki equation. The method of uniform approximation is a promising semi-analytic approach to solve this equation with the important features that it is both systematically improvable and does not assume the constancy of the slow-roll parameters. In this work, we study the divergences in one significant implementation of this method in the calculation of the power spectrum. In particular, we find that the nature of all divergences in this implementation are logarithmic in nature. Furthermore, we discover that in this implementation, the power spectrum is finite only up to second order in the slow-roll parameters; from the third order onwards, it is logarithmically divergent.

Future Prospect. Beyond uncovering the nature of the divergence problem is the question of properly dealing with this problem—how do we solve the power spectrum using the method of uniform approximation up to *any* order in the slow-roll parameters without hitting divergence in the final result? The insight we gained in our study tells us that the root cause of the seemingly non-removable infinities is the ill-constructed expansion scheme for the slow-roll parameters. It would be interesting to explore other possible expansion schemes and consider constructing new inflationary parameters, that could possibly lead to a power spectrum free from divergent artifacts of our chosen method of calculation.

Adiabatic Regularization. The two-point function of primordial cosmological perturbations has an ultraviolet divergence in the spatial coincidence limit. The method of adiabatic regularization solves this problem by performing a mode-by-mode subtraction scheme thereby removing the divergent parts. Such a regularization procedure is correspondingly reflected in the power spectrum, the physical form of which (called the regularized power spectrum,) is the difference between the "bare" power spectrum and the subtraction term. In this study, we calculate the regularized power spectrum within the framework of the two inflation models mentioned above. In both of these cases, we find that the regularized power spectrum is simply the "bare" power spectrum. The expansion of the Universe during (and right after) inflation washes out the subtraction term; it exponentially decays with the number of e-folds. This study together with that of Urakawa and Starobinsky dealing with the canonical case, justifies the use of the "bare" power spectrum in standard calculation.

Future Prospect. The adiabatic regularization of the power spectrum we cover

in this work extends the result in the canonical case to two different directions—one including a variable sound speed, and the other one adding a nonminimal coupling term. Considering these two models, the natural next step is a generalization encompassing these two—a nonminimally coupled general single-field inflation. For this generalization, one has to deal with challenges involving (a) variable sound speed, (b) time-dependent nonminimal coupling functional of the inflaton, and (c) new slow-roll parameters due to the nonminimal coupling term. With these complexities, one has to answer the question of the effect of the subtraction term on the regularized power spectrum. If it would not have a trivial effect as what the current study suggests, one may ask under what conditions (eg., near scale-invariance) the regularized power spectrum is simply the "bare" power spectrum.

Appendices

A Codes

A.1 Code for Figure 3.1

```
gnuplot> set pm3d \# splot style for drawing graphs/surfaces
gnuplot> set hidden3d \# hidden line removal
gnuplot> set isosample 80,80 \# interval of sampling for graphs
gnuplot> unset key \# remove legends
gnuplot> unset tics \# remove tics on axes
gnuplot> unset border \# remove bounding box/border
gnuplot> unset colorbox \# remove color legend box
gnuplot> set xrange [-5:5]
gnuplot> set yrange [-5:5]
gnuplot> splot x**2 + y**2,x**2 + y**2 + 20,x**2 + y**2 + 40, x**2
+ y**2 + 60, x**2 + y**2 + 80
```

A.2 Code for Figure 6.2

```
plot2d(
    [airy_ai(ξ),airy_bi(ξ)],
    [ξ,-12.0,5.0],[y,-0.5,1.0],
    [legend,"Ai(ξ)","Bi(ξ)"],
    [style,[linespoints,1.0,1.5,2],[lines,2.5,1]],
    [adapt_depth, 1],
    [nticks, 28],
    [plot_format,gnuplot]
);
```

A.3 Maple Codes for the Calculation of the Power Spectra in the Uniform Approximation

```
# load packages
with(combinat):

# The var max_index is the maximum index in the expression
# involving e[i] and d[i]
max_index := 25:
printf("The maximum index is %d", max_index);

# This function differentiates an expression involving
# e[i] and d[i] wrt N where e[i] and d[i] are the Hubble
# and sound flow functions, respectively.
fExpand2 := proc (expr)
     local n, i, j, m, iterm, newterm, hold_expr, hold_expr2, pow;
     n := nops(expr+x__unique)-1;
     hold_expr := expr;
     for i to n do
         if n = 1 then
             iterm := expr
         else
             iterm := op(i, expr)
         end if;

         hold_expr := hold_expr-iterm;

         for j to max_index do
             if has(iterm, e[j]) then
                 m := degree(iterm, e[j]);
                 newterm := subs(e[j]^m = m*e[j]^m*e[j+1], iterm);
                 hold_expr := hold_expr+newterm
             end if;

             if has(iterm, d[j]) then
                 m := degree(iterm, d[j]);
                 newterm := subs(d[j]^m = m*d[j]^m*d[j+1], iterm);
                 hold_expr := hold_expr+newterm
```

```
            end if;
        end do;
    end do;

    hold_expr2 := expr;

    for i to n do
        if n = 1 then
            iterm := expr
        else iterm := op(i, expr) end if;

        hold_expr2 := hold_expr2-iterm;
        pow := degree(iterm, k__d);

        if has(iterm, k__d) then
            hold_expr2
            :=
            hold_expr2+subs(
                k__d^pow = pow*k__d^pow*(-d[1]-1+e[1]), iterm
            )
        end if ;
    end do;

    hold_expr+hold_expr2;
end proc:



#####################################################################
#####################################################################
# This function trims an expression up to order uptoj
fPrune := proc(expr, uptoj)
    local n, i, j, hold_expr, iterm, order;
    # add one and minus one to avoid counting multiplicands
    n := nops(expr+x__unique)-1;
    hold_expr := expr;
    for i to n do
        order := 0;
```

```
        if n = 1 then
            iterm := expr
        else
            iterm := op(i, expr)
        end if;

        for j to max_index do
            if has(iterm, e[j]) then
                order := order + degree(iterm, e[j])
            end if;

            if has(iterm, d[j]) then
                order := order + degree(iterm, d[j])
            end if;
        end do;
        if order > uptoj then
            hold_expr := hold_expr - iterm
        end if;
    end do;
    hold_expr;
end proc:



#####################################################################
#####################################################################
# This function performs binomial expansion
fBinom := proc(expr, binom_power, first_term, uptoj, order)
    local i, j, hold_expr, sec_term, jterm;

    if not(has(expr, first_term)) then
        printf("Error :  First term, not found!");
        return;
    end if;

    sec_term := expand(expr/first_term - 1);
    hold_expr := 0;
```

```
    for i from 0 to uptoj do
        jterm := 1;
        for j to i do
            jterm := jterm*(binom_power - j + 1)
        end do;
        hold_expr
        :=
        hold_expr + jterm*fPrune(expand(sec_term^i),order)/i!;
    end do;

    expand(first_term^binom_power*hold_expr);
end proc:



#################################################################
#################################################################
# This function picks the nth order terms
fPick := proc(expr, urOrder)
    local n, hold_expr, i, j, iterm, order;

    # add one and minus one to avoid counting
    n := nops(expr+x__unique)-1; multiplicands
    hold_expr := 0;
    for i to n do
        order := 0;
        if n = 1 then
            iterm := expr
        else
            iterm := op(i,expr)
        end if;

        for j to max_index do
            if has(iterm, e[j]) then
                order := order + degree(iterm, e[j])
            end if;
            if has(iterm, d[j]) then
                order := order + degree(iterm, d[j])
```

```
            end if;
        end do;

        if order = urOrder then
            hold_expr := hold_expr + iterm
        end if;
    end do;
    hold_expr;
end proc:
```

B Calculation of the Integral F_3

We wish to calculate the integral F_3 given by

$$F_3 = \int_1^w \mathrm{d}u \, \frac{u^5 \ln^3 u}{(1-u^2)^{\frac{5}{2}}}. \tag{135}$$

Maple 2015.2 cannot produce an analytical expression for this integral. Moreover, the online Mathematica integrator gives result in terms of generalized hypergeometric functions and some other functions; but the limit of this result as $w \to 0^+$ vanishes[20]. Although we know by following the argument in **Sec. 6.5** that the integral is not divergent, numerical calculations indicate that its value is not vanishing.

In order to evaluate the integral, we change our variable from u to x as

$$u = \sqrt{1-(1-x)^2} \quad \Rightarrow \quad \mathrm{d}u = \frac{1-x}{\sqrt{2x-x^2}}\mathrm{d}x. \tag{136}$$

Note that this is the same substitution trick used in the much simpler integral C_2 discussed as a representative example in **Sec. 6.4**. Unlike that of C_2 however, the integral F_3 cannot be readily solved using Maple and Mathematica online integrator even after the above substitution. Here, our aim is to demonstrate how to carry out the integration of the innocent-looking integral above by performing some simple but helpful additional trick based on integration by parts.

[20] We verified this using Maple 2015.2 through the Mathematica-to-Maple converter and the limit functions available. We do not have a copy of Mathematica

After the change of variable from u to x, the integral F_3 becomes

$$F_3 = \int_1^{0^+} \mathrm{d}x \frac{x^2(2-x)^2\big[\ln x + \ln(2-x)\big]^3}{8(1-x)^4},$$

$$F_3 = \int_1^{0^+} \mathrm{d}x \frac{x^2(2-x)^2 \ln^3 x}{8(1-x)^4} + \int_1^{0^+} \mathrm{d}x \frac{3x^2(2-x)^2 \ln^2 x \ln(2-x)}{8(1-x)^4}$$
$$+ \int_1^{0^+} \mathrm{d}x \frac{3x^2(2-x)^2 \ln x \ln^2(2-x)}{8(1-x)^4} + \int_1^{0^+} \mathrm{d}x \frac{x^2(2-x)^2 \ln^3(2-x)}{8(1-x)^4},$$

$$F_3 = F_{3A} + F_{3B} + F_{3C} + F_{3D} \tag{137}$$

For brevity, we have called the four integrals above in the second equality as F_{3A}, F_{3B}, F_{3C}, and F_{3D} respectively.

The first and the fourth integrals can be readily evaluated using the online Mathematica integrator. The result can be written as

$$F_{3A} + F_{3D} \tag{138}$$
$$= \frac{1}{48(-1+x)^3}\Big\{ -72 - 72x^4 - 60\mathrm{Li}_3(x) + 60\ln(2-x) + 32\ln^3(2-x)$$
$$- 24\ln^2(2-x) + 288x^3 + 6\ln(x-1) - 432x^2 - 54x^2\ln(2-x)\ln(x-1)$$
$$- 6(x-1)^3(3+10\ln x)\mathrm{Li}_2(x) + 54x\ln(2-x)\ln(x-1)$$
$$- 90x^2\ln^2(2-x)\ln(x-1) - 54x\ln(1-x)\ln x - 18x^3\ln(1-x)\ln x$$
$$+ 90x\ln^2(2-x)\ln(x-1) + 18x^3\ln(2-x)\ln(x-1)$$
$$- 30x^3\ln(1-x)\ln^2 x + 30x^3\ln^2(2-x)\ln(x-1) + 54x^2\ln(1-x)\ln x$$
$$+ 6(x-1)^3[3+10\ln(2-x)]\mathrm{Li}_2(2-x) + 90x^2\ln(1-x)\ln^2 x$$
$$- 90x\ln(1-x)\ln^2 x + 60\mathrm{Li}_3(2-x) - 60x^3\mathrm{Li}_3(2-x) + 180x^2\mathrm{Li}_3(2-x)$$
$$- 180x\mathrm{Li}_3(2-x) - 222x\ln(2-x) + 300x^2\ln(2-x) - 174x^3\ln(2-x)$$
$$+ 36x^4\ln(2-x) + 90x\ln^2(2-x) - 129x^2\ln^2(2-x) + 81x^3\ln^2(2-x)$$
$$- 18x^4\ln^2(2-x) - 96x\ln^3(2-x) + 6x^4\ln^3(2-x) + 96x^2\ln^3(2-x)$$
$$- 40x^3\ln^3(2-x) - 18x^2\ln(1-x) + 6x^3\ln(1-x) + 18x\ln(1-x)$$

$$
\begin{aligned}
&- 6x^3\ln(x-1) - 18x\ln(x-1) + 18x^2\ln(x-1)\\
&- 30\ln^2(2-x)\ln(x-1) - 18\ln(2-x)\ln(x-1) - 180x^2\mathrm{Li}_3(x)\\
&+ 180x\mathrm{Li}_3(x) + 60x^3\mathrm{Li}_3(x) - 8x^3\ln^3 x - 42x\ln x - 114x^3\ln x - 18x^4\ln^2 x\\
&+ 63x^3\ln^2 x + 30x\ln^2 x - 75x^2\ln^2 x + 36x^4\ln x + 120x^2\ln x\\
&+ 6x^4\ln^3 x + 30\ln(1-x)\ln^2 x + 18\ln(1-x)\ln x - 6\ln(1-x) + 288x\Big\}\Big|_1^{0^+},
\end{aligned}
$$

where $\mathrm{Li}_s(x)$ is the polylogarithm of order s. Note that ignoring the limits, the expression above for $F_{3A}+F_{3D}$ is not real; see e.g., the term $\ln(-1+x)$. However, the imaginary part is constant so this should not be a problem.

The integral F_{3B} cannot be directly solved by the online Mathematica integrator (nor by Maple). However, it can be evaluated by applying the technique of integration by parts. The trick is to segment the integrand such that the resulting integral can be evaluated by our integrator. With good insight about the capability of the integrator we can find the appropriate segmentation that works, after few attempts.

$$
\begin{aligned}
F_{3B} &= \int_1^{0^+} \mathrm{d}x \frac{3x^2(2-x)^2\ln^2 x\ln(2-x)}{8(1-x)^4},\\
&= \int_1^{0^+} \ln^2 x\left[\frac{3x^2(2-x)^2\ln(2-x)}{8(1-x)^4}\mathrm{d}x\right],\\
&= \left[\frac{1}{16(1-x)^2} - \frac{1}{8(1-x)} - \frac{3x}{8} - \frac{(3x^4-15x^3+33x^2-33x+11)\ln(2-x)}{8(1-x)^3}\right.\\
&\quad \left. - \frac{5\ln(x-2)}{8} + \frac{5\ln(-1+x)}{8}\right]\ln^2 x\Big|_1^{0^+}\\
&\quad + \int_1^{0^+}\mathrm{d}x\Big[-\frac{\ln x}{8x(-1+x)^2} - \frac{2\ln x}{x(-8+8x)} + \frac{3\ln x}{4}\\
&\qquad - \frac{(3x^4-15x^3+33x^2-33x+11)\ln(2-x)\ln x}{4x(-1+x)^3} + \frac{5\ln x\ln(x-2)}{4x}\\
&\qquad - \frac{5\ln x\ln(-1+x)}{4x}\Big],
\end{aligned}
$$

$$
F_{3B} = F_{3B}^{(1)} + F_{3B}^{(2)}. \tag{139}
$$

We have labeled the integral in the right hand side of the second to the last equality above as $F_{3B}^{(2)}$ and the remaining terms as $F_{3B}^{(1)}$.

Unlike F_{3B}, Mathematica online integrator can evaluate $F_{3B}^{(2)}$. The result of integration is given by

$$
\begin{aligned}
F_{3B}^{(2)} = \frac{1}{16(x-1)^2}\Bigg[& 3 + 10\ln\frac{2(x-1)}{x-2}\ln^2\frac{x}{2-x} + 32x^2\ln 2\ln^2 x - 64x\ln 2\ln^2 x \\
& + 20x^2\ln x\mathrm{Li}_2(x) - 40x\ln x\mathrm{Li}_2(x) - 20x\ln(x-2)\ln^2 x \\
& + 10x^2\ln(x-2)\ln^2 x + 40x\ln(x-1)\ln^2 x - 20x^2\ln(x-1)\ln^2 x \\
& + 20\ln(x-1)\ln x\ln\frac{x}{2-x} - 20\ln(1-x)\ln(2-x)\ln x \\
& - 30x^2\ln(1-x)\ln(x-2) + 40x\ln\frac{x}{2-x}\mathrm{Li}_2(x) - 54\ln(x-2) \\
& - 60x\ln(x-2)\ln(x-1) + 30x^2\ln(x-2)\ln(x-1) \\
& - 40x\ln(x-1)\ln x\ln\frac{x}{2-x} + 20x^2\ln(x-1)\ln x\ln\frac{x}{2-x} \\
& - 10x^2\ln^2\ln(x-1)\frac{x}{2-x} + 20x\ln^2\ln(x-1)\frac{x}{2-x} \\
& - 20x^2\ln(1-x)\ln x\ln\frac{x}{2-x} - 20x^2\ln\frac{x}{2-x}\mathrm{Li}_2(x) - 12x^3\ln(2-x)\ln x \\
& + 8\ln\frac{2}{2-x} + 30x^2\ln(2-x)\ln x - 10x^2\ln\frac{2}{2-x}\ln^2\frac{x}{2-x} \\
& + 128x\ln x\mathrm{Li}_2\left(\frac{x}{2}\right) - 20\ln(1-x)\ln x\ln\frac{x}{2-x} + 40x\ln(1-x)\ln x\ln\frac{x}{2-x} \\
& + 40x\ln(1-x)\ln(2-x)\ln x - 20x^2\ln(1-x)\ln(2-x)\ln x \\
& + 24x^2\ln\left(1-\frac{x}{2}\right)\ln x - 20\mathrm{Li}_3\left(\frac{x}{2-x}\right) + 20\mathrm{Li}_3\left(\frac{x}{x-2}\right) + 8\mathrm{Li}_2\left(\frac{x}{x-2}\right) \\
& + 64\mathrm{Li}_3\left(\frac{x}{2}\right) - 20x^2\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{x-2}\right) + 24x^2\mathrm{Li}_2\left(\frac{x}{2}\right) - 48x\mathrm{Li}_2\left(\frac{x}{2}\right) \\
& - 64x^2\ln x\mathrm{Li}_2\left(\frac{x}{2}\right) - 4\ln^2\frac{x}{2-x} - 3\ln^2 x + 10x^2\ln\frac{2(x-1)}{x-2}\ln^2\frac{x}{2-x} \\
& - 20x^2\ln(2-x)\mathrm{Li}_2(x) - 10x^2\ln(2-x)\ln^2 x + 64x^2\mathrm{Li}_3\left(\frac{x}{2}\right)
\end{aligned}
$$

$$
\begin{aligned}
&+ 2(x-1)^2\mathrm{Li}_2(1-x) + 30\ln(1-x)\ln(2-x) - 10\ln(x-1)\ln^2\frac{x}{2-x} \\
&+ 108x\ln(x-2) - 30\ln(1-x)\ln(x-2) + 30\ln(x-2)\ln(x-1) \\
&+ 2x^2\mathrm{Li}_2(x) - 4x\mathrm{Li}_2(x) - 20\ln(2-x)\mathrm{Li}_2(x) - 20\ln\frac{x}{2-x}\mathrm{Li}_2(x) \\
&+ 24\ln\left(1-\frac{x}{2}\right)\ln x - 10\ln(2-x)\ln^2 x - 20\ln(x-1)\ln^2 x \\
&+ 10\ln(x-2)\ln^2 x + 20\ln x\mathrm{Li}_2(x) + 8\ln x\ln\frac{x}{2-x} + 32\ln 2\ln^2 x \\
&- 20x^2\mathrm{Li}_3\left(\frac{x}{2-x}\right) + 40x\mathrm{Li}_3\left(\frac{x}{2-x}\right) + 20x^2\mathrm{Li}_3\frac{x}{x-2} - 40x\mathrm{Li}_3\frac{x}{x-2} \\
&- 16x\mathrm{Li}_2\left(\frac{x}{x-2}\right) + 8x^2\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 16x\ln\frac{2}{2-x} + 8x^2\ln\frac{2}{2-x} \\
&- 4x^2\ln^2\frac{x}{2-x} - 4x^2\ln\frac{x}{2-x} + 8x\ln^2\frac{x}{2-x} + 8x\ln\frac{x}{2-x} \\
&+ 20\ln\frac{x}{2-x}\mathrm{Li}_2\frac{x}{2-x} - 20\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 10\ln\frac{2}{2-x}\ln^2\frac{x}{2-x} \\
&+ 8\ln\frac{2}{2-x}\ln\frac{x}{2-x} - 128x\mathrm{Li}_3\left(\frac{x}{2}\right) - 20x\ln(2-x)\ln x + 8x^2\ln x\ln\frac{x}{2-x} \\
&- 16x\ln x\ln\frac{x}{2-x} + 60x\ln(1-x)\ln(x-2) + 24\mathrm{Li}_2\left(\frac{x}{2}\right) \\
&- 48x\ln\left(1-\frac{x}{2}\right)\ln x - 4\ln\frac{x}{2-x} + 30x^2\ln(1-x)\ln(2-x) \\
&- 54x^2\ln(x-2) - 60x\ln(1-x)\ln(2-x) + 2\mathrm{Li}_2(x) + 38\ln(2-x) - 36x^3 \\
&- 24\ln(x-1) + 75x^2 + 4\ln x - 36x^2\ln(2-x)\ln(x-1) \\
&+ 72x\ln(2-x)\ln(x-1) - 4x\ln(1-x)\ln x + 2x^2\ln(1-x)\ln x \\
&+ 20x^2\ln(1-x)\ln^2 x - 40x\ln(1-x)\ln^2 x + 40x\ln(2-x)\mathrm{Li}_2(x) \\
&+ 20\mathrm{Li}_3(2-x) + 20x^2\mathrm{Li}_3(2-x) - 40x\mathrm{Li}_3(2-x) - 62x\ln(2-x) \\
&+ 12x^2\ln(2-x) + 12x^3\ln(2-x) + 18x^2\ln(1-x) - 36x\ln(1-x) \\
&+ 48x\ln(x-1) - 24x^2\ln(x-1) - 36\ln(2-x)\ln(x-1) + 12x\ln x
\end{aligned}
$$

$$
\begin{aligned}
&+\ 24x^3\ln x + 6x\ln^2 x - 3x^2\ln^2 x - 40x^2\ln x + 20\ln(1-x)\ln^2 x \\
&+\ 2\ln(1-x)\ln x + 18\ln(1-x) + 40x\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{x-2}\right) \\
&-\ 40x\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{2-x}\right) - 42x + 20x^2\ln\frac{x}{2-x}\mathrm{Li}_2\frac{x}{2-x} \\
&+\ 20x\ln\frac{2}{2-x}\ln\frac{x}{2-x}^2 + 8x^2\ln\frac{2}{2-x}\ln\frac{x}{2-x} - 16x\ln\frac{2}{2-x}\ln\frac{x}{2-x} \\
&-\ 2(x-1)^2\left(3 + 10\ln x - 10\ln\frac{x}{2-x}\right)\mathrm{Li}_2(2-x) \\
&-\ 20x\ln\frac{2(x-1)}{x-2}\ln^2\frac{x}{2-x} - 64\ln x\mathrm{Li}_2\left(\frac{x}{2}\right) \\
&+\ 20x\ln(2-x)\ln^2 x\Big]. \qquad (140)
\end{aligned}
$$

Similar to the sum $F_{3A}+F_{3D}$, we observe that F_{3B} is not real even though the corresponding integrand is real. This is however, not a problem since as before, the imaginary part of F_{3B} is simply a constant.

The integral F_{3C} cannot also be directly evaluated using the Mathematica online integrator so we apply the same trick we have used for F_{3B} namely, segment the integrand into manageable parts in performing integration by parts.

$$
\begin{aligned}
F_{3C} &= \int_1^{0^+}\mathrm{d}x\frac{3x^2(2-x)^2\ln x\ln^2(2-x)}{8(1-x)^4} \\
&= \int_1^{0^+}\ln^2(2-x)\left[\frac{3x^2(2-x)^2\ln x}{8(1-x)^4}\mathrm{d}x\right] \\
&= \frac{\ln^2(2-x)}{16(x-1)^3}\Big[3 + x - 16x^2 + 18x^3 - 6x^4 - 10(x-1)^3\ln(1-x) \\
&\qquad\qquad +\ 2x^3(-4+3x)\ln x\Big]_1^{0^+} \\
&\quad +\int_1^{0^+}\mathrm{d}x\Big[\frac{(-6x^4+18x^3-16x^2+x+3)\ln(2-x)}{8(2-x)(x-1)^3} \\
&\qquad -\ \frac{5\ln(1-x)\ln(2-x)}{4(2-x)} + \frac{x^3(-4+3x)\ln x\ln(2-x)}{4(2-x)(x-1)^3}\Big],
\end{aligned}
$$

$$F_{3C} = F_{3C}^{(1)} + F_{3C}^{(2)} \tag{141}$$

In the last equality we have labeled the integral in the second-to-the-last equality in the right hand side as $F_{3C}^{(2)}$ and the remaining terms as $F_{3C}^{(1)}$.

The integral $F_{3C}^{(2)}$ can be directly evaluated using the Mathematica online integrator. The result is given by

$$\begin{aligned}
F_{3C}^{(2)} = \frac{1}{16(x-1)^2}\Bigg[&24 - 10x^2 \ln\frac{2(x-1)}{x-2}\ln^2\frac{x}{2-x} + 20x\ln\frac{2(x-1)}{x-2}\ln^2\frac{x}{2-x} \\
&- 20x^2\ln(x-1)\ln x\ln\frac{x}{2-x} + 40x\ln(x-1)\ln x\ln\frac{x}{2-x} \\
&+ 20x^2\ln(1-x)\ln(2-x)\ln x - 40x\ln(1-x)\ln(2-x)\ln x \\
&+ 20x^2\ln(1-x)\ln x\ln\frac{x}{2-x} - 40x\ln(1-x)\ln x\ln\frac{x}{2-x} \\
&- 2\ln(2-x)\ln(x-1) + 11\ln^2(2-x) - 4\ln^2 x + 40x\mathrm{Li}_3\left(\frac{x}{x-2}\right) \\
&- 4\ln^2\frac{x}{2-x} + 6x^2\mathrm{Li}_2(x) - 12x\mathrm{Li}_2(x) + 20\ln(2-x)\mathrm{Li}_2(x) + 4\ln\frac{x}{2-x} \\
&- 34\ln(2-x) - 4\ln x - 8x\ln\frac{x}{2-x} + 20\ln\frac{x}{2-x}\mathrm{Li}_2(x) + 20\mathrm{Li}_3\left(\frac{x}{2-x}\right) \\
&+ 4x^2\ln\frac{x}{2-x} - 20\mathrm{Li}_3(x) + 10\ln(x-1)\ln^2 x - 10\ln(1-x)\ln^2 x, \\
&- 32\ln^2(2-x)\ln x - 10\ln\frac{2(x-1)}{x-2}\ln^2\frac{x}{2-x} + 12x^3\ln x + 40x\mathrm{Li}_3(x) \\
&- 20x^2\mathrm{Li}_3(x) + 24x^2\mathrm{Li}_2\left(\frac{x}{2}\right) - 2\mathrm{Li}_2(x-1) + 20\ln(1-x)\ln x\ln\frac{x}{2-x} \\
&+ 20\ln(1-x)\ln(2-x)\ln x - 10x^2\ln(1-x)\ln^2 x + 26x^2\ln(2-x)\ln x \\
&- 40x\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 64x\ln^2(2-x)\ln\frac{x}{2} \\
&+ 20x\ln^2(2-x)\ln(x-1) - 12x\ln(2-x)\ln x + 10x^2\ln\frac{2}{2-x}\ln^2\frac{x}{2-x} \\
&+ 20x^2\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 40x\ln(2-x)\mathrm{Li}_2(x) - 40x\ln\frac{x}{2-x}\mathrm{Li}_2(x)
\end{aligned}$$

$$
\begin{aligned}
&- 12x^3 \ln(2-x)\ln x + 32x^2 \ln^2(2-x)\ln\frac{x}{2} - 20x\ln(x-1)\ln^2\frac{x}{2-x} \\
&+ 64x\ln^2(2-x)\ln x, -32x^2\ln^2(2-x)\ln x - 2x^2\ln(2-x)\ln(x-1) \\
&+ 64(x-1)^2\ln(2-x)\mathrm{Li}_2\left(1-\frac{x}{2}\right) + 20x^2\ln(2-x)\mathrm{Li}_2(x) \\
&- 20x\ln(1-x)\ln^2(2-x) - 10x^2\ln^2(2-x)\ln(x-1) \\
&- 20x\ln\frac{2}{2-x}\ln^2\frac{x}{2-x} + 8x^2\ln x\ln\frac{x}{2-x} + 20x^2\ln\frac{x}{2-x}\mathrm{Li}_2(x) \\
&- 48x\ln\left(1-\frac{x}{2}\right)\ln x + 10x^2\ln(x-1)\ln^2\frac{x}{2-x} - 16x\ln\frac{2}{2-x}\ln\frac{x}{2-x} \\
&- 16x\ln x\ln\frac{x}{2-x} + 4x\ln(2-x)\ln(x-1) + 8x^2\ln\frac{2}{2-x}\ln\frac{x}{2-x} \\
&- 2(x-1)^2(1+10\ln(2-x) - 10\ln x + 10\ln\frac{x}{2-x})\mathrm{Li}_2(2-x) \\
&+ 24x^2\ln\left(1-\frac{x}{2}\right)\ln x + 10x^2\ln(1-x)\ln^2(2-x) - 30x^2\ln x + 8x\ln^2 x \\
&- 4x^2\ln^2 x + 10\ln\frac{2}{2-x}\ln^2\frac{x}{2-x} + 20x^2\mathrm{Li}_3\left(\frac{x}{2-x}\right) + 128x\mathrm{Li}_3\left(1-\frac{x}{2}\right) \\
&- 64x^2\mathrm{Li}_3\left(1-\frac{x}{2}\right) - 16x\mathrm{Li}_2\left(\frac{x}{x-2}\right) + 4x\mathrm{Li}_2(x-1) + 8x^2\mathrm{Li}_2\left(\frac{x}{x-2}\right) \\
&+ 22x\ln x + 24\ln\left(1-\frac{x}{2}\right)\ln x + 8\ln x\ln\frac{x}{2-x} + 8\ln\frac{2}{2-x}\ln\frac{x}{2-x} \\
&+ 20\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 20\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{2-x}\right) - 8x^2\ln\frac{2}{2-x} \\
&+ 16x\ln\frac{2}{2-x} - 26\ln(x-2) - 40x\mathrm{Li}_3\left(\frac{x}{2-x}\right) \\
&- 20x^2\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{2-x}\right) + 32\ln^2(2-x)\ln\frac{x}{2} - 26x^2\ln(x-2) \\
&+ 52x\ln(x-2) - 20x^2\mathrm{Li}_3\left(\frac{x}{x-2}\right) + 40x\ln\frac{x}{2-x}\mathrm{Li}_2\left(\frac{x}{2-x}\right) \\
&- 64\mathrm{Li}_3\left(1-\frac{x}{2}\right) - 2x^2\mathrm{Li}_2(x-1) + 8x\ln^2\frac{x}{2-x} - 4x^2\ln^2\frac{x}{2-x}
\end{aligned}
$$

$$
\begin{aligned}
&- 20\mathrm{Li}_3\left(\frac{x}{x-2}\right) - 36x^3 + 11x^2\ln^2(2-x) - 10\ln^2(2-x)\ln(x-1)\\
&+ 96x^2 - 22x\ln^2(2-x) + 20x\ln(1-x)\ln^2 x + 6x^2\ln(1-x)\ln x\\
&- 12x\ln(1-x)\ln x - 20\ln(x-1)\ln x\ln\frac{x}{2-x} - 20x\ln(x-1)\ln^2 x\\
&- 84x + 24x^3\ln(2-x) + 10x^2\ln(x-1)\ln^2 x + 24\mathrm{Li}_2\left(\frac{x}{2}\right) - 48x\mathrm{Li}_2\left(\frac{x}{2}\right)\\
&+ 10\ln(1-x)\ln^2(2-x) + 10\ln(x-1)\ln^2\frac{x}{2-x} + 88x\ln(2-x)\\
&- 78x^2\ln(2-x) + 6\ln(1-x)\ln x - 12x\ln(x-1) + 6x^2\ln(x-1)\\
&+ 8\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 8\ln\frac{2}{2-x} + 6\ln(x-1) + 6\mathrm{Li}_2(x)\Big]_1^{0^+}
\end{aligned}
\tag{142}
$$

Note that the integral F_{3C} carries the imaginary constant artifact of integration also present in F_{3A}, F_{3B}, and F_{3D}.

The sum $F_{3A} + F_{3B} + F_{3C} + F_{3D}$ can be simplified by canceling some terms common in the addends. The overall result for F_3 prior to taking the limits is given by

$$
\begin{aligned}
F_3 = \frac{1}{48(x-1)^3}\Big[&- 153 + 288x^2\ln(2)\ln^2(2-x) + 270x\ln(x-2)\ln(x-1)\\
&+ 270x^2\ln(1-x)\ln(x-2) - 90x^3\ln(2-x)\ln(x-1)\\
&- 270x\ln(1-x)\ln(x-2) + 576x^2\ln x\mathrm{Li}_2\left(\frac{x}{2}\right) - 270x^2\ln(x-2)\ln(x-1)\\
&+ 288x^2\ln(2-x)\ln^2 x + 288x\ln(2)\ln^2 x - 576x\ln x\mathrm{Li}_2\left(\frac{x}{2}\right)\\
&- 288x\ln(2-x)\ln^2 x - 288x^2\ln(2)\ln^2 x + 90x^3\ln(1-x)\ln(2-x)\\
&+ 144x^2\ln(2)\ln(2-x) - 288x\ln(2)\ln^2(2-x) + 288x^2\ln(2)\ln x\\
&+ 192x^3\mathrm{Li}_2\left(1-\frac{x}{2}\right)\ln(2-x) + 576x\ln(2-x)\mathrm{Li}_2\left(1-\frac{x}{2}\right)\\
&- 144x\ln(2)\ln(2-x) - 90x^3\ln(1-x)\ln(x-2) - 96x^3\ln(2)\ln x
\end{aligned}
$$

$$
\begin{aligned}
&- 192x^3 \ln x \mathrm{Li}_2\left(\frac{x}{2}\right) + 90x^3 \ln(x-2)\ln(x-1) - 72x^4 \ln(2-x)\ln x \\
&- 288x\ln(2)\ln x + 180x\ln(1-x) - 24x^3 \ln^2(2-x)\ln x \\
&- 576x^2 \mathrm{Li}_2\left(1-\frac{x}{2}\right)\ln(2-x) - 48x^3\ln(2-x)\ln(2) + 90\ln(2-x)\ln(x-1) \\
&- 72\ln^2(2-x) + 96\ln(2-x)\ln^2 x + 192\ln x \mathrm{Li}_2\left(\frac{x}{2}\right) + 48\ln(2-x) \\
&- 90\ln(x-2)\ln(x-1) + 192x^3\mathrm{Li}_3\left(\frac{x}{2}\right) + 48x^3\mathrm{Li}_2\left(\frac{x}{x-2}\right) \\
&- 240x^3\ln(x-2) + 96\ln(2)\ln^2(2-x) - 432x^3\ln x \\
&+ 90\ln(1-x)\ln(x-2) - 432x^2\mathrm{Li}_2\left(\frac{x}{2}\right) - 192\mathrm{Li}_3\left(\frac{x}{2}\right) \\
&- 552x^2\ln(2-x)\ln x + 384x\ln(2-x)\ln x + 336x^3\ln(2-x)\ln x \\
&+ 270x^2\ln(2-x)\ln(x-1) - 96x^3\ln(2)\ln^2(2-x) + 96x^3\ln(2)\ln^2 x \\
&- 270x\ln(2-x)\ln(x-1) + 432x^2\ln x - 192x^3\mathrm{Li}_3\left(1-\frac{x}{2}\right) + 48x\ln^2 x \\
&- 132x^2\ln^2 x - 192\ln(2-x)\mathrm{Li}_2\left(1-\frac{x}{2}\right) - 576x\mathrm{Li}_3\left(1-\frac{x}{2}\right) \\
&- 96x\ln^3(2-x) + 576x^2\mathrm{Li}_3\left(1-\frac{x}{2}\right) + 144x\mathrm{Li}_2\left(\frac{x}{x-2}\right) \\
&- 144x^2\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 90\ln(2-x)\ln(1-x) - 96\ln(2-x)\ln x - 144x\ln x \\
&+ 144x^3\mathrm{Li}_2\left(\frac{x}{2}\right) - 96\ln(2)\ln^2 x + 96x^2\ln^3(2-x) + 240\ln(x-2) \\
&+ 18x^4\ln^2 x\ln(2-x) + 96\ln(2)\ln x + 48\ln(2)\ln(2-x) + 576x\mathrm{Li}_3\left(\frac{x}{2}\right) \\
&+ 720x^2\ln(x-2) - 576x^2\mathrm{Li}_3\left(\frac{x}{2}\right) - 720x\ln(x-2) - 120x^3\ln^2 x\ln(2-x) \\
&+ 192\mathrm{Li}_3\left(1-\frac{x}{2}\right) + 18x^4\ln^2(2-x)\ln x + 1017x^3 + 270x\ln(2-x)\ln(1-x)
\end{aligned}
$$

$$
\begin{aligned}
&- 348x^2\ln^2(2-x) - 270x^2\ln(1-x)\ln(2-x) - 1323x^2 + 264x\ln^2(2-x)\\
&+ 747x - 480x^3\ln(2-x) + 144x^4\ln(2-x) - 144\mathrm{Li}_2\left(\frac{x}{2}\right) + 432x\mathrm{Li}_2\left(\frac{x}{2}\right)\\
&+ 192x^3\ln^2(2-x) - 36x^4\ln^2(2-x) + 6x^4\ln^3(2-x) - 40x^3\ln^3(2-x)\\
&- 288x\ln(2-x) - 180x^2\ln(1-x) + 576x^2\ln(2-x) + 60x^3\ln(1-x)\\
&- 60x^3\ln(x-1) - 8x^3\ln^3 x - 36x^4\ln^2 x + 120x^3\ln^2 x - 180x\ln(x-1)\\
&+ 144x^4\ln x + 180x^2\ln(x-1) + 6x^4\ln^3 x - 288x^4 + 32\ln^3(2-x)\\
&- 48\mathrm{Li}_2\left(\frac{x}{x-2}\right) - 60\ln(1-x) + 60\ln(x-1)\Big]_1^{0^+}
\end{aligned}
\tag{143}
$$

Ignoring the limits, we have verified that the derivative of the right hand side reduces to the original integrand involving x given by the first of (137). After this verification, all that is left is to evaluate the limits and perform simplification of the result. We find

$$
F_3 = \int_1^{0^+} \mathrm{d}u\, \frac{u^5\,\ln^3 u}{(1-u^2)^{\frac{5}{2}}} = -4\zeta(3) + 6 + 2\ln^2 2 - \frac{8}{3}\ln^3 2 + \frac{2\pi^2}{3}\ln 2 - 6\ln 2 - \frac{\pi^2}{6},
$$

which was to be calculated. We have verified that this analytical result (in fact, all the listed integrals A, B, $\cdots$, F in **Sec. 6.5**) agrees with that from numerical quadrature.

C Ricci Scalar in Einstein and Jordan frames

In this appendix, we wish to show the relationship between the Ricci scalar in the Jordan frame, R, and the Ricci scalar in the Einstein frame, $\widehat{R}$, given by

$$
R = \Omega^2\big[\widehat{R} + 6\widehat{\Box}\ln\Omega - 6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu\ln\Omega)(\widehat{\nabla}_\nu\ln\Omega)\big], \tag{144}
$$

where the hatted quantities are expressed in terms of the hatted metric in the conformal transformation $\mathrm{d}s^2 \to \mathrm{d}\widehat{s}^2 = \Omega^2\mathrm{d}s^2$. In so doing, we follow the logic pathway laid down in refs. [8, 114].

The equation above relating R and $\widehat{R}$ can be interpreted in two ways. The first one corresponds to taking $\widehat{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$ and keeping the coordinates the

same in both frames. Needless to say, for this one, all derivatives in the equation above relating R and $\widehat{R}$ are evaluated with respect to $\{x^\mu\}$ (which is equal to $\{\widehat{x}^\mu\}$). The second one corresponds to defining new hatted coordinates as in for instance, the first of (8.70) namely, $\mathrm{d}\widehat{t} = \Omega \mathrm{d}t$. In this case, the metric *components* are not rescaled by the same factor Ω^2, following the condition $\mathrm{d}\widehat{s}^2 = \Omega^2 \mathrm{d}s^2$. In the following calculation, we first consider the first case where $\widehat{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$ and then verify that the resulting equation, that is, (144), also holds for the second case for the metric rescaling $\mathrm{d}\widehat{s}^2 = -\mathrm{d}\widehat{t}^{\,2} + \widehat{a}^2 \delta_{ij} \mathrm{d}x^i \mathrm{d}x^j$, where $\mathrm{d}\widehat{t} = \Omega \mathrm{d}t$ and $\widehat{a} = \Omega a$.

To relate $\widehat{R}$ with R we first find the relationship between the Riemann tensors in the two frames. The hatted Riemann tensor can be written in terms of the hatted Christoffel symbols which in turn can be expressed in terms of the hatted metric components. We have

$$\widehat{R}^{\rho}_{\sigma\mu\nu} = -\widehat{\Gamma}^{\rho}_{\sigma\mu,\nu} + \widehat{\Gamma}^{\rho}_{\sigma\nu,\mu} - \widehat{\Gamma}^{\lambda}_{\sigma\mu}\widehat{\Gamma}^{\rho}_{\nu\lambda} + \widehat{\Gamma}^{\lambda}_{\sigma\nu}\widehat{\Gamma}^{\rho}_{\mu\lambda}, \tag{145}$$

where

$$\begin{aligned}
\widehat{\Gamma}^{\rho}_{\mu\nu} &= \tfrac{1}{2}\,\widehat{g}^{\rho\sigma}\big(\widehat{g}_{\sigma\mu,\nu} + \widehat{g}_{\nu\sigma,\mu} - \widehat{g}_{\mu\nu,\sigma}\big), \\
&= \tfrac{1}{2}\,\Omega^{-2} g^{\rho\sigma}\big(\Omega^2 g_{\sigma\mu,\nu} + 2\Omega\Omega_{,\nu} g_{\sigma\mu} + \Omega^2 g_{\nu\sigma,\mu} + 2\Omega\Omega_{,\mu} g_{\nu\sigma} \\
&\qquad\qquad - \Omega^2 g_{\mu\nu,\sigma} - 2\Omega\Omega_{,\sigma} g_{\mu\nu}\big), \\
&= \Gamma^{\rho}_{\mu\nu} + \Omega^{-1}\big(\delta^{\rho}_{\mu}\Omega_{;\nu} + \delta^{\rho}_{\nu}\Omega_{;\mu} - g_{\mu\nu} g^{\rho\sigma}\Omega_{;\sigma}\big), \\
\widehat{\Gamma}^{\rho}_{\mu\nu} &= \Gamma^{\rho}_{\mu\nu} + Y^{\rho}_{\mu\nu},
\end{aligned} \tag{146}$$

with $Y^{\rho}_{\mu\nu} \equiv \Omega^{-1}\big(\delta^{\rho}_{\mu}\Omega_{;\nu} + \delta^{\rho}_{\nu}\Omega_{;\mu} - g_{\mu\nu} g^{\rho\sigma}\Omega_{;\sigma}\big)$. The transformation $g_{\mu\nu} \to \widehat{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$ induces a transformation of Christoffel symbol from $\Gamma^{\rho}_{\mu\nu}$ to $\widehat{\Gamma}^{\rho}_{\mu\nu}$ where $\delta\Gamma^{\rho}_{\mu\nu} \equiv \widehat{\Gamma}^{\rho}_{\mu\nu} - \Gamma^{\rho}_{\mu\nu} = Y^{\rho}_{\mu\nu}$. While neither Christoffel symbols is a tensor, their difference is a tensor. This fact will be useful in a short while.

With the decomposition of hatted Christoffel symbol in hand, we can express the hatted Riemann tensor in terms of the Riemann tensor without a hat and some additional terms.

$$\begin{aligned}
\widehat{R}^{\rho}_{\sigma\mu\nu} = R^{\rho}_{\sigma\mu\nu} &- Y^{\rho}_{\sigma\mu,\nu} + Y^{\rho}_{\sigma\nu,\mu} - \Gamma^{\lambda}_{\sigma\mu} Y^{\rho}_{\nu\lambda} - \Gamma^{\rho}_{\nu\lambda} Y^{\lambda}_{\sigma\mu} - Y^{\lambda}_{\sigma\mu} Y^{\rho}_{\nu\lambda}, \\
&+ \Gamma^{\lambda}_{\sigma\nu} Y^{\rho}_{\mu\lambda} + \Gamma^{\rho}_{\mu\lambda} Y^{\lambda}_{\sigma\nu} + Y^{\rho}_{\mu\lambda} Y^{\lambda}_{\sigma\nu},
\end{aligned}$$

$$= R^{\rho}_{\sigma\mu\nu} - (Y^{\rho}_{\sigma\mu,\nu} + \Gamma^{\rho}_{\nu\lambda}Y^{\lambda}_{\sigma\mu} - \Gamma^{\lambda}_{\sigma\nu}Y^{\rho}_{\mu\lambda} - \Gamma^{\lambda}_{\mu\nu}Y^{\rho}_{\sigma\lambda})$$
$$+ (Y^{\rho}_{\sigma\nu,\mu} + \Gamma^{\rho}_{\mu\lambda}Y^{\lambda}_{\sigma\nu} - \Gamma^{\lambda}_{\sigma\mu}Y^{\rho}_{\nu\lambda} - \Gamma^{\lambda}_{\mu\nu}Y^{\rho}_{\sigma\lambda}) - Y^{\lambda}_{\sigma\mu}Y^{\rho}_{\nu\lambda} + Y^{\rho}_{\mu\lambda}Y^{\lambda}_{\sigma\nu}. \quad (147)$$

In the last equality, we have added and subtracted the term $\Gamma^{\lambda}_{\mu\nu}Y^{\rho}_{\sigma\lambda}$. This is based on the insight that since, as we have pointed above, $Y^{\rho}_{\sigma\mu}$ is a tensor, then $Y^{\rho}_{\sigma\mu,\nu}$ can be considered as a part of $Y^{\rho}_{\sigma\mu;\nu}$ (and for $Y^{\rho}_{\sigma\nu}$, the term $Y^{\rho}_{\sigma\nu,\mu}$ can be considered as a part of $Y^{\rho}_{\sigma\nu;\mu}$). It turns out we have all the ingredients of $Y^{\rho}_{\sigma\mu;\nu}$ (and $Y^{\rho}_{\sigma\nu;\mu}$) in the first equality in the calculation above for $\widehat{R}^{\rho}_{\sigma\mu\nu}$ except for the terms we have added and subtracted in the second equality. It follows that

$$\widehat{R}^{\rho}_{\sigma\mu\nu} = R^{\rho}_{\sigma\mu\nu} - Y^{\rho}_{\sigma\mu;\nu} + Y^{\rho}_{\sigma\nu;\mu} - Y^{\lambda}_{\sigma\mu}Y^{\rho}_{\nu\lambda} + Y^{\rho}_{\mu\lambda}Y^{\lambda}_{\sigma\nu},$$
$$\widehat{R}^{\rho}_{\sigma\mu\nu} = R^{\rho}_{\sigma\mu\nu} + H^{\rho}_{\sigma\mu\nu}. \quad (148)$$

Here, $H^{\rho}_{\sigma\mu\nu} \equiv Y^{\rho}_{\sigma\mu;\nu} + Y^{\rho}_{\sigma\nu;\mu} - Y^{\lambda}_{\sigma\mu}Y^{\rho}_{\nu\lambda} + Y^{\rho}_{\mu\lambda}Y^{\lambda}_{\sigma\nu}$.

It remains for us to determine $H^{\rho}_{\sigma\mu\nu}$ in terms of $g_{\mu\nu}$ and Ω. For the covariant derivative we have from the definition of $Y^{\rho}_{\sigma\mu}$ given above,

$$Y^{\rho}_{\sigma\mu;\nu} = \left[\Omega^{-1}(\delta^{\rho}_{\sigma}\Omega_{;\mu} + \delta^{\rho}_{\mu}\Omega_{;\sigma} - g_{\sigma\mu}g^{\rho\alpha}\Omega_{;\alpha})\right]_{;\nu},$$
$$= -\Omega_{;\nu}\Omega^{-2}(\delta^{\rho}_{\sigma}\Omega_{;\mu} + \delta^{\rho}_{\mu}\Omega_{;\sigma} - g_{\sigma\mu}g^{\rho\alpha}\Omega_{;\alpha})$$
$$+ \Omega^{-1}(\delta^{\rho}_{\sigma}\Omega_{;\mu\nu} + \delta^{\rho}_{\mu}\Omega_{;\sigma\nu} - g_{\sigma\mu}g^{\rho\alpha}\Omega_{;\alpha\nu}),$$
$$Y^{\rho}_{\sigma\mu;\nu} = -\Omega_{;\nu}\Omega^{-1}Y^{\rho}_{\sigma\mu} + \Omega^{-1}(\delta^{\rho}_{\sigma}\Omega_{;\mu\nu} + \delta^{\rho}_{\mu}\Omega_{;\sigma\nu} - g_{\sigma\mu}g^{\rho\alpha}\Omega_{;\alpha\nu}). \quad (149)$$

Plugging this expression together with the expression for $Y^{\rho}_{\sigma\mu}$ in the definition of $H^{\rho}_{\sigma\mu\nu}$ will certainly produce a lengthy expression. To ease our way here, we use a computer algebra system (Maxima). With the correspondence,

$$\begin{array}{llll} \Omega & \to W & \rho \to r & \mu \to m \\ Y^{\rho}_{\sigma\mu} & \to C & \sigma \to s & \nu \to n \\ Y^{\rho}_{\sigma\mu;\nu} & \to D & \alpha \to a & \text{etc.} \end{array} \quad (150)$$

we write and execute the following code:

```
load(itensor);
imetric(g);
components(C([m,n],[r]), W([],[])^(-1)*(
```

```
        kdelta([m],[r])*W([n],[])
        +
        kdelta([n],[r])*W([m],[])
        -
        g([m,n],[])*g([],[r,s])*W([s],[])
        )
);
ishow(C([m,n],[r]))$
components(D([s,m,n],[r]),
        -W([n],[])/W([],[])*C([s,m],[r])
        +
        W([],[])^(-1)*(
            kdelta([s],[r])*W([m,n],[])
            +
            kdelta([m],[r])*W([s,n],[])
            -
            g([s,m],[])*g([],[r,a])*W([a,n],[])
        )
);
ishow(D([s,m,n],[r]))$
ishow(
        -D([s,m,n],[r])
        +
        D([s,n,m],[r])
        -
        C([s,m],[l])*C([n,l],[r])
        +
        C([s,n],[l])*C([m,l],[r])
)$
ishow(expand(%))$
nterms(%);
defcon(g,kdelta,g);
ishow(contract(rename(%th(3))))$
nterms(%);
decsym(g,2,0,[sym(all)],[]);
decsym(g,0,2,[],[sym(all)]);
ishow(canform(%th(4)))$
```

The output of the code above written in terms of our notation is given by

$$H^{\rho}_{\sigma\mu\nu} = \Omega^{-1}\big(- \delta^{\rho}_{\mu}\Omega_{;\sigma\nu} - g_{\sigma\nu}g^{\rho\alpha}\Omega_{;\alpha\mu} + \delta^{\rho}_{\nu}\Omega_{;\sigma\mu} + g_{\sigma\mu}g^{\rho\alpha}\Omega_{;\alpha\nu} + \delta^{\rho}_{\sigma}\Omega_{;\nu\mu} - \delta^{\rho}_{\sigma}\Omega_{;\mu\nu}\big)$$

$$+\ \Omega^{-2}\big(-2\delta^\rho_\nu\Omega_{;\mu}\Omega_{;\sigma}+2\delta^\rho_\mu\Omega_{;\nu}\Omega_{;\sigma}-g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}\delta^\rho_\mu g_{\nu\sigma}$$
$$+\ 2g_{\nu\sigma}g^{\rho\alpha}\Omega_{;\alpha}\Omega_{;\mu}+g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}g_{\mu\sigma}\delta^\rho_\nu-2g_{\mu\sigma}g^{\rho\alpha}\Omega_{;\alpha}\Omega_{;\nu}\big) \tag{151}$$

The second line vanishes because $\Omega_{;\mu\nu}=\Omega_{;\nu\mu}$.

$$H^\rho_{\sigma\mu\nu}=\Omega^{-1}\big(-\delta^\rho_\mu\Omega_{;\sigma\nu}-g_{\sigma\nu}g^{\rho\alpha}\Omega_{;\alpha\mu}+\delta^\rho_\nu\Omega_{;\sigma\mu}+g_{\sigma\mu}g^{\rho\alpha}\Omega_{;\alpha\nu}\big)$$
$$+\ \Omega^{-2}\big(-2\delta^\rho_\nu\Omega_{;\mu}\Omega_{;\sigma}+2\delta^\rho_\mu\Omega_{;\nu}\Omega_{;\sigma}-g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}\delta^\rho_\mu g_{\nu\sigma}$$
$$+\ 2g_{\nu\sigma}g^{\rho\alpha}\Omega_{;\alpha}\Omega_{;\mu}+g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}g_{\mu\sigma}\delta^\rho_\nu-2g_{\mu\sigma}g^{\rho\alpha}\Omega_{;\alpha}\Omega_{;\nu}\big) \tag{152}$$

We now proceed to contract the indices of $H^\rho_{\sigma\mu\nu}$ to find $\widehat{R}$ in terms of R and Ω.

$$\begin{aligned}
H^\rho_{\sigma\rho\nu}&=\Omega^{-1}\big(-4\Omega_{;\sigma\nu}-g_{\sigma\nu}g^{\rho\alpha}\Omega_{;\alpha\rho}+\Omega_{;\sigma\nu}+\Omega_{;\sigma\nu}\big)\\
&\quad+\ \Omega^{-2}\big(-2\Omega_{;\nu}\Omega_{;\sigma}+8\Omega_{;\nu}\Omega_{;\sigma}-4g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}g_{\nu\sigma}\\
&\qquad+\ 2g_{\nu\sigma}g^{\rho\alpha}\Omega_{;\alpha}\Omega_{;\rho}+g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}g_{\nu\sigma}-2\Omega_{;\sigma}\Omega_{;\nu}\big),\\
&=-\Omega^{-1}(2\Omega_{;\sigma\nu}+g_{\sigma\nu}g^{\rho\alpha}\Omega_{;\alpha\rho})+\Omega^{-2}(4\Omega_{;\nu}\Omega_{;\sigma}-g^{\alpha\beta}\Omega_{;\alpha}\Omega_{;\beta}g_{\nu\sigma}),\\
g^{\mu\nu}H^\rho_{\mu\rho\nu}&=6\Omega^{-1}g^{\mu\nu}\Omega_{;\mu\nu}+4\Omega^{-2}g^{\mu\nu}\Omega_{;\mu}\Omega_{;\nu}-4\Omega^{-2}g^{\mu\nu}\Omega_{;\mu}\Omega_{;\nu},\\
g^{\mu\nu}H^\rho_{\mu\rho\nu}&=6\Omega^{-1}g^{\mu\nu}\Omega_{;\mu\nu}.
\end{aligned} \tag{153}$$

Consequently, contracting the indices in the second of (148) and performing substitution in the resulting equation we find

$$\widehat{R}=\Omega^{-2}R+6\Omega^{-3}g^{\mu\nu}\Omega_{;\mu\nu}. \tag{154}$$

The final expression that we wish to prove involves R written in terms of the hatted quantities so we have to express $6\Omega^{-3}g^{\mu\nu}\Omega_{;\mu\nu}$ in terms of the hatted quantities; in particular, $\widehat{\Box}\ln\Omega$ and $\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu\ln\Omega)(\widehat{\nabla}_\nu\ln\Omega)$. To do this, we first calculate $\widehat{\Box}\ln\Omega$.

$$\begin{aligned}
\widehat{\nabla}_\mu\widehat{\nabla}_\nu\ln\Omega&=\widehat{\nabla}_\mu\big(\ln\Omega\big)_{;\nu},\\
&=\big(\ln\Omega\big)_{,\nu\mu}-\widehat{\Gamma}^\alpha_{\mu\nu}\big(\ln\Omega\big)_{;\alpha},\\
&=\nabla_\mu\nabla_\nu\ln\Omega-Y^\alpha_{\mu\nu}\big(\ln\Omega\big)_{;\alpha},
\end{aligned}$$

$$= \nabla_\mu \nabla_\nu \ln\Omega - \Omega^{-1}\left[\delta^\alpha_\mu \Omega_{,\nu} + \delta^\alpha_\nu \Omega_{,\mu} - g_{\mu\nu} g^{\alpha\beta} \Omega_{,\beta}\right] (\ln\Omega)_{;\alpha},$$

$$= \nabla_\mu \nabla_\nu \ln\Omega - \left[2(\ln\Omega)_{;\mu} (\ln\Omega)_{;\nu} - g_{\mu\nu} g^{\alpha\beta} (\ln\Omega)_{;\alpha} (\ln\Omega)_{;\beta}\right],$$

$$\widehat{\Box} \ln\Omega = \Omega^{-2} \Box \ln\Omega + 2\Omega^{-2} g^{\mu\nu} (\ln\Omega)_{;\mu} (\ln\Omega)_{;\nu}. \tag{155}$$

Then, we relate $\Box \ln\Omega$ to $g^{\mu\nu}\Omega_{;\mu\nu}$.

$$\Box \ln\Omega = g^{\mu\nu} \nabla_\mu (\ln\Omega)_{;\nu},$$

$$= g^{\mu\nu} \left(\frac{\Omega_{;\nu}}{\Omega}\right)_{;\mu},$$

$$\Box \ln\Omega = g^{\mu\nu} \Omega^{-1} \Omega_{;\mu\nu} - g^{\mu\nu} (\ln\Omega)_{;\mu} (\ln\Omega)_{;\nu}. \tag{156}$$

Substitution in the equation above for $\widehat{\Box} \ln\Omega$ yields

$$\widehat{\Box} \ln\Omega = g^{\mu\nu} \Omega^{-3} \Omega_{;\mu\nu} + \Omega^{-2} g^{\mu\nu} (\ln\Omega)_{;\mu} (\ln\Omega)_{;\nu},$$

$$\widehat{\Box} \ln\Omega = g^{\mu\nu} \Omega^{-3} \Omega_{;\mu\nu} + \widehat{g}^{\mu\nu} (\ln\Omega)_{;\mu} (\ln\Omega)_{;\nu}, \tag{157}$$

Finally, upon using the last equation above in the expression for $\widehat{R}$ given by (154) above we find

$$R = \Omega^2 \left[\widehat{R} + 6\widehat{\Box} \ln\Omega - 6\widehat{g}^{\mu\nu} (\widehat{\nabla}_\mu \ln\Omega)(\widehat{\nabla}_\nu \ln\Omega)\right], \tag{158}$$

which was to be shown.

Let us now verify that the above equation relating R and $\widehat{R}$ also holds for the case where

$$\widehat{g}_{00} = g_{00}, \quad \widehat{g}_{ij} = \Omega^2 g_{ij}, \tag{159}$$

and

$$\mathrm{d}\widehat{t} \equiv \Omega \, \mathrm{d}t \quad \text{and} \quad \widehat{a} \equiv \Omega a, \tag{160}$$

corresponding to the FLRW background metric $\mathrm{d}\widehat{s}^2 = -\mathrm{d}\widehat{t}^{\,2} + \widehat{a}^2 \delta_{ij} \mathrm{d}x^i \mathrm{d}x^j$. To see this, note that for $\mathrm{d}s^2 = -\mathrm{d}t^2 + \delta_{ij} a^2 \mathrm{d}x^i \mathrm{d}x^j$, the Ricci scalar is given by

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right). \tag{161}$$

It follows that

$$\widehat{R} = 6\left[\frac{1}{\widehat{a}}\frac{\mathrm{d}^2\widehat{a}}{\mathrm{d}\widehat{t}^{\,2}} + \frac{1}{\widehat{a}^2}\left(\frac{\mathrm{d}\widehat{a}}{\mathrm{d}\widehat{t}}\right)^2\right]. \tag{162}$$

We expand the latter equation together with $6\widehat{\Box}\ln\Omega - 6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu \ln\Omega)(\widehat{\nabla}_\nu \ln\Omega)$ to see if the sum would reduce to the former expression stating R in terms of a and its derivatives. For $\widehat{R}$ we have

$$\begin{aligned}\widehat{R} &= 6\left[\frac{1}{\Omega a}\frac{\mathrm{d}}{\mathrm{d}\widehat{t}}\left(\dot{a} + a\frac{\dot{\Omega}}{\Omega}\right) + \frac{1}{\Omega^2 a^2}\left(\dot{a} + a\frac{\dot{\Omega}}{\Omega}\right)^2\right] \\ \widehat{R} &= \frac{6}{\Omega^2}\left[\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2} + 3\frac{\dot{a}}{a}\frac{\dot{\Omega}}{\Omega} + \frac{\ddot{\Omega}}{\Omega}\right].\end{aligned} \tag{163}$$

For the calculation of $6\widehat{\Box}\ln\Omega$ note that

$$\widehat{\Gamma}^i_{0j} = \frac{1}{\widehat{a}}\frac{\mathrm{d}\widehat{a}}{\mathrm{d}\widehat{t}}\delta^i_j, \qquad \widehat{\Gamma}^0_{ij} = \widehat{a}\frac{\mathrm{d}\widehat{a}}{\mathrm{d}\widehat{t}}\delta_{ij}, \tag{164}$$

and all other components of the hatted Christoffel symbol vanish.

$$\begin{aligned}6\widehat{\Box}\ln\Omega &= 6\widehat{g}^{\mu\nu}\widehat{\nabla}_\mu(\ln\Omega)_{;\nu} \\ &= 6\widehat{g}^{\mu\nu}\left[(\ln\Omega)_{,\mu\nu} - \nabla\Gamma^\alpha_{\mu\nu}(\ln\Omega)_{;\alpha}\right] \\ &= 6\widehat{g}^{00}\left[(\ln\Omega)_{,00} - \widehat{\Gamma}^\alpha_{00}(\ln\Omega)_{;\alpha}\right] + 6\widehat{g}^{ij}\left[(\ln\Omega)_{,ij} - \widehat{\Gamma}^\alpha_{ij}(\ln\Omega)_{;\alpha}\right] \\ &= -6\frac{\mathrm{d}^2}{\mathrm{d}\widehat{t}^{\,2}}\ln\Omega - \frac{6}{\widehat{a}^2}\delta^{ij}\cdot\delta_{ij}\,\widehat{a}\frac{\mathrm{d}\widehat{a}}{\mathrm{d}\widehat{t}}\frac{\mathrm{d}}{\mathrm{d}\widehat{t}}\ln\Omega \\ 6\widehat{\Box}\ln\Omega &= -\frac{6}{\Omega^2}\left(\frac{\ddot{\Omega}}{\Omega} + \frac{\dot{\Omega}^2}{\Omega^2} + 3\frac{\dot{a}}{a}\frac{\dot{\Omega}}{\Omega}\right).\end{aligned} \tag{165}$$

Observe that all differentiation in the calculation for $6\widehat{\Box}\ln\Omega$ above is with respect to the hatted coordinates although we did not put a hat on the derivative indices for brevity. For $-6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu \ln\Omega)(\widehat{\nabla}_\nu \ln\Omega)$ we have

$$\begin{aligned}-6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu \ln\Omega)(\widehat{\nabla}_\nu \ln\Omega) &= -6\widehat{g}^{00}\left(\frac{\mathrm{d}}{\mathrm{d}\widehat{t}}\ln\Omega\right)^2 \\ -6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu \ln\Omega)(\widehat{\nabla}_\nu \ln\Omega) &= \frac{6}{\Omega^2}\frac{\dot{\Omega}}{\Omega^2}.\end{aligned} \tag{166}$$

Summing up the three sub-results above for $\widehat{R}$, $6\widehat{\Box}\ln\Omega$, and $-6\widehat{g}^{\mu\nu}(\widehat{\nabla}_\mu \ln\Omega)\times(\widehat{\nabla}_\nu \ln\Omega)$, and multiplying the result by Ω^2 we get

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right), \tag{167}$$

which was to be verified.

D Power Spectrum of Primordial Cosmological Perturbations and CMB Radiation

The primordial cosmological perturbations through inflation and the ensuing processes related to the evolution of the Universe served as seeds for the large-scale structures such as galaxies and clusters of galaxies we observe in the current era. If this is true, the distribution of these (essentially) matter clusters must bear resemblance with the that of primordial perturbations. On the other hand, since matter and radiation were tightly coupled in the past, then the radiation remnant namely, CMB radiation, should also bear resemblance with the distribution of primordial cosmological perturbations. More specifically, given sufficient knowledge of the evolution of the Universe and accompanying physical processes such as photon decoupling, reheating, cooling, structure formation, among others, we may be able to relate the matter or radiation distribution with that of the primordial cosmological perturbations.

In this appendix, we relate the CMB temperature fluctuation to the scalar power spectrum. A similar approach although we may say more complicated, can be done with CMB polarization and tensor power spectrum. Interested readers who wish to probe further the relationship between primordial cosmological perturbations and today's measurable physical quantities may consult refs. [1, 2, 6, 48]. Here, we do not deal with intricacies that should be properly left to the mentioned references. It is enough that we focus on one, that is, CMB temperature fluctuation and scalar power spectrum. While we shun away from rigorous details in this appendix, the relations coupled with short comments that we will write below shall serve as a testament (mainly for the uninitiated and/or curious) that such a relation exist.

What our instruments can measure is temperature of CMB radiation coming from different positions in the sky. We take the current time as τ_0 and

the origin corresponding to the location of our measuring instrument as $\mathbf{x}_0$. Furthermore, with respect to this location, we can look at or "point" our measuring instrument to any direction in the sky denoted by $\hat{\mathbf{n}} \equiv \mathbf{p}/p$, where $\mathbf{p}$ is photon momentum. With the foregoing, let $\Theta(\tau_0, \mathbf{x}_0, \hat{\mathbf{n}})$ be the brightness function associated with the CMB temperature fluctuation defined as

$$\Theta(\tau_0, \mathbf{x}_0, \hat{\mathbf{n}}) \equiv \frac{T(\tau_0, \mathbf{x}_0, \hat{\mathbf{n}}) - T(\tau_0)}{T(\tau_0)}, \tag{168}$$

where T stands for temperature and $T(\tau_0)$ is some average temperature evaluated at the current time.

The brightness function can be decomposed into a series of spherical harmonics.

$$\Theta(\tau_0, \mathbf{x}_0, \hat{\mathbf{n}}) = \sum_{\ell m} (-1)^\ell a_{\ell m}(\tau_0, \mathbf{x}_0) Y_{\ell m}(\hat{\mathbf{n}}). \tag{169}$$

This is like the usual Fourier transformation except that the "wave" expansion corresponds to spherical space instead of a rectangular space. The value $\ell = 0$ corresponds to monopole moment, $\ell = 1$ corresponds to dipole moment, $\ell = 0$ corresponds to quadrupole moment, and so on. Assuming a (nearly) Gaussian distribution, we can take $\langle a_{\ell m} \rangle = 0$. The two-point function of $a_{\ell m}$ then (almost) completely specifies the statistics of the brightness function. Let C_ℓ be defined as

$$\langle a_{\ell m} a_{\ell' m'} \rangle = \delta_{\ell \ell'} \delta_{m m'} C_\ell. \tag{170}$$

Since we can measure CMB temperature fluctuation, we can determine C_ℓ from this measurement. Noting that C_ℓ is essentially the value of the two-point function of $a_{\ell m}$, we may relate it to the two-point function of the scalar modes ζ_k with the latter being essentially the power spectrum $\Delta_s^2(k)$. The "transformation" from primordial cosmological perturbation ζ_k to $a_{\ell m}$ telling us the CMB temperature fluctuation, is done through a transfer function $T_\ell(k)$. We will not be detailing here the form of this function; suffice it to say that it depends on the way primordial perturbation evolves and "becomes" CMB

radiation. With all these considerations in hand, we write [48]

$$C_\ell = 4\pi \int \frac{\mathrm{d}k}{k} \Delta_s^2(k)\, T_\ell^2(k). \tag{171}$$

Note that although the expression above involves integration over all k, the power spectrum that explicitly contributes to C_ℓ involves only those modes stretched and amplified, or in some other ways affected by inflation. (The idea about adiabatic regularization is that the subtraction due to the UV divergence might affect the power spectrum of these contributing modes as well; but as we found, for the models we considered in this work, the effect is essentially trivial.)

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